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conference
abstracts

9th EUROPEAN CONFERENCE ON ATOMS MOLECULES & PHOTONS

ECAMP IX

6-11th MAY 2007

HERAKLION

Editors: D. Charalambidis, S. Farantos and P. Lambropoulos

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ECAMP IX

6-11th MAY 2007
Heraklion, Crete

ABSTRACTS

Editors: D. Charalambidis, S. Farantos and P. Lambropoulos

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CONTACT ADDRESS:

FORTH - IESL
PO Box 1527, 71110 Heraklion, Crete, GREECE
Tel: +30 2810 391300, Fax: +30 2810 391305
Email: ecamp9@iesl.forth.gr

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This book contains all abstracts received before March 1st

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The poster abstracts are arranged by topics, in the order of their presentation at the conference. They are labelled with the day and topic number (Mo1, Mo2, ..., Tu1, Tu2.....) followed by a serial number.

Oral presentations and hot topics are not assigned as their selection was finalized after this book went to press.

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ECAMP IX

6-11th May 2007, Heraklion, Crete

Conference Programme

Sunday 6/5

Welcome Reception 20:30-21:30

Monday 7/5

Opening 08:45-09:00

Plenary session *Chair: Lars Andersen*

1. PRECISION MASS MEASUREMENT: $\omega_{cyclotron}$ IS NOT qB/m, DOES $E=mc^2$?
David E. Pritchard 09:00-10:00

Coffee Break 10:00-10:30

Parallel Sessions

1a: Coherent control *Chair: Gustav Gerber*

1a-1 QUANTUM CONTROL OF CHEMICAL REACTIONS AND FUNCTIONS
Leticia González *(Invited)* 10:30-11:00

1a-2 QUANTUM AND MIXED QUANTUM/CLASSICAL APPROACHES TO THE CONTROL OF ULTRAFAST MOLECULAR WAVE PACKET INTERFERENCES
Christoph Meier *(Invited)* 11:00-11:30

1a-3 DRESSED STATE TAILORING WITH ULTRASHORT LIGHT PULSES
Matthias Wollenhaupt *(Invited)* 11:30-12:00

1a-4 COHERENTLY CONTROLLED ADIABATIC PASSAGE TO MULTICHANNEL CONTINUUM STRUCTURE
Ioannis Thanopulos and Moshe Shapiro *(Oral)* 12:00-12:15

1a-5 NEW WAY TO INDUCE AND CONTROL ELEMENTARY CHEMICAL TRANSFORMATIONS ON A GAS-SOLID INTERPHASE BY MEANS OF RESONANT LASER RADIATION
V. V. Petrunin *(Oral)* 12:15-12:30

1b: Clusters *Chair: Wolfgang Ernst*

1b-1 PROPERTIES OF CLUSTER IONS PROBED BY MASS SPECTROMETRY, LASER SPECTROMETRY, ELECTRON DIFFRACTION AND QUANTUM CHEMISTRY
M. M. Kappes, O. Hampe, M. Neumaier, D. Schooss, A. Lechtken, M. Kordel, P. Weis, E. Oger, O. Ehrler, K. Matheis, C. Rensing and A. Glöss *(Invited)*
10:30-11:15

1b-2 NEAR-INRARED SPECTROSCOPY ON C60 ANIONS
J.U. Andersen *(Invited)* 11:15-11:45

1b-3 MOLECULAR DYNAMICS FOR FISSION PROCESSES
O.I. Obolensky, A. Lyalin, I.A. Solov’yov, A. Yakubovich, E. Henriques, A.V. Solov’yov, W. Greiner *(Invited)* 11:45-12:15

1b-4 FEMTOSECOND OPTICAL SPECTROSCOPY OF A SINGLE METAL NANOPARTICLE
Natalia Del Fatti, Otto Muskens, and Fabrice Valée *(Invited)* 12:15-12:45

Lunch 12:30-15:00

Parallel Sessions

2a: Attosecond Physics *Chair: George Tsakiris*

2a-1 ATTOSECOND PHYSICS
Ferenc Krausz *(Invited)* 15:00-15:45

2a-2 THE OTHER HALF OF THE STORY: ATTOSECOND TIME-RESOLVED ELECTRON DYNAMIC
Marc Vrakking *(Invited)* 15:45-16:15

2a-3 ATTOSECOND METROLOGY IN THE SINGLE-CYCLE REGIME
G. Sansone, E. Benedetti, F. Calegari, C. Vozzi, S. Stagira, S. De Silvestri, M. Nisoli, L. Avaldi, R. Flammini, L. Poletto, P. Villoresi, C. Altucci, R. Velotta *(Invited)* 16:15-16:45

2a-4 AUTOCORRELATION MEASUREMENT OF ATTOSECOND PULSES BY XUV TWO-PHOTON PROCESS
Yasuo Nabekawa, Toshihiko Shimizu, Hirokazu Hasegawa, and Katsumi Midorikawa *(Invited)* 16:45-17:15

2b: Cold atoms and molecules

Chair: Wolfgang von Klitzing

2b-1 NOVEL INTERACTIONS IN QUANTUM GASES
Tilman Pfau *(Invited)* 15:00-15:30

2b-2 QUANTUM DEGENERATE GASES OF METASTABLE HELIUM-3 AND HELIUM-4 ATOMS
Wim Vassen *(Invited)* 15:30-16:00

2b-3 SCATTERING LENGTH OF SPIN-POLARIZED HELIUM
Bogumił Jeziorski *(Invited)* 16:00-16:30

2b-4 SIGNATURES OF EFIMOV’S EFFECT IN ULTRACOLD GASES
Thorsten Köhler *(Invited)* 16:30-17:00

Coffee Break & **Poster Session** 17:00-20:00

Tuesday 8/5

Plenary session

Chair: Andrey Solov’yov

2. SWEETNESS AND LIGHT: FROM GLUCOSE TO GLYCOBIOLOGY
John P. Simons 9:00-10:00

Coffee Break 10:00-10:30

Parallel Sessions

3a: Biophysics

Chair: Frederik Merkt

3a-1 CONICAL INTERSECTIONS AND PHOTOSTABILITY OF THE BUILDING BLOCKS OF LIFE
Wolfgang Domcke and Andrzej L. Sobolewski *(Invited)* 10:30-11:15

3a-2 PROBING THE SECONDARY STRUCTURES OF SHORT PEPTIDE CHAINS IN THE GAS PHASE: IR / UV DOUBLE RESONANCE STUDIES
E Gloaguen, F. Pagliarulo, F. Piuzzi, V. Brenner, I. Dimicoli and M. Mons *(Invited)* 11:15-11:45

3a-3 IR AND UV SPECTROSCOPY OF COLD, BIOMOLECULAR IONS
Thomas R. Rizzo *(Invited)* 11:45-12:15

3a-4 ON MAGNETORECEPTION MECHANISMS IN BIRDS

Ilia A. Solov'yov, Danielle Chandler, Klaus Schulten and Walter Greiner *(Oral)* 12:15-12:30

3b: Cavity QED, Quantum information *Chair: Fernande Vedel*

3b-1 OPTICAL CAVITY QED
Gerhard Rempe *(Invited)* 10:30-11:00

3b-2 SINGLE PHOTONS FROM STRONGLY COUPLED ATOM-CAVITY SYSTEMS
Axel Kuhn *(Invited)* 11:00-11:30

3b-3 QED THEORY OF HEAVY IONS AND ATOMS
V.M. Shabaev *(Invited)* 11:30-12:00

3b-4 INDIVIDUAL ADDRESSING AND ERROR RESISTANT SINGLE QUBIT GATES WITH TRAPPED Yb^+ IONS
A. Braun, V. Elman, M. Johanning, W. Neuhauser, N. Timoney, C. Weiß, Chr. Wunderlich *(Oral)* 12:00-12:15

3b-5 A SCHEME FOR CAVITY COOLING OF INTERNAL AND EXTERNAL DEGREES OF FREEDOM OF MOLECULES
P.W.H. Pinkse, G. Morigi, M. Kowalewski, R. de Vivie-Riedle *(Oral)*
12:15-12:30

Lunch 12:30-15:00

Parallel Sessions

4a: Electron collisions *Chair: Reinhold Schuch*

4a-1 ANION RESONANCES, THRESHOLD PHENOMENA, AND CHEMICAL CHANGE REVEALED BY ELECTRON-SCATTERING
Michael Allan, Bogdan C. Ibănescu and Olivier May *(Invited)* 15:00-15:30

4a -2 THEORY OF ELECTRON COLLISIONS WITH POLAR MOLECULES
Roman Čurík and David Field *(Invited)* 15:30-16:00

4a -3 SYNTHESIS OF AMINO ACIDS BY LOW-ENERGY ELECTRONS IN MOLECULAR ICES
A. Lafosse, M. Bertin, I. Martin, E. Illenberger, and R. Azria *(Invited)*
16:00-16:30

4a -4 STRUCTURAL ASPECTS OF THE RADIOLYSIS OF PROTEINS AND PEPTIDES: THE EXAMPLE OF DISULFIDE BONDS
Chantal Houée-Levin *(Invited)* 16:30-17:00

4b: Rydberg and cold plasmas *Chair: Uwe Becker*

4b-1 RYDBERG EXCITATION AND PLASMA FORMATION IN AN ULTRACOLD ATOMIC ENVIRONMENT
Jan M. Rost *(Invited)* 15:00-15:30

4b-2 DIPOLE BLOCKADE IN HIGH-RESOLUTION LASER EXCITATION OF RYDBERG STATES
Pierre Pillet *(Invited)* 15:30-16:00

4b-3 COHERENT PHENOMENA IN ULTACOLD RYDBERG GASES
Matthias Weidemüller *(Invited)* 16:00-16:30

4b-4 ZEEMAN DECELERATION OF NEUTRAL GROUND STATE ATOMS
S. D. Hogan, N. Vanhaecke, M. Andrist, U. Meier, D. Sprecher, B. H. Meier and F. Merkt *(Oral)* 16:30-16:45

4b-5 MESOSCOPIC PHYSICS WITH ULTRACOLD ATOMS: FROM CONFINED SCATTERING TO RYDBERG ATOMS IN MAGNETIC TRAPS
P. Schmelcher *(Oral)* 16:45-17:00

Coffee Break & **Poster Session** 17:00-20:00

Wednesday 9/5

Plenary session *Chair: Hartmut Hotop*

3. THE OPTICAL FREQUENCY COMB - A REMARKABLE TOOL WITH MANY USES
John L. Hall 09:00-10:00

Coffee Break 10:00-10:30

Plenary session *Chair: Hartmut Hotop*

4. QUANTUM INFORMATION PROCESSING WITH TRAPPED CA$^+$ IONS - MULTI-PARTICLE ENTANGLEMENT AND QUANTUM METROLOGY -
Rainer Blatt 10:30-11.30

ECAMP assembly 11:30-12:30

Lunch 12:30-15:00

Poster Session 20:00-22:00

Thursday 10/5

Plenary session *Chair: Christophe Blondel*

5. COLD QUANTUM GASES: WHEN ATOMIC PHYSICS MEETS CONDENSED MATTER
Jean Dalibard 09:00-10:00

Coffee Break 10:00-10:30

Parallel Sessions

5a: Alignment and polarization *Chair: Gerard Meijer*

5a-1 CONTROLLING THE ROTATIONAL MOTION OF ASYMMETRIC TOP MOLECULES BY LASER PULSES
Henrik Stapelfeldt *(Invited)* 10:30-11:15

5a-2 NEW METHODS FOR THE PRODUCTION AND DETECTION OF SPIN-POLARIZED HYDROGEN
T. Peter Rakitzis *(Invited)* 11:15-11:45

5a-3 KINEMATICALLY COMPLETE STUDY OF DISSOCIATIVE IONIZATION OF D_2 BY ION IMPACT
G. Laurent, J. Fernández, S. Legendre, M. Tarisien, L. Adoui, A. Cassimi, X. Fléchard, F. Frémont, B. Gervais, E. Giglio, J. P. Grandin, and F. Martín *(Invited)* 11 :45-12:15

5a-4 LASER INDUCED MOLECULAR ALIGNMENT OF ETHYLENE
A. Rouzée, S. Guérin, B. Lavorel, and O. Faucher *(Oral)* 12:15-12:30

5b: Quantum information *Chair: Krystof Pachucki*

5b -1 QUANTUM COMMUNICATION IN OPTICAL NETWORKS
Nicolas Gisin *(Invited)* 10:30-11:15

5b-2 LARGE HOT ATOMIC GASSES AS IDEAL QUANTUM SYSTEMS FOR QUANTUM INFORMATION
Klaus Mølmer *(Invited)* 11:15-11:45

5b-3 QUANTUM TELEPORTATION BETWEEN LIGHT AND MATTER
J. F. Sherson, H. Krauter, R. K. Olsson, B. Julsgaard, K. Hammerer, J.I. Cirac, and E.S. Polzik *(Invited)* 11:45-12:15

5b-4 COLLECTIVE EXCITATIONS AND INSTABILITY OF AN OPTICAL LATTICE DUE TO UNBALANCED PUMPING
P. Domokos, J. K. Asbóth, H. Ritsch *(Oral)* 12:15-12:30

Lunch 12:30-15:00

Parallel Sessions

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6a-1 REALIZATION AND APPLICATION OF FREQUENCY COMBS
Thomas Udem, Akira Ozawa, Christoph Gohle, Jens Rauschenberger, Ronald Holzwarth, Maximilian Herrmann, Elisabeth Peters, Birgitta Bernhardt, and Theodor W. Hänsch *(Invited)* 15:00-15:30

6a-2 MEASURING THE ELECTRON’S ELECTRIC DIPOLE MOMENT WITH HEAVY, POLAR MOLECULES.
J.J. Hudson, D. Kara, H.T. Ashworth, M.R. Tarbutt, B.E. Sauer, E.A. Hinds *(Invited)* 15:30-16:00

6a-3 ON A VARIATION OF THE PROTON-ELECTRON MASS RATIO
W. Ubachs *(Invited)* 16:00-16:30

6a-4 MATTER-ANTIMATTER CHEMISTRY WITH ANTIPROTONS
E. Lodi Rizzini, L. Venturelli, N. Zurlo *(Invited)* 16:30-17:00

6b: Molecular spectroscopy *Chair: Fernando Martin*

6b-1 AB INITIO QUANTUM DEFECT THEORY: FROM X-RAY EXCITATION TO MILLIMETER WAVE SPECTROSCOPY
R. Guérout, H. Oueslati, Ch. Jungen and M. Telmini *(Invited)* 15:00-15:30

6b-2 INTERSTELLAR POLYCYCLIC AROMATIC HYDROCARBONS: FROM SPACE TO THE LABORATORY
C. Joblin *(Invited)* 15:30-16:00

6b-3 BIOMOLECULES STUDIED BY HIGH RESOLUTION LASER SPECTROSCOPY: STATE OF THE ART
W. Leo Meerts *(Invited)* 16:00-16:30

6b-4 VACUUM ULTRAVIOLET PHOTODISSOCIATION IMAGING OF HeH^+ USING INTENSE FREE ELECTRON LASER PULSES
H. B. Pedersen, S. Altevogt, B. Jordon-Thaden, O. Heber, M. L. Rappaport, D. Schwalm, J. Ullrich, D. Zajfman, R. Treusch, N, Guerassimova, M. Martins, J.-T Hoeft, M. Wellhöfer and A. Wolf *(Oral)* 16:30-16:45

6b-5 SINGLE PHOTON-INDUCED SYMMETRY BREAKING OF H_2 DISSOCIATION
F. Martín, J. Fernández, T. Havermeier, L. Foucar, Th. Weber, K. Kreidi, M. Schöffler, L. Schmidt, T. Jahnke, O. Jagutzki, A. Czasch, E. P. Benis, T.

Osipov, A. L. Landers, A. Belkacem, M. H. Prior, H. Schmidt-Böcking, C. L. Cocke, R. Dörner *(Oral)* 16:45-17:00

Coffee Break & **Poster Session** 17:00-19:00

Conference Dinner 19:30

Friday 11/5

Plenary session *Chair: Ken Taylor*

6. FEW-PHOTON MULTIPLE IONIZATION OF ATOMS BY INTENSE FEL RADIATION
R. Moshammer, L. Foucar, A. Rudenko, Th. Ergler, C.D. Schröter, K. Zrost, S. Lüdemann, D. Fischer, J. Tietze, T. Jahnke, M. Schöffler, T. Weber, R. Dörner, T. Zouros, A. Dorn,T. Ferger, K.U. Kühnel, R. Treusch, P. Radcliff, E. Plönjes, Y.H. Jiang, and J. Ullrich 09:00-10:00

Coffee Break 10:00-10:30

Parallel Sessions

7a: Few-body dynamics *Chair: Horst Schmidt Böcking*

7a-1 COINCIDENCE STUDIES OF PHOTOIONIZATION PROCESSES
P. Bolognesi and L. Avaldi *(Invited)* 10:30-11:00

7a-2 DOUBLE PHOTOIONIZATION OF SMALL MOLECULES AND RELATED PHENOMENA
A. Belkacem *(Invited)* 11:00-11:30

7a-3 UNRAVELING MODE-SPECIFIC REACTIVITY BY PRODUCT PAIR - CORRELATION MEASUREMENTS
Kopin Liu *(Invited)* 11:30-12:00

7a-4 EFFECT OF THE GEOMETRIC PHASE ON CHEMICAL REACTION DYNAMICS
Stuart C. Althorpe *(Invited)* 12:00-12:30

7b: Cold atoms and molecules *Chair: Jaques Vigue*

7b-1 EVIDENCE FOR EFIMOV QUANTUM STATES IN EXPERIMENTS WITH ULTRACOLD CESIUM GASES
Hans-Christoph Nägerl *(Invited)* 10:30-11:00

7b-2 DECELERATION AND TRAPPING OF NEUTRAL POLAR MOLECULES

Sebastiaan Y.T. van de Meerakker *(Invited)* 11:00-11:30

7b-3 TRAPPING RYDBERG ATOMS AND MOLECULES USING ELECTRIC FIELDS
E. Vliegen and F. Merkt *(Invited)* 11:30-12:00

7b-4 MANY-BODY DYNAMICS OF REPULSIVELY BOUND PAIRS OF PARTICLES IN A PERIODIC POTENTIAL
David Petrosyan, Bernd Schmidt, James R. Anglin, and Michael Fleischhauer *(Oral)* 12:00-12:15

7b-5 CREATION OF AN ULTRACOLD MIXTURE OF FERMIONIC LITHIUM AND POTASSIUM
F.M. Spiegelhalder, E. Wille, G. Kerner, D. Naik, A. Trenkwalder, C. Aiello, R. Chulia Jordan, G. Hendl, F. Schreck and R. Grimm *(Oral)* 12:15-12:30

Lunch 12:30-14:00

Parallel Sessions

8a: Hot Topics *Chair: Ninolay Kabachnik*

8a-1 ATTOSECOND IONIZATION DYNAMICS
P. Johnsson, J. Mauritsson, T. Remetter, K. J. Schafer and A. L'Huillier 14:00-14:20

8a-2 A FEMTOSECOND IMAGING STOPWATCH FOR THE BOND BREAKAGE OF A POLYATOMIC MOLECULE
R. de Nalda, J.G. Izquierdo, J. Durá, L. Bañares 14:20-14:40

8a-3 VISUALIZING AND CONTROLING ULTRAFAST WAVE-PACKET INTERFERENCE IN DIATOMIC MOLECULES
Hiroyuki Katsuki, Hisashi Chiba, Kenji Ohmori, Christoph Meier, and Bertrand Girard 14:40-15:00

8a-4 MAPPING THE VIBRATION OF FAST MOLECULES WITH ULTRASHORT LASER PULSES
C R Calvert, J McKenna, D S Murphy, W A Bryan, E M L English, J Wood, I C E Turcu, J F McCann, W R Newell and I D Williams 15:00-15:20

8a-5 FEMTOSECOND LASER INDUCED FUSION OF GAS PHASE FULLERENES
K.Hansen, M.Kjellberg, A.V.Bulgakov, E.E.B.Campbell 15:20-15:40

8a-6 BEYOND MEAN FIELD: USING LASER PULSES TO PROBE PAIR CORRELATIONS IN CONDENSATES
J. Mur-Petit, P. Naidon, E. Luc-Koenig, and F. Masnou-Seeuws 15:40-16:00

8b: Hot Topics

Chair: Christian Bordas

8b-1 ELECTRON SPIN RELAXATION IN ALKALI SAMPLES ON THE SURFACE OF HELIUM NANODROPLETS
Johann Nagl, Gerald Auböck, Carlo Callegari, and Wolfgang E. Ernst
14:00-14:20

8b-2 RESONANCES IN TRANSITION METAL COMPLEXES BY TDDFT CALCULATIONS
P. Decleva, G. Fronzoni and M. Stener 14:20-14:40

8b-3 NON-METALLIC BEHAVIOR OF C_{60} ELECTRON SHELL
M. Ya. Amusia and A. S. Baltenkov 14:40-15:00

8b-4 ^{87}Sr OPTICAL LATTICE CLOCK USING SPIN-POLARIZED ATOMS
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8b-5 PHOTOIONIZATION MICROSCOPY: EXPERIMENT AND SIMULATIONS
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8b-6 FLUORESCENCE OF HELIUM DOUBLY EXCITED STATES BELOW $N = 2$ IN HOMOGENEOUS ELECTRIC FIELD
Andrej Mihelič and Matjaž Žitnik 15:40-16:00

POSTERS

(Few of the contributions listed bellow were presented as oral or hot topic contributions at the conference. Those are not indicated here as their selection was finalized after this book went to press)

Monday 7/5

1. Attosecond Physics

Mo1-1 ATTOSECOND REAL-TIME OBSERVATION OF ELECTRON TUNNELLING AND MULTI-ELECTRON DYNAMICS IN ATOMS
M. Schultze, M. Uiberacker, Th. Uphues, A.J. Verhoef, V. Yakovlev, M.F. Kling, J. Rauschenberger, N.M. Kabachnik, H. Schröder, M. Lezius, K.L. Kompa, H.-G. Muller, M.J.J. Vrakking, S. Hendel, U. Kleineberg, U. Heinzmann, M. Drescher & F. Krausz.

Mo1-2 THE ROUTE TO INTENSE ATTOSECOND PULSES USING HIGH POWER LASERS
R. Hörlein, Y. Nomura, S. Rykovanov, M.. Geissler, P. Tzallas, S. Karsch, Zs. Major, J. Osterhoff, D. Charalambidis, F. Krausz, and G. D. Tsakiris

Mo1-3 TOWARDS INTENSE ISOLATED ATTOSECOND PULSES
P. Tzallas, E. Skantzakis, C. Kalpouzos, E. P. Benis, A. Bonarou, G. D. Tsakiris and D. Charalambidis

Mo1-4 SPATIOTEMPORAL EFFECTS IN ATTOSECOND PULSE TRAINS METROLOGY
E.P. Benis, J. Kruse, P. Tzallas, E. Skantzakis, G.D.Tsakiris and D. Charalambidis

Mo1-5 SINGLE ATTOSECOND PULSES FROM SURFACE HARMONICS USING POLARIZATION GATING TECHNIQUE
S.G. Rykovanov, M. Geissler, J. Meyer-ter-Vehn, and G. D. Tsakiris

Mo1-6 FULL TEMPORAL RECONSTRUCTION OF LOWER ORDER HARMONIC SUPERPOSITIONS
E. Skatzakis, P. Tzallas, , E. Papalazarou, C. Kalpouzos, A. Bonarou, E. P. Benis, G. D. Tsakiris and D. Charalambidis

Mo1-7 ATTOSECOND ELECTRON PULSES FROM INTERFERENCE OF ABOVE-THRESHOLD DE BROGLIE WAVES
Sándor Varró and Győző Farkas

Mo1-8 ATTOSECOND IONIZATION DYNAMICS
P. Johnsson, J. Mauritsson, T. Remetter, K. J. Schafer and A. L'Huillier

Mo1-9 THEORETICAL STUDY OF ATOMIC PHOTOIONIZATION BY ATTOSECOND XUV PULSES IN A STRONG LASER FIELD

A.K. Kazansky and N.M. Kabachnik

Mo1-10 MECHANISMS FOR EFFICIENT PRODUCTION OF SINGLE ATTOSECOND PULSE: BREMSSTRAHLUNG VERSUS RECOMBINATION
M. Yu. Emelin, A. A. Gonoskov, M. Yu. Ryabikin and A. M. Sergeev

Mo1-11 SUPER INTENSE LASER FIELD ON SURFACE WITH FORMING THE ATTO-SECOND LASER PLASMA AND NEW LASER SPECTROSCOPY OF NUCLEAR ISOMERS
Alexander V. Glushkov

2. Advanced Radiation and Particle Sources

Mo2-1 A BRIGHT ULTRACOLD ATOMS - BASED ELECTRON SOURCE
G. Taban, M.P. Reijnders, S.B. van der Geer, O.J. Luiten, and E.J.D. Vredenbregt

Mo2-2 AN INTENSE CHANNELING RADIATION X-RAY SOURCE
W. Wagner, B. Azadegan and J. Pawelke

Mo2-3 ON THE POSSIBILITY OF A CRYSTALLINE “UNDULATOR” FOR LOW-ENERGY ELECTRONS
A.V. Korol, M. Tabrizi, A.V. Solov’yov, W. Greiner

Mo2-4 ULTRASHORT TUNABLE UV PULSES FROM SELF-FOCUSING OF FEW-CYCLE PULSES IN ARGON AND APPLICATION FOR PUMP-PROBE SPECTROSCOPY
W. Fuß, K. Kosma, W.E. Schmid, S.A. Trushin

Mo2-5 CRYSTALLINE UNDULATOR BASED GAMMA-LASER: CURRENT SATUS AND PROSPECTS
Andriy Kostyuk, Andrei Korol, Andrey Solov’yov, Walter Greiner

Mo2-6 LASER-COOLED ION SOURCE
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Mo2-7 COLLIDING LASER PRODUCED PLASMAS AS ATOMIC, MOLECULAR AND CLUSTER SOURCES: A PROGRESS REPORT
P. Hough, C. McLoughin, J.P. Mosnier, J. Costello

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N. de Ruette, X. Gillon, B. Fabre, X. Urbain

Mo2-9 FEASIBILITY OF A CRYSTALLINE UNDULATOR FOR ULTRA-HIGH-ENERGY ELECTRONS
A.V. Korol, M. Tabrizi, A.V. Solov’yov, W. Greiner

3. Clusters and Nanoparticles

Mo3-1	SPECTRUM AND DYNAMICS OF A TWO-ELECTRON DOUBLE QUANTUM DOT MOLECULE R. Nepstad, V. Popsueva and J. P. Hansen
Mo3-2	NON-METALLIC BEHAVIOR OF C_{60} ELECTRON SHELL M. Ya. Amusia and A. S. Baltenkov
Mo3-3	SURFACE PHOTOCHEMISTRY FROM FIRST PRINCIPLES Thorsten Klüner
Mo3-4	KINETIC MODEL FOR NANOTUBES GROWTH O. I. Obolensky, I. A. Solov’yov, A. V. Solov’yov, W. Greiner
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Mo3-6	CLUSTER ORIGIN OF TRANSFER OF NANOTUBES Francisco Torrens and Gloria Castellano
Mo3-7	MULTIPLY CHARGED NEON CLUSTER IONS: CRITICAL SIZE AND COULOMB EXPLOSION I. Mähr, F. Zappa, S. Denifl, D. Kubala, O. Echt, T. D. Märk and P. Scheier
Mo3-8	ELECTRON SPIN RELAXATION IN ALKALI SAMPLES ON THE SURFACE OF HELIUM NANODROPLETS Johann Nagl, Gerald Auböck, Carlo Callegari, and Wolfgang E. Ernst
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Mo3-10	RADIATIVE COOLING OF Al_4^- Y. Toker, O. Aviv, M. Eritt, M.L. Rappaport, O. Heber, D. Schwalm, D. Zajfman
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Mo3-13	ATOM DECAY WITHIN CLUSTERS OF DIELECTRIC AND METALLIC NANOPARTICLES V. Yannopapas and N. V. Vitanov

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Mo3-15 RESONANCES IN TRANSITION METAL COMPLEXES BY TDDFT CALCULATIONS
P. Decleva, G. Fronzoni and M. Stener

Mo3-16 DIFFRACTION OF keV ATOMS AND MOLECULES ON SURFACES
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Mo3-17 GUIDED TRANSMISSION OF LOW ENERGY ELECTRONS BY HIGHLY ORDERED Al_2O_3 NANOCAPILLARIES
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Mo3-18 ELECTRONIC STRUCTURE AND STABILITY OF C_{70}^{q+} (q=0-14)
H. Zettergren, G. Sánchez, S. Díaz-Tendero, M. Alcamí and F. Martín

Mo3-19 FEMTOSECOND LASER INDUCED FUSION OF GAS PHASE FULLERENES
K.Hansen, M.Kjellberg, A.V.Bulgakov, E.E.B.Campbell

Mo3-20 EFFECT OF DIFFUSION ON NANOCLUSTER NUCLEATION
D.N. Korolev, M.V. Sorokin, A.E. Volkov

Mo3-21 PROBING FINITE-SIZE PROPERTIES OF SMALL CARBON CLUSTERS WITH DELAYED DETACHMENT PROCESS.
F. Pagliarulo, B. Baguenard, F. Calvo, P. Parneix, B. Concina, F. Lépine and C. Bordas

Mo3-22 SCREENING OF A CONFINED ATOM BY A FULLERENE OF FINITE THICKNESS
S. Lo, A.V. Korol and A.V. Solov'yov

Mo3-23 SPECIFIC FEATURES OF POLARIZATION BREMSSTRAHLUNG ON ELECTRON SCATTERING BY XENON CLUSTERS
E.V. Gnatchenko, A.N. Nechay, A.A. Tkachenko

Mo3-24 THE PHOTON-ASSISTED TRANSPORT AND MAXWELL POTENTIAL IN MESOSCOPIC DEVICES
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Mo3-25 IS CADMIUM DIMER A TRULY VAN DER WAALS MOLECULE: ROTATIONS AT THE $^{1}0_u^+ (5^1P_1) \leftarrow X^1 0_g^+$ AND $^{1}1_u(5^1P_1) \leftarrow X^1 0_g^+$ TRANSITIONS
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Mo3-26 FERROMAGNETIC COUPLING IN FINITE Mn LINEAR CHAINS
Andrey Lyalin, Andrey Solov’yov, and Walter Greiner

Mo3-27 VAPORIZATION OF RUBIDIUM AND POTASSIUM CLUSTERS BY A LOW POWER CW ATOMIC RESONANT LASER RADIATION
Alexander Plekhanov, Sergey Atutov, Roberto Calabrese, Lucca Tomassetti, Vincenzo.Guidi, Anatoly Shalagin

Mo3-28 TWO-DIMENSIONAL DISTRIBUTIONS OF SLOW Ne^{7+} TRANSMITTED THROUGH SiO_2-NANO-CAPILLARIES
P. Skog, H. Q. Zhang, and R. Schuch

Mo3-29 POLAR MOLECULES IN HELIUM CLUSTERS: BOSONIC VERSUS FERMIONIC ENVIRONMENTS
M. P. de Lara-Castells, R. Prosmiti, G. Delgado-Barrio, D. López-Durán, and P. Villarreal

Mo3-30 SWEEPING-OUT-ELECTRONS EFFECT UNDER IMPACT OF LARGE MOLECULES AND CLUSTERS
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Mo3-31 FRAGMENTATION AND FORMATION AS PHASE TRANSITION IN FULLERENES
Adilah Hussien, Ilia Solov'yov, Andrey V. Solov'yov and Walter Greiner

Mo3-32 DFT CALCULATIONS OF GOLD CLUSTERS WITH S, Se and Te COMPOUNDS
Pablo López-Tarifa, Fernando Martín and Manuel Alcamí

Mo3-33 QUANTUM MONTE CARLO SIMULATION OF SMALL BOSON-HELIUM CLUSTERS WITH FERMION-HELIUM IMPURITIES
Dr. Cono Di Paola, Prof. Gabriele Morosi, Dr. Dario Bressanini

Mo3-34 QUANTUM STRUCTURING AND MICROENERGETICS OF IONIC DOPANTS IN ^{4}HE DROPLETS FROM STOCHASTIC CALCULATIONS
E. Coccia, E. Bodo, F.A. Gianturco

Mo3-35 SPATIAL ARRANGEMENTS AND STABILITY SHELLS FOR BOSONIC He CLUSTERS AROUND IONIC IMPURITIES: A GENETIC ALGORITHM STUDY.
F. Marinetti, E. Bodo, F.A. Gianturco, E. Yurtserver, M. Yurtserver, E. Yildrim

Mo3-36 STRUCTURE OF THE PCBM FULLERENE DERIVATIVE AND ITS DIMERS
Yang Wang, Manuel Alcamí, Fernando Martín

Mo3-37 PHOTO – ATOMIC INDUCED PROCESSES IN DRYFILM COATINGS AND NANOPOROUS SILICA
A. Burchianti, A. Bogi, A. Cappello, C. de Mauro, S. Di Renzone, A. Khanbekyan, C. Marinelli, C. Maibohm, E. Mariotti, L. Moi

Mo3-38 EXCITATION AND IONIZATION OF CLUSTERS OF CHIRAL FLUORINATED MOLECULES BY R2PI SPECTROSCOPY
A. Giardini, F. Rondino, A. Paladini, M. Speranza, S. Piccirillo, M. Satta

Mo3-39 PHOTOABSORPTION CROSS SECTIONS FOR THE FULLERENE IONS C_{60}^{+} AND C_{60}^{++} .
A.K. Belyaev, V.K. Ivanov, R.G. Polozkov, A.S. Tiukanov, A.V. Solov'yov and W. Greiner

Mo3-40 STABILITY OF MULTIPLY CHARGED FULLERENE DIMERS
H. Zettergren, S. Díaz-Tendero, M. Alcamí and F. Martín

Mo3-41 AB INITIO INTERMOLECULAR POTENTIALS AND DYNAMICS OF Rg_2-DIHALOGEN CLUSTERS
R. Prosmiti, A. Valdés, C. DiezPardos, P. Villarreal, G. DelgadoBarrio

Mo3-42 ATOM-SURFACE VAN DER WAALS INTERACTION IN THE NANOMETRIC RANGE
A. Laliotis, I. Maurin, P. Todorov, I. Hamdi, G. Dutier, S. Saltiel, M.-P. Gorza, M. Fichet, D. Bloch and M. Ducloy

Mo3-43 THE LATTICE PHONON STUDIES OF CCVD GROWN CnTs
R. Malekfar and H. Asadi

Mo3-44 ENERGETICS AND STABILITY OF CARBON NANOTUBES OF DIFFERENT CHIRALITIES
Maneesh Mathew, Ilia A. Solov'yov, Andrey V. Solov'yov and Walter Greiner

Mo3-45 PRODUCTION, ANALYSIS AND MANIPULATION OF SILICON NANOPARTICLE FILMS
S. Jaksch, F. Zappa, P. Scheier

Mo3-46 NONADIABATIC PHOTODISSOCIATION DYNAMICS IN $(HI)_2$ INDUCED BY INTRACLUSTER COLLISIONS
S. López-López, R. Prosmiti and A. García-Vela

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Mo4-2 PUMP-PROBE SPECTROSCOPY IN DEGENERATE TWOLEVEL ATOMS WITH ARBITRARILY STRONG FIELDS
T. Zigdon, A. D. Wilson-Gordon, and H. Friedmann

Mo4-3 MANIPULATION OF DARK STATES WITH WHITE LIGHT

M.Auzinsh, N.N.Bezuglov , K.Miculis

Mo4-4 COHERENTLY CONTROLLED ADIABATIC PASSAGE TO MULTICHANNEL CONTINUUM STRUCTURE
Ioannis Thanopulos and Moshe Shapiro

Mo4-5 QUANTUM DYNAMICS OF A KICKED HARMONIC OSCILLATOR
Calvin Stubbins

Mo4-6 CONTROL OF WAVEPACKET INTERFERENCE AND VIBRATIONAL DISTRIBUTION BY CONTROL OF PHASE BETWEEN ULTRASHORT PULSES
Anindita Bhattacharjeei and Krishna Rai Dastidarii

Mo4-7 A GENERAL SCHEME FOR CONSTRUCTION OF COHERENT STATES OF ANHARMONIC OSCILLATORS
Marcin Molski

Mo4-8 SELECTION OF UNRESOLVED HYPERFINE STATES OF MOLECULES USING THE AUTLER-TOWNES EFFECT
T. Kirova, A. Ekers, M. Auzinsh, N. Bezuglov, K. Blushs

Mo4-9 ELECTROMAGNETICALLY INDUCED TRANSPARENCIES IN CIRCULARLY POLARIZED LIGHT IN CROSS MAGNETIC FIELDS
J. Dimitrijević, A. J. Krmpot, M. M. Mijailović, Z. D. Grujić, D. Arsenović, and B. M. Jelenković

Mo4-10 ANALYTICAL SOLUTION OF THE DEGENERATE LANDAU-ZENER MODEL
G. S. Vasilev, S. S. Ivanov and N. V. Vitanov

Mo4-11 ENHANCED FOUR-WAVE MIXING IN MERCURY ISOTOPES, PREPARED BY STARK-CHIRPED RAPID ADIABATIC PASSAGE
Martin Oberst, Jens Klein, and Thomas Halfmann

Mo4-12 CONTROLLING STATISTICAL PROPERTIES OF STORED LIGHT
Sylwia Zielińska-Kaniasty, Andrzej Raczyński, Karolina Słowik and Jarosław Zaremba

Mo4-13 COHERENT CONTROL OF LIGHT-SHIFTS AND APPLICATION TO SLOW-LIGHT AND PULSE AMPLIFICATION.
M.A.Bouchene , J-C.Delagnes, F.A. Hashmi

Mo4-14 STIMULATED RAMAN ADIABATIC PASSAGE (STIRAP) IN A Pr:YSO CRYSTAL
Jens Klein, Fabian Beil, and Thomas Halfmann

Mo4-15 PICOSECOND TO NANOSECOND PULSE SHAPING VIA A CHIRP-TRANSFORM SCALING TECHNIQUE

N. Forget, A. Cotel, T. Oksenhendler, C. Le Blanc, D. Kaplan and P. Tournois

Mo4-16 NEW WAY TO INDUCE AND CONTROL ELEMENTARY CHEMICAL TRANSFORMATIONS ON A GAS-SOLID INTERPHASE BY MEANS OF RESONANT LASER RADIATION
V. V. Petrunin

Mo4-17 LASERCONTROLLED PORPHYRIN BASED MOLECULAR CURRENT ROUTER
Ioannis Thanopulos and Emmanuel Paspalakis

Mo4-18 THE IMPORTANCE OF CARRIER BEAMS IN THE LOSSLESS PROPAGATION OF NONADIABATIC PULSES
A. Eilam, A. D. Wilson-Gordon, and H. Friedmann

Mo4-19 COMPLETE POPULATION INVERSION BY A PHASE JUMP: AN EXACTLY SOLUBLE MODEL
B. T. Torosov and N. V. Vitanov

Mo4-20 ANALYSIS OF THE TRANSIENT EFFECTS OF TWO-LEVEL ATOM IN LASER LIGHT
Saud AL-Awfi, Smail Bougouffa

Mo4-21 MANIPULATION OF SPATIAL DISTRIBUTION OF EXCITED MOLECULES IN A BEAM VIA DRESSED-STATE INTERFERENCE.
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L. P. Yatsenko and K. Bergmann

Mo4-22 DEPHASING-DECOHERENCE IN TWO-STATES TRANSITION
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Mo4-23 INTENSITY DEPENDENT LINE-WIDTHS OF HANLE ELECTROMAGNETICALLY INDUCED ABSORPTION TO TRANSVERSE MAGNETIC FIELDS
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Mo4-24 CONTROL OF PROBE RESPONSE AND DISPERSION IN A THREE LEVEL CLOSED-SYSTEM: INTERPLAY BETWEEN SPONTANEOUSLY GENERATED COHERENCE AND DYNAMICALLY INDUCED COHERENCE
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Mo4-25 EFFECT OF A TWO COLOUR LASER FIELD AND COHERENT PHASE CONTROL ON ELECTRON IMPACT EXCITATION OF A HYDROGENIC ION
A. Sinha

Mo4-26 RAPID ADIABATIC PASSAGE IN A Pr^{3+}:Y_2SiO_5 CRYSTAL

Fabian Beil, Jens Klein, and Thomas Halfmann

Mo4-27 COHERENT POPULATION TRANSFER AMONG QUANTUM STATES BY MULTIPHOTON STIRAP
H. K. Avetissian and G. F. Mkrtchian

Mo4-28 CONTROLLED POPULATION TRANSFER IN INTERSUBBAND TRANSITIONS OF QUANTUM WELL STRUCTURES
E. Paspalakis, A. Kanaki and A. F. Terzis

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Mo5-2 THE EFFECT OF VIBRATIONAL AND ROTATIONAL EXCITATION OF THE REAGENTS ON DYNAMICS OF THE INTERACTION IN THE SYSTEM CsCl + RbJ
V.M. Azriel, L.Yu. Rusin

Mo5-3 METASTABLE FRAGMENT AND VUV FLUORESCENCE YIELD FOLLOWING O 1s EXCITATION OF H_2O
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Mo5-4 OBSERVATION OF CONSECUTIVE PHOTOREACTIONS OF SINGLE ANILINE CATIONS
K. Højbjerre, D. Offenberg, A. Mortensen, P. Staanum, M. Drewsen

Mo5-5 SINGLE PHOTON-INDUCED SYMMETRY BREAKING OF H_2 DISSOCIATION
F. Martín, J. Fernández, T. Havermeier, L. Foucar, Th. Weber, K. Kreidi, M. Schöffler, L. Schmidt, T. Jahnke, O. Jagutzki, A. Czasch, E. P. Benis, T. Osipov, A. L. Landers, A. Belkacem, M. H. Prior, H. Schmidt-Böcking, C. L. Cocke, R. Dörner

Mo5-6 KINETIC STUDY OF THE REACTION $H_2O_2 + O(^3P) \rightarrow OH + HO_2$ BY AB INITIO CALCULATION
H. Koussa, M. Bahri, Y. Tarchouna, N. Jaidane

Mo5-7 PHOTOFRAGMENT SPACE DISTRIBUTION IN THE PHOTODISSOCIATION OF NAI IN THE SPECTRAL RANGE 315 - 370 NM: THE ROLE OF MOLECULAR AXIS ROTATION
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Mo5-8 ROLE OF SYMMETRY IN DISSOCIATION OF HIGHLY SYMMETRIC MOLECULES
Vandana Sharma and Bhas Bapat

Mo5-9 ULTRAFAST DISSOCIATION OF $M(CO)_6$: WAVELENGTH INDEPENDENT COHERENT OSCILLATIONS EXCLUDE A TRIPLET PATH
K. Kosma, W. Fuß, S.A. Trushin, W.E. Schmid, B. Schneider

Mo5-10 APPLICATION OF THE FEW BODY QUANTUM THEORY FOR GUIDED CONTROL OF CHEMICAL REACTIONS AND CREATION OF THE NEW MOLECULAR STRUCTURES
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Mo5-11 COULOMB EXPLOSION IMAGING OF NEGATIVE MOLECULAR HYDROGEN IONS
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Mo5-12 FEMTOSECOND WAVE PACKET DYNAMICS IN Na_2 REVEALED BY FOUR-WAVE MIXING.
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Mo5-13 ON THE STABILITY, LIFETIME AND REACTIVITY OF MOLECULAR DICATIONS IN THE GAS PHASE
M. Yáñez and O. Mó

Mo5-14 INTRAMOLECULAR VIBRATIONAL REDISTRIBUTION IN $Ne\text{-}Br_2$: THE SIGNATURE OF INTERMEDIATE RESONANCES
A. Garcia-Vela

Mo5-15 SOLVENT EFFECT ON THE 0-0 PHOSPHORESCENCE BAND AND CHANGE OF POLARIZABILITY UNDER THE $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ TRANSITION IN MOLECULAR OXYGEN
Vladimir S. Pavlovich

Mo5-16 EJECTION ANISOTROPY IN THE COULOMB EXPLOSION OF SOME ALKYL HALIDES UNDER STRONG PS LASER IRRADIATION
S. Kaziannis, C. Kosmidis

Mo5-17 THEORETICAL STUDY OF THE PHOTOIONIZATION CROOSS SECTION NEAR THE *CK*-IONIZATION THRESHOLD OF THE C_2H_2 MOLECULE
V.A.Yavna, A.M.Nadolinsky, A.N.Hopersky

Mo5-18 VALENCE SHELL DOUBLE PHOTOIONIZATION OF ALKALINE-EARTH ATOMS
A. S. Kheifets and Igor Bray

Mo5-19 ISOTOPE EFFECTS IN THE $Mg^+(3p) + HD \rightarrow MgD^+ (MgH^+) + H(D)$ REACTION
K. Højbjerre, P. Staanum, R. Wester1, M. Drewsen

Mo5-20 TIME-RESOLVED STIMULATED EMISSION SPECTROSCOPY TRHOUGH SUB-PICOSECOND PUMP-PROBE EXPERIMENTS
L. Guidoni, S. Orlando, A. Paladini, G.P. Parisi, A. Santagata, R. Teghil, A.De Bonis, A. Giardini, P. Villani, S. Piccirillo

Mo5-21 HIGH-RESOLUTION SLICE IMAGING OF QUANTUM STATE-TO-STATE PHOTODYNAMICS
M. Laura Lipciuc , T. P. Rakitzis and M .H. M. Janssen

Mo5-22 DISSOCIATION DYNAMICS OF SMALL MOLECULES UNDER STRONG LASER FIELD
A. Diner, A. Natan, U. Lev, I. Ben-Itzhak, O. Heber, D. Schwalm, Y. Silberberg, D. Zajfman

Mo5-23 HIGH-ORDER HARMONIC GENERATION IN LASER IRRADIATED LIGHT MOLECULAR DIMERS
Vladimir I. Usachenko, Pavel E. Pyak and Shih-I Chu

Mo5-24 SINGLE PHOTON–INDUCED SYMMETRY BREAKING IN H_2 DISSOCIATIVE IONIZATION
F. Martín, J. Fernández, T. Havermeier, L. Foucar, Th. Weber, K. Kreidi, M. Schöffler, L. Schmidt, T. Jahnke, O. Jagutzki, A. Czasch, E. P. Benis, T. Osipov, A. L. Landers, A. Belkacem, M. H. Prior, H. Schmidt-Böcking, C. L. Cocke, R. Dörner

Mo5-25 HIGH-RESOLUTION UV-LASERSPECTROSCOPY ON JET-COOLED 9-CYANO-ANTHRACENE IN ELECTRIC FIELDS
Markus Glugla, Elke Heinecke

Mo5-26 CAN 2D PHOTON ECHO SPECTROSCOPY DISTINGUISH ELECTRONIC AND VIBRATIONAL COHERENCES IN MOLECULAR SYSTEMS?
Dassia Egorova, Maxim Gelin and Wolfgang Domcke

Mo5-27 A FEMTOSECOND IMAGING STOPWATCH FOR THE BOND BREAKAGE OF A POLYATOMIC MOLECULE
R. de Nalda, J.G. Izquierdo, J. Durá, L. Bañares

Mo5-28 SINGLY DIFFERENTIAL CROSS SECTION FOR Ps-FRAGMENTATION WITH EXCHANGE
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Mo5-29 TRANSITION STATE SPECTROSCOPY OF OPEN SHELL SYSTEMS: ANGLE-RESOLVED PHOTODETACHMENT SPECTRA FOR THE ADIABATIC SINGLET STATES OF OHF.
Susana Gómez-Carrasco, Alfredo Aguado, Miguel Paniagua, Octavio Roncero

Mo5-30 DISSOCIATIVE ELECTRON ATTACHMENT OF SOME CYCLIC DIOLS
Bogdan Catalin Ibanescu, Olivier May, Michael Allan

6. Plasma

Mo6-1 COLLISIONAL-RADIATIVE MODELS FOR DIAGNOSIS OF Xe PLASMAS
K. Katsonis, Ch. Berenguer, R.E.H. Clark, M. Cornille, M. Ganciu

Mo6-2 IMAGING AND SPECTROSCOPY OF COLLISIONS BETWEEN HOT DENSE PLASMAS
J. Dardis, C. L. S. Lewis, J. T. Costello

Mo6-3 AN INDIUM COLLISIONAL-RADIATIVE MODEL FOR DIAGNOSTICS OF PLASMA THRUSTERS
K. Katsonis, J. Bonnet, D. Packan , Ch. Berenguer, A. Ndiaye

Mo6-4 ANGLE-RESOLVED ABSOLUTE OUT-OF-BAND RADIATION STUDIES OF TIN-BASED LASER-PRODUCED PLASMA SOURCES.
O Morris, P Dunne, F O'Reilly, G O'Sullivan, and P Hayden

Mo6-5 PLASMA CHARACTERISTICS COMPARISSON OF N_2 AND (N_2+HE) HOLLOW CATHODE GLOW DISCHARGES
V.Gencheva and R. Djulgerova

Mo6-6 IMPOSSIBILITY OF IONIZATION EQUILIBRIUM IN SWIFT HEAVY ION TRACKS
A.E. Volkov, N.A. Medvedev

Mo6-7 REACTIVE INTERACTIONS OF SMALL HYDROCARBONS WITH FUSION RELEVANT MATERIALS
N. Endstrasser, B. Rasul, W. Schustereder, F. Zappa, P. Scheier, T.D. Märk

Mo6-8 TIME RESOLVED STUDY OF LOW TEMPERATURE COLLIDING LINE PLASMAS
J. Pedregosa-Gutierrez, K. D. Kavanagh and J. T. Costello.

Mo6-9 ELECTRICAL AND OPTICAL CHARACTERIZATION OF PULSED PLASMA OF $N_2 - H_2$ MIXTURE
H. Martínez and F. B. Yousif

Mo6-10 APPLICATION OF COLLISIONAL-RADIATIVE MODELS TO SPECTROSCOPIC DIAGNOSTICS OF WEGA
K. Katsonis[1], D. Zhang, R. König, WEGA Team, Ch. Berenguer, R.E.H. Clark, M. Cornille

Mo6-11 QED EFFECTS IN INTERACTION OF ENERGETIC ELECTRONS AND PHOTONS WITH STRONG PLASMA FIELDS
I. Kostyukov and E. Nerush

Mo6-12 KINETIC ENERGY DISTRIBUTIONS OF IONS PRODUCED BY LASER ABLATION OF METALS
Borja Sierra, Jon I. Apiñániz, Roberto Martínez, Fernando Castaño

Mo6-13 LASER PULSE INTERACTION WITH INHOMOGENEOUS CYLINDRICAL PLASMA
N. Mirnes and A. H. Belbachir

Mo6-14 CORRECTION OF MEASURED EMISSION SPECTRA OF LASER INDUCED PLASMA
K. Yu. Catsalap, E. A. Ershov-Pavlov, Yu. A. Stankevich, K. L. Stepanov

Mo6-15 3D SIMULATIONS OF LASER ELECTRON ACCELERATION
Michael Geissler, Sergey Rykovanov, Jörg Schreiber and Jürgen Meyer-ter-Vehn

Mo6-16 Investigation of x-ray and high energy ions produced by laser-generated plasma in H2- and He-droplets
Nikos Petridis, Rui A. Costa Fraga, Robert E. Grisenti and Reinhard Dörner

Mo6-17 MEASUREMENTS OF ELECTRON TEMPERATURE AND DENSITY, IN AN AC PULSED OXYGEN PLASMA DISCHARGE
H Martínez, F. B. Yousif and F Castillo

Mo6-18 APPLICATION OF A LASER-INDUCED-PLASMA TO THE STUDY OF STARK WIDTHS OF Pb III SPECTRAL LINES
A.Alonso-Medina and C. Colón

Mo6-19 ATOMIC DATA FOR FUSION REACTOR IMPURITIES
K. Katsonis, R.E.H. Clark, M. Cornille, Ch. Berenguer, D. Humbert, A. Ndiaye, G. Maynard

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1. Electron, atom, molecule and ion collisions

Tu1-1 ELECTRON-IMPACT DISSOCIATIVE IONIZATION OF $CClF_3$ AND CCl_3F
Borja Sierra, Roberto Martínez, Fernando Castaño

Tu1-2	ELECTRON IMPACT EXCITATION OF THE INITIALLY EXCITED ATOMS: A FULLY RELATIVISTIC APPROACH Rajesh Srivastava, Lalita Sharma and A. D. Stauffer
Tu1-3	EFFECT OF FINITE DETECTION EFFICIENCY ON THE OBSERVATION OF DIPOLE-DIPOLE INTERACTION OF A FEW RYDBERG ATOMS I.I.Ryabtsev, D.B.Tretyakov, I.I.Beterov, and V.M.Entin
Tu1-4	A HIGH RESOLUTION STUDY OF THE $N_2^{-}(^{2}\Sigma_g^{+})$ RESONANCE IN ELECTRON SCATTERING T. H. Hoffmann, M. Allan, G. Sauter, W. Meyer, K. Franz, M.-W. Ruf , H. Hotop
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Alexander A. Kamnev

Tu3-15 ABSOLUTE CROSS SECTIONS OF ION PRODUCTION IN ELECTRON COLLISION WITH CYTOSINE MOLECULES
M.I.Sukhoviya, M.I.Shafranyosh, V.V. Medulych, P.M.Vichniy, L.L.Shimon, I.I.Shafranyosh

Tu3-16 NEW METHOD TO STUDY THE FRAGMENTATION PROCESSES UNDER WELL CONTROLLED INTERNAL ENERGY.
S. Martin, L. Chen, R. Brédy, J. Bernard, X. Ma, B.Li

Tu3-17 EXCITON DYNAMICS IN LIGHT-HARVESTING COMPLEXES AND REACTION CENTERS: CONCEPTION OF HYSTONS USED FOR SPECTRAL BROADENING AND ELECTRON TRANSFER
Vladimir S. Pavlovich

Tu3-18 ON THE ENERGETICS OF keV ION-INDUCED RADIATION DAMAGE TO DEOXYRIBOSE
Fresia Alvarado, Sadia Bari, Przemek Sobocinski, Ronnie Hoekstra, Thomas Schlathölter, Li Chen, Richard Bredy, Jerome Bernard, Serge Martin

Tu3-19 ELECTRON INDUCED CAPTURE DISSOCIATION OF PEPTIDE CATIONS.
Anne I. S. Holm, Preben Hvelplund, Umesh Kadhane, Steen Brøndsted Nielsen, Subhasis Panja, Kristian Støchkel and Esben S. Worm

Tu3-20 QUANTUM MECHANICAL SELFASSEMBLING OF ARTIFICIAL MINIMAL CELLS AND CONTROL BY MOLECULAR ELECTRONICS AND SPINTRONICS LOGICAL DEVICES
Arvydas Tamulis and Vykintas Tamulis

Tu3-21 QUANTUM MECHANICAL MODELING OF MINIMAL LIVING ORGANISMS AND PROGRAMMABLE NANO BIOROBOTS
Arvydas Tamulis and Vykintas Tamulis

Tu3-22 QUANTUM PROCESSES OF SELFASSEMBLY, PHOTOSYNTHESIS AND MOLECULAR COMPUTING IN ARTIFICIAL MINIMAL LIVING CELLS
Arvydas Tamulis and Vykintas Tamulis

Tu3-23 DETERMINATION OF TRACE ELEMENTS OF PHYTOCOMPOSITION WITH USING HERB BY INDUCTIVELY COUPLED PLASMA OPTICAL SPECTROMETRY (HYDRIDE GENERATION)
Alena Muravitskaya, Michail Belkov

Tu3-24 DIRECT FORMATION OF AMINO ACID BY UV IRRADIATION TO SIMPLE ORGANIC MOLECULES
A. Hiraya, M. Morita, Y. Harada, H. Tamaki, M. Kuwajima

Tu3-25 INELASTIC SCATTERING AND STOPPING POWER OF ELECTRONS IN BIOMOLECULAR SYSTEMS
A. Muñoz, J. C. Oller, F. Blanco, P Limão-Vieira and G. García

Tu3-26 IMAGING OF ISOLATED GASEOUS BIOMOLECULES PRODUCED BY LASER DESORPTION
T L Merrigan, C A Hunniford, R W McCullough and D J Timson

Tu3-27 LOW ENERGY ION DAMAGE TO DNA
L. Sellami, S. Lacombe, Z. Deng, M. Imhoff, I. Bald, E. Illenberger, and M. A. Huels

Tu3-28 METASTABLE DECAYS OF NEGATIVE IONS FORMED UPON ELECTRON ATTACHMENT TO SMALL BIOMOLECULES AND EXPLOSIVES
A. Mauracher, M. Beikircher, S. Denifl, F. Zappa, A. Bacher, O. Echt, T.D. Märk, P. Scheier

Tu3-29 GAS-PHASE STUDIES OF THE PHOTOABSORPTION DYNAMICS IN CHROMOPHORE IONS
L. Lammich, I.B. Nielsen, H. Sand, A. Svendsen and L.H. Andersen

Tu3-30 EPOTRAN: A FULL-DIFFERENTIAL MONTE CARLO CODE FOR ELECTRON AND POSITRON TRANSPORT IN LIQUID WATER
Champion Christophe

Wednesday 9/5

1. Alignment-Orientation-Polarization

We1-1 ON THE ANGULAR DISTRIBUTION AND SPIN POLARIZATION OF PHOTOELECTRONS FROM SEMI-FILLED SHELL ATOMS
M. Ya. Amusia and L. V. Chernysheva

We1-2 MOLECULAR IONIZATION PROBABILITY MEASURED BY MOLECULAR ALIGNMENT
V. Loriot, E. Hertz, A. Rouzée, B. Lavorel, and O. Faucher

We1-3 EFFICIENT ORIENTATION OF MOLECULES
S. Guérin, D. Sugny, H.R. Jauslin

We1-4 LASER CONTROL OF PHOTOINDUCED PROCESSES. I. ALIGNMENT AND REACTIVITY
D. Sugny, M. Desouter-Lecomte, Y. Justum L. Bomble and M. Ndong

We1-5 FIELD-FREE DYNAMIC ALIGNMENT OF DEUTERIUM WITH INTENSE FEW-CYCLE PULSES
J Wood, E M L English, C R Calvert, J McKenna, W A Bryan, R Torres, I C E Turcu, I D Williams and W R Newell

We1-6 NEW METHODS FOR THE PRODUCTION AND DETECTION OF POLARIZED ATOMS: HYDROGEN AND CHLORINE
Dimitris Sofikitis, Luis Rubio-Lago, Andrew J. Alexander, Marion R. Martin, Davida J. Ankeny Brown, Antonis Koubenakis, Nathaniel C.-M. Bartlett, Richard. N. Zare, Theofanis N. Kitsopoulos and T. Peter Rakitzis

We1-7 LASER INDUCED MOLECULAR ALIGNMENT OF ETHYLENE
A. Rouzée, S. Guérin, B. Lavorel, and O. Faucher

We1-8 ELECTRON RE-SCATTERING IN ALIGNED H_2 AND CO_2 USING THE R-MATRIX METHOD
Alex Harvey and Jonathan Tennyson

We1-9 PULSE SHAPING FOR OPTIMIZING FIELD-FREE MOLECULAR ALIGNMENT
E. Hertz, A. Rouzée, B. Lavorel, and O. Faucher

We1-10 DETERMINATION OF ATOMIC LEVEL POLARIZATION TIME DECAY
E.G. Kanetsyan, G.G. Adonts

We1-11 ALIGNMENT DEPENDENCE IN STRONG-FIELD IONIZATION OF LASER IRRADIATED MOLECULAR DIMERS
Vladimir I. Usachenko, Pavel E. Pyak and Shih-I Chu

We1-12 CIRCULAR DICHROISM IN TWO-PHOTON IONIZATION OF ORIENTED AND ALIGNED ATOMS
M. Ya. Agre

2. BEC-Quantum Gases

We2-1 GENERALIZED MEAN FIELD THEORY OF RESONANT BOSE-FERMI MIXTURES
Alexander V.Avdeenkov, Daniele C. E. Bortolotti, and John.L.Bohn

We2-2 TIME-AVERAGED ADIABATIC POTENTIALS (TAAP) FOR MATTER-WAVE INTERFEROMETRY
M. Baker, V. Bolpasi, P. Condylis, G. Konstantinidis, N. Lagos, A. Lazoudis, I. Lesanovsky, O. Morizot, M. Pappa, A. Protopapadakis, D. Sanchez, W. von Klitzing

We2-3 CREATION OF SOLITONS IN ATOMIC BEC
G. Juzeliūnas, P. Öhberg, J. Rusecka and M. Fleischhauer

We2-4 ROUTES TOWARDS Cs ATOM BEC VIA HIGH DENSITY DIPOLE TRAP.
G. Stern, D. Sofikitis, E. Dimova, A. Fioretti, D. Comparat and P. Pillet

We2-5 INTERACTION OF A RYDBERG ATOM WITH A TRAPPED BOSE-EINSTEIN CONDENSATE
Cenap Ates and Jan-Michael Rost

We2-6 MULTICOMPONENT GAP SOLITONS IN SPINOR BOSE-EINSTEIN CONDENSATES
Beata J. Dąbrowska-Wüster, Elena A. Ostrovskaya, Tristram J. Alexander, Yuri S. Kivshar

We2-7 GROUND STATE PROPERTIES AND ELEMENTARY EXCITATION OF ^{85}Rb BOSE- EINSTEIN CONDENSATE : ANALYTICAL METHOD FOR MODIFIED THOMAS-FERMI MODEL WITH LARGE GAS-PARAMETER
Moumita Gupta and Krishna Rai Dastidar

We2-8 BEYOND MEAN FIELD: USING LASER PULSES TO PROBE PAIR CORRELATIONS IN CONDENSATES
J. Mur-Petit, P. Naidon, E. Luc-Koenig, and F. Masnou-Seeuws

We2-9 DYNAMICAL INTERFERENCES AS A PROBE OF SHORT-PULSE PHOTOASSOCIATION
J. Mur-Petit, E. Luc-Koenig, and F. Masnou-Seeuws

We2-10 GAP SOLITON SELF-FORMATION IN BOSE-EINSTEIN CONDENSATE
Michal Matuszewski, Wieslaw Krolikowski, Marek Trippenbach, Yuri S. Kivshar

We2-11 GROUND STATES OF SPIN-3 BOSE-EINSTEIN CONDENSATES FOR CONSERVED MAGNETIZATION
H. Mäkelä and K.-A. Suominen

We2-12 NON-MARKOVIAN DYNAMICS IN ATOM-LASER OUTCOUPLING FROM A DOUBLE-WELL BOSE-EINSTEIN CONDENSATE
G. M. Nikolopoulos, C. Lazarou and P. Lambropoulos

3. Cold atoms and molecules

We3-1 PRODUCTION, STATE SELECTION AND DECELERATION OF COLD LITHIUM HYDRIDE
S. K. Tokunaga, J. O. Stack, J. J. Hudson, B. E. Sauer, E. A. Hinds and M. R. Tarbutt

We3-2 ATOM TRAP TRACE ANALYSIS OF CALCIUM ISOTOPES
Albert K. Mollema, Lorenz Willmann, Klaus Jungmann and Ronnie Hoekstra

We3-3 ZEEMAN DECELERATION OF NEUTRAL GROUND STATE ATOMS
S. D. Hogan, N. Vanhaecke, M. Andrist, U. Meier, D. Sprecher, B. H. Meier and F. Merkt

We3-4 QUANTUM ENGINEERING OF ULTRACOLD ATOMS IN ONE-DIMENSIONAL TRAPPING POTENTIALS
D.S. Murphy and J.F. McCann

We3-5 A SCHEME FOR CAVITY COOLING OF INTERNAL AND EXTERNAL DEGREES OF FREEDOM OF MOLECULES.
P.W.H. Pinkse, G. Morigi, M. Kowalewski, R. de Vivie-Riedle

We3-6 CREATION OF AN ULTRACOLD MIXTURE OF FERMIONIC LITHIUM AND POTASSIUM
F.M. Spiegelhalder, E. Wille, G. Kerner, D. Naik, A. Trenkwalder, C. Aiello, R. Chulia Jordan, G. Hendl, F. Schreck and R. Grimm

We3-7 COHERENT LIGHT TRANSPORT IN ULTRACOLD ATOMIC VAPORS
G. Labeyrie, D. Wilkowski, R. Kaiser, C. Miniatura, D. Delande

We3-8 PHOTOASSOCIATION OF METASTABLE HELIUM REVISITED
B. Dequilhem, F.X. Gadéa, T. Leininger, A.S. Dickinson

We3-9 AN ELECTRODYNAMIC TRAP FOR NEUTRAL ATOMS
Sophie Schlunk, Adela Marian, Peter Geng, Allard Mosk, Gerard Meijer, and Wieland Schöllkopf

We3-10	A TOOLBOX FOR THE THEORETICAL DESCRIPTION OF ULTRACOLD ATOMIC COLLISIONS Yulian V. Vanne and Alejandro Saenz
We3-11	ENHANCING RAMAN ANALYSIS IN OPTICAL TWEEZERS BY PHASE-SENSITIVE DETECTION. A. C. De Luca, G. Pesce, G. Rusciano and A. Sasso
We3-12	PHOTO-ASSOCIATIVE SPECTROSCOPY OF WEAKLY BOUND MOLECULES. LU-FANO ANALYSIS. H. Jelassi, B. Viaris de Lesegno and L. Pruvost
We3-13	TRANSPORT AND LOCALIZATION IN TILTED AND DRIVEN OPTICAL LATTICES Dirk Witthaut, Friederike Trimborn, and Hans Jürgen Korsch
We3-14	SYMPATHETIC COOLING OF MOLECULAR IONS AT ULTRALOW ENERGIES: INTERACTION AND DYNAMICS FOR $MgH^+(X^1\Sigma^+)$ WITH $Rb(^+S)$. M. Tacconi, E. Bodo, F.A. Gianturco
We3-15	MESOSCOPIC PHYSICS WITH ULTRACOLD ATOMS: FROM CONFINED SCATTERING TO RYDBERG ATOMS IN MAGNETIC TRAPS P. Schmelcher
We3-16	DETERMINATION OF THE SCATTERING LENGTH OF THE $a^3\Sigma^+$ POTENTIAL OF ^{87}RbCs E. Tiesinga, M. Anderlini, and E. Arimondo
We3-17	ELECTROMAGNETICALLY INDUCED TRANSPARENCY OF COLD Rb ATOMS IN A MAGNETO-OPTICAL TRAP K. Kowalski, S. Gateva, M. Głódź, M. Janowicz, J. Szonert, K. Vaseva
We3-18	STIMULATED RAMAN TRANSITIONS IN A CO_2 LATTICE M. G. Bason, K. J. Weatherill and C. S. Adams
We3-19	UNIVERSAL METHOD FOR COOLING/HEATING OF THE ULE FABRY-PEROT CAVITES TO THE ZERO EXPANSION TEMPERATURE J. Alnis, A. Matveev, N. Kolachevsky, Th. Udem, T.W. Hänsch
We3-20	TRANSPORT PROPERTIES IN A MOTT-LIKE STATE OF MOLECULES D.M. Bauer, N. Syassen, T. Volz, M. Lettner, D. Dietze, S. Dürr, and G. Rempe
We3-21	FEMTOSECOND LASER INDUCED FLUORESCENCE IN DENSE RbCs VAPOR

Nataša Vujičić, Ticijana Ban, Silvije Vdović, Damir Aumiler, Hevoje Skenderović and Goran Pichler,

We3-22 SPIN EXCHANGE SHIFTS IN MAGNETIC RESONANCE OF COLD ATOMIC HYDROGEN GAS
J. Ahokas, J. Järvinen, S. Vasiliev

We3-23 TRAPPING AND GUIDING ULTRACOLD ATOMS WITH THE HELP OF QUANTUM REFLECTION
Javier Madrõnero1, Florian Arnecke and Harald Friedrich

We3-24 COLD AND PURE GUIDED BEAMS OF POLAR MOLECULES
P.W.H. Pinkse, L.D. van Buuren, M. Motsch, S. Pohle, T. Rieger, C. Sommer and G. Rempe

We3-25 PHOTOASSOCIATION OF COLD CESIUM ATOMS: ANALYSIS OF THE LONG-RANGE 0_g^- STATE REVISITED.
Nadia Bouloufa, Anne Crubellier, and Olivier Dulieu

We3-26 THEORETICAL STUDY OF THE OPTICAL MANIPULATION OF COLD ATOMS
Naceur Gaaloul

We3-27 ULTRACOLD ATOM-ATOM COLLISIONS IN TRAP WITH TIME-DEPENDENT WAVE-PACKET METOD
V.S. Melezhik

We3-28 AUTOIONIZATION OF SPIN-POLARIZED METASTABLE HELIUM IN TIGHT ANISOTROPIC HARMONIC TRAPS
T. J. Beams, G. Peach and I. B. Whittingham

We3-29 COLLECTIVE EXCITATIONS AND INSTABILITY OF AN OPTICAL LATTICE DUE TO UNBALANCED PUMPING
P. Domokos, J. K. Asbóth, H. Ritsch

We3-30 HIGH SENSITIVE DETECTION SYSTEM FOR WEAK Fr MAGNETO-OPTICAL TRAP
S.N. Atutov, R. Calabrese, L. Corradi, A. Dainelli, C. de Mauro, A. Khanbekyan, E. Mariotti, L. Moi, P. Minguzzi, S. Sanguinetti, G. Stancari, L. Tomassetti, S.Veronesi

We3-31 DIPOLE-DIPOLE INSTABILITY OF ATOM CLOUDS IN AN OPTICAL DIPOLE TRAP
D. Nagy and P. Domokos

We3-32 ATOM INTERACTIONS WITH THE EVANESCENT FIELD OF A SUBMICRON FIBRE
K. Deasy, M. J. Morrissey, T. N. Bandi, B. J. Shortt, S. Nic Chormaic

We3-33 PRODUCTION AND QUANTUM CONTROL OF MOLECULES WITH OPTICAL AND MICROWAVE FIELDS
Svetlana Kotochigova

We3-34 POLARIZATION-DEPENDENT EFFECTS ON OPTICALLY PUMPED COLD CESIUM ATOMS
Yu. S. Domnin, G. A. Elkin, A.V. Novoselov, L. N. Kopylov, Yu. M. Malychev, V. N. Baryshev , V. G. Pal'chikov

We3-35 PERFORMANCE OF AN INERTIAL SENSOR BASED ON COLD ATOMS INTERFEROMETRY
A. Gauguet, W. Chaibi, B. Canuel, N. Dimarcq, D. Holleville, A. Landragin

We3-36 LOW-DENSITY, ONE DIMENSIONAL TONKS-GIRARDEAU GAS IN A SPLIT TRAP
J. Goold and Th. Busch

We3-37 GRAVITATIONAL STATES OF COLD ANTIHYDROGEN ATOMS REFLECTED FROM A SOLID SURFACE
P. Froelich and A. Voronin

We3-38 ULTRA-THIN COHERENT ATOM BEAM BY STERN-GERLACH INTERFEROMETRY
F. Perales, J. Robert, J. Baudon, J. Grucker, J.-C. Karam, V. Bocvarski, G. Vassilev, M. Ducloy

We3-39 NOVEL SURFACES FOR ATOM CHIPS
T. David, R. Salem, S. Machluf, E. Fleminger, S. Younnis, O. Arzouan, P. Petrov, V. Dikovsky, M. Rosenblit, Y. Japha, D. Groswasser, M. Keil, and R. Folman

We3-40 DEMONSTRATION OF A THREE-DIMENSIONAL RYDBERG ATOM TRAP
S. D. Hogan and F. Merkt

We3-41 PHOTOASSOCIATION OF METASTABLE HELIUM REVISITED
B. Deguilhem, F.X. Gadea, T. Leininger and A.S. Dickinson

4. Quantum Information-Cavity QED

We4-1 ENTANGLED EFFECT OF THREE-LEVEL ATOMS WITH Ξ, V AND Λ CONFIGURATIONS IN QUANTUM BIMODAL CAVITY FIELD
Ciobanu Nellu and Enaki Nicolae A.

We4-2 INDIVIDUAL ADDRESSING AND ERROR RESISTANT SINGLE QUBIT GATES WITH TRAPPED Yb^{+} IONS

A. Braun, V. Elman, M. Johanning, W. Neuhauser, N. Timoney, C. Weiß, Chr. Wunderlich

We4-3 PERFECT STATE TRANSFER IN NETWORKS OF ARBITRARY TOPOLOGY AND INTERACTIONS
G. M. Nikolopoulos, V. Košták and I. Jex

We4-4 PHOTONIC PHASE TRANSITIONS, MANY BODY SPIN MODELS, AND QIP IN COUPLED CAVITY ARRAYS
Dimitris G. Angelakis, Marcelo F. Santos, and Sougato Bose

We4-5 HIGH-FIDELITY LOGIC GATES FOR SQUID QUBITS IN A MICROWAVE CAVITY
E. Paspalakis, Z. Kis, N. Sangouard, J. Janszky and M. Fleischhauer

We4-6 FACTORING NUMBERS WITH ULTRASHORT LASER PULSES
B. Chatel, D. Bigourd, E. Baynard, C. Meier, B. Girard, W. Merkel, and W. P. Schleich

We4-7 NAVIGATION IN HILBERT SPACE BY QUANTUM STATE REFLECTIONS
P. A. Ivanov, E. S. Kyoseva, B. T. Torosov and N. V. Vitanov

We4-8 LASER CONTROL OF PHOTOINDUCED PROCESSES II. LOGICAL GATES
M. Desouter-Lecomte, D. Sugny, D. Lauvergnat L. Bomble and M. Ndong

We4-9 PERSISTENT SUPERCURRENT AS A RESOURCE FOR ATOM CHIP POTENTIAL
Tetsuya Mukai, Christoph Hufnagel, and Fujio Shimizu

We4-10 ADIABATIC PASSAGE TECHNIQUE FOR QUANTUM INFORMATION
X. Lacour, S. Guérin, H.R. Jauslin

5. Precision measurements

We5-1 DETERMINING THE ANTIPROTON MAGNETIC MOMENT FROM MEASUREMENTS OF THE HYPERFINE STRUCTURE OF ANTIPROTONIC HELIUM
Dimitar Bakalov, Eberhard Widmann

We5-2 MATTER WAVE EXPERIMENTS WITH POTASSIUM MOLCULES
Horst Knöckel, Sha Liu, I. Sherstov, C. Lisdat, E. Tiemann

We5-3 PROGRESS TOWARDS A HIGH-PRECISION MEASUREMENT OF THE *g*-FACTOR OF A SINGLE ISOLATED (ANTI)PROTON IN A HYBRID DOUBLE PENNING-TRAP

S. Ulmer, K. Blaum, H. Kracke, S. Kreim, C. C. Rodegheri, W. Quint, S. Stahl, J. Verdu, J. Walz

We5-4 VISUALISATION OF INSTABILITIES IN A STABLE TRAPPING AREA OBSERVED ON PR IONS STORED IN A PAUL TRAP
W. Koczorowski, G. Szawioła, A. Walaszyk, A. Buczek, E. Stachowska

We5-5 OPTICAL LATTICE POLARIZATION EFFECTS ON HYPERPOLARIZABILITY AND LATTICE-FIELD-INDUCED $^1S_0$- $^3P_0$ TRANSITIONS IN EVEN ISITOPES OF ALKALINE-EARTH ATOMS
Ovsiannikov V. D., Pal'chikov V. G, Taichenachev A. V and Yudin V. I

We5-6 PRECISION SPECTROSCOPY OF ANTIPROTONIC HELIUM
E. Widmann

We5-7 NEW PECULIARITIES OF SATURATED-ABSORPTION AND MAGNETO-OPTICAL RESONANCES IN ELLIPTICALLY POLARIZED LIGHT FIELDS
D.V. Brazhnikov, A.V. Taichenachev, A.M. Tumaikin, V.I. Yudin, S.A. Zibrov, Ya.O. Dudin, A.G. Radnaev, V.V. Vasil’ev, V.L. Velichansky

We5-8 LINE BROADENING BY OPTICAL PUMPING IN THE WEAK EXCITATION LIMIT
E. Saks, I. I. Beterov, P. Spels, I. Sydoryk, K. Miculis, A. Janovs, N. N. Bezuglov, I. I. Ryabtsev, A. Ekers

We5-9 COMPARISON OF DOUBLE RESONANCE MAGNETOMETERS BASED ON ATOMIC ALIGNMENT AND ORIENTATION
A. Weis, G. Di Domenico, G. Bison, P. Knowles, M. Loutsch, and H. Saudan

We5-10 ^{3}HE METASTABILITY EXCHANGE OPTICAL PUMPING STUDIES AT HIGH MAGNETIC FIELD
A. Nikiel , T. Pałasz , M. Suchanek, M. Abboud, A. Sinatra, Z. Olejniczak, T. Dohnalik, G. Tastevin , P-J. Nacher

We5-11 I.C.E.: A BOSON-FERMION ATOM INTERFEROMETER FOR MICROGRAVITY
RA Nyman, G Varoquaux, J-F Clément, J-P Brantut, T Bourdel, A Aspect, P Bouyer, N Zahzam, Y Bidel, A Bresson, F Pereira Dos Santos, A Landragin, M Rouzé, L Mondin, J Mignot

We5-12 RESONANT FEMTOSECOND PULSE-TRAIN EXCITATION OF RUBIDIUM ATOMS
D. Aumiler, T. Ban, S. Vdović, N. Vujičić, H. Skenderović and G. Pichler

We5-13 EXPERIMENTAL DEMONSTRATION OF THE FLUCTUATION-DISSIPATION THEOREM IN A THERMAL RUBIDIUM VAPOR
G. E. Katsoprinakis, A. T. Dellis and I. K. Kominis

We5-14 FEMTOSECOND LASER FREQUENCY COMB TREATMENT OF VELOCITY GROUPS BY USING ATOMIC HYPERFINE FILTER WITH PURE RUBIDIUM ISOTOPES
Goran Pichler, Ticijana Ban, Damir Aumiler, Hrvoje Skenderović, Nataša Vujičić and Silvije Vdović

We5-15 STRONGLY INTERACTING ATOMS IN OPTICAL LATTICES
Servaas Kokkelmans, Johan Mentink

We5-16 ENHANCED SENSITIVITY RUBIDIUM VELOCITY COMB MEASUREMENTS
T. Ban, S. Vdović, D. Aumiler, H. Skenderović, N. Vujičić and G. Pichler

We5-17 HIGH RESOLUTION LASER SPECTROSCOPY OF Cs-VAPOUR LAYERS WITH THICKNESS COMPARABLE TO THE WAVELENGTH OF THE IRRADIATING LIGHT
S. Cartaleva, K. Koynov, S. Saltiel, D. Sarkisyan, D. Slavov, P.Todorov, K.Vaseva

We5-18 ^{87}Sr OPTICAL LATTICE CLOCK USING SPIN-POLARIZED ATOMS
X. Baillard, M. Fouché, R. Le Targat, P. Westergaard, A. Lecallier, F. Chapelet, S. Bize, P. Rosenbusch, M. Abgrall, P. Laurent, Y. Lecoq, G.D. Rovera, A. Clairon, P. Lemonde, B. Lipphardt, G. Grosche, H. Schnatz

We5-19 HIGH-RESOLUTION SPECTROSCOPY OF FORMALDEHYDE FOR DIAGNOSTICS OF GUIDED COLD MOLECULES
P.W.H. Pinkse, M. Motsch, M. Schenk, M. Zeppenfeld, and G. Rempe

We5-20 PRECISION ELECTRONICS FOR PRECISION EXPERIMENTS
S. Stahl and S. Djekic

We5-21 EVIDENCE FOR LASER-INDUCED RELAXATION IN METASTABILITY EXCHANGE OPTICAL PUMPING OF ^{3}HE
M. Batz, W. Heil, P.-J. Nacher, G. Tastevin

We5-22 HYPERFINE STRUCTURE OF THE ONE- AND TWO-PHOTON TRANSITION LINES IN HD^+
Dimitar Bakalov, Vladimir I. Korobov, Stephan Schiller

We5-23 FROM NEWTON TO CASIMIR AND BACK: FUNDAMENTAL PHYSICS USING ATOMIC BEAM SPIN ECHO.
M.F.M. DeKieviet

We5-24 A Ca^+ SINGLE ION FOR FREQUENCY METROLOGY IN THE OPTICAL RANGE
C. Zumsteg, C. Champenois, G. Hagel, M. Houssin, M. Knoop, M. Vedel and F. Vedel

We5-25 JONES EFFECT ON ATOMS WITH DOUBLET STRUCTURE OF LEVELS

V.V. Chernushkin, P.V. Mironova and V.D. Ovsiannikov

We5-26 HIGH-ACCURACY MASS AND *g*-FACTOR MEASUREMENTS ON HIGHLY-CHARGED IONS IN PENNING TRAPS
K. Blaum, J. Alonso, I. Bergström, T. Fritioff, H.-J. Kluge, Sz. Nagy, W. Quint, B. Schabinger, R. Schuch, A. Solders, M. Suhonen, G. Werth

We5-27 ATOM INTERFEROMETRY EXPERIMENTS WITH LITHIUM
M. Jacquey, A. Miffre , M. Büchner, G. Trénec and J. Vigué

Thursday 10/5

1. Atomic and Molecular Astrophysics

Th1-1 RELATIVISTIC CORRECTION TO LYMAN AND WERNER BAND SYSTEMS OF HYDROGEN MOLECULE
E.A.Pazyuk, A.N.Drozdova, V.V.Meshkov, A.V.Stolyarov, M. Tamanis

Th1-2 TRANSITION FREQUENCY SHIFTS WITH FINE STRUCTURE CONSTANT VARIATION FOR Fe II
K. V. Koshelev, S. G. Porsev, I. I. Tupitsyn, M. G. Kozlov, D. Reimers, and S. A. Levshakov

Th1-3 THE FERRUM-PROJECT: EXPERIMENTAL AND THEORETICAL TRANSITION RATES OF FORBIDDEN [ScII] LINES AND RADIATIVE LIFETIMES OF METASTABLE ScII LEVELS
Hartman H., Gurell J., Lundin P., Schef P.,Hibbert A, Lundberg H., Mannervik S, Norlin L-O. and Royen P.

Th1-4 INFRARED EMISSION SPECTRUM OF INTERSTELLAR MOLECULAR HYDROGEN FORMED ON THE SURFACE OF DUST
Junko Takahashi

Th1-5 COLLISIONAL EXCITATION OF AMMONIA BY HELIUM AND MOLECULAR HYDROGEN IN SPACE
E. Scifoni, P. Valiron, A. Faure, C. Rist

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L. U. Ancarani and G. Gasaneo

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Kh.Yu. Rakhimov and Kh.T. Butanov

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Th3-15 DISSOCIATIVE DOUBLE CAPTURE IN $^{15}N^{4+}$ AND H_2 COLLISIONS
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Th3-16 TWO ELECTRON RESONANT EMISSION FROM ATOMS AND CLUSTERS IN THE MULTIPLE SCATTERING APPROACH
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Th3-17 TEMPERATURE EFFECTS ON DISSOCIATIVE ELECTRON ATTACHMENT TO HBr AND DBr
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C. G. Floare

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4. General Physics

Th4-1 DECOMPOSITION OF THE BOSE DISTRIBUTION OF BLACK-BODY RADIATION IN TERMS OF FERMION BINARY PHOTONS
Sándor Varró

Th4-2 MONTE CARLO SIMULATIONS OF NON-MARKOVIAN OPEN SYSTEMS
J. Piilo, S. Maniscalco, and K.-A. Suominen

Th4-3 MEASUREMENT INDUCED MANIPULATION OF THE QUANTUM-CLASSICAL BORDER
Sabrina Maniscalco, Jyrki Piilo, and Kalle-Antti Suominen

Th4-4 PHASE SPACE SUB-PLANCK STRUCTURES: EXPERIMENTAL REALIZATION IN TIME-FREQUENCY DOMAIN
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Th4-5 THE UNIVERSAL VIEW OF THE HAMILTONIAN OF THE EXCANGE INTERACTION FOR THE SYSTEM OF PARTICLES WITH ARBITRARY SPINS.
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Th4-6 EINSTEIN COEFFICIENTS FOR ACTIVATION BARRIER
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Th4-7 LOSCHMIDT ECHO IN A SYSTEM OF INTERACTING ELECTRONS
G. Manfredi and P.-A. Hervieux

POST DEADLINE ABSTRACTS

FORMATION AND TIME-RESOLVED FLUORESCENCE OF Cs^*He_n EXCIPLEXES IN SOLID ^4He
A. Hofer, P. Moroshkin, A. Weis Mo 7/5, (Clusters and Nanoparticles)

SELF-SUSTAINED OSCILLATING MODE OF OPERATION OF A HOLLOW CATHODE DISCHARGE AT POSITIVE DYNAMIC RESISTANCE
V. Steflekova, E. Dimova and D. Zhechev Mo 7/5, (Plasma)

ONE- AND TWO-PHOTON COHERENT CONTROL OF ATOMIC IONIZATION YIELDS IN THE PRESENCE OF A DC FIELD
A. Bolovinos, S. Cohen Mo 7/5, (Coherent Control)

EXACT SOLUTION OF THE THREE-BODY SCHRÖDINGER EQUATION FOR COULOMB PROBLEMS
S. Paul Thu 10/5, (Few body dynamics)

TWO-COLOR PUMP-PROBE STUDIES COMBINING EUV FREE ELECTRON AND IR/VISIBLE LASER RADIATION
P. Radcliffe, S. Düsterer, H. Redlin, A. Azima, W. Li, J. Feldhaus, J. Dardis, K. Kavanagh, H. Luna, J. Pedregosa Gutierrez, P. Yeates, E.T. Kennedy, J.T. Costello, A. Delserieys, C.L.S. Lewis, R. Taïeb, A. Maquet, A.N. Grum-Grzhimailo, E.V. Gryzlova, S.I. Strakhova, D. Cubaynes, D. Glijer, and M. Meyer
Mo 7/5, (Coherent Control)

AB INITIO STUDY OF THE PHOTODISSOCIATION OF METHANE
Rob van Harrevelt Mo 7/5, (Molecular dynamics)

TWO-PHOTON IONIZATION OF He USING EXTERIOR COMPLEX SCALING
F. Morales, F. Martín, C.W. McCurdy, Dan Horner Thu 10/5, (Few body dynamics)

OZONE MOLECULE: GLOBAL VARIATIONAL CALCULATION AND ASSIGNMENT OF HIGHLY EXCITED RO-VIBRATIONAL STATES
Vladimir Tyuterev, Sergei Tashkun, Habib Seghir, and Alain Barbe
Thu 10/5, (Atomic and Molecular Spectroscopy)

PHOTODISSOCIATION OF ALKALI DIMER MOLECULES AND DIATOMIC BUBBLES IN SOLID ^4HE
P. Moroshkin, A. Hofer, and A. Weis Mo 7/5, (Clusters and Nanoparticles)

ATOM-DIMER RESONANCE IN AN ULTRACOLD GAS
F. Ferlaino, M. Mark, M. Berninger, J. G. Danzl, S. Knoop, T. Kraemer, H. Schöbel, H. C. Nägerl, and R. Grimm We 9/5, (Cold atoms and molecules)

STRUCTURAL PATTERNS IN FULLERENES: C_{20} TO C_{102}
Yang Wang, Goar Sánchez, Sergio Díaz-Tendero, Fernando Martín and Manuel Alcamí Mo 7/5, (Clusters and Nanoparticles)

STATE SELECTIVE DIFFERENTIAL CROSS SECTIONS FOR SINGLE ELECTRON CAPTURE IN H^+-, He^+- and He^{2+} -COLLISIONS WITH He

M.S. Schöffler, J. Titze, L.Ph.H. Schmidt, O. Jagutzki, T. Jahnke, R. Dörner, H. Schmidt-Böcking and I. Mancev Thu 10/5, (Few body dynamics)

MESOSCOPIC COHERENT QUANTUM DYNAMICS IN THE STRONG BLOCKADE REGIME

Tilman Pfau

PAULI’S APPROACH OF HYDROGEN ATOM IN NONCOMMUTATIVE QUANTUM MECHANICS

Y. Grandati, A. Bérard, H. Mohrbach, H. Boumrar and F. Menas

We 9/5, (Precision Measurements)

PLENARY TALKS

Plenary 1

Precision Mass Measurement: $\omega_{cyclotron}$ is not qB/m, does $E=mc^2$?

Prof. Dave Pritchard, MIT.

We have developed an *ion balance* that has improved atomic and molecular mass measurement accuracy to ~ 10^{-11}. It compares the cyclotron frequency of *two individual* molecular or atomic ions trapped in a uniform magnetic field to find the mass ratio. Besides improving the mass of fundamental particles, this has led to discovery of a correction to the cyclotron resonance formula, a new route to determining the fine structure constant using simple physics, the best measurement of the dipole moment of any charged molecule, recalibration of the x-ray wavelength standard, a possible route to replace the artifact kilogram with an atomic mass standard, and a precise test of $E=mc^2$. We can also weigh chemical bonds.

Plenary 2

SWEETNESS AND LIGHT: FROM GLUCOSE TO GLYCOBIOLOGY

John P Simons
Chemistry Department, Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, UK

The functional importance of carbohydrates in biological processes, particularly those involving specific molecular recognition, is immense. The molecular interactions involved in the recognition of carbohydrates by proteins mediate an extraordinarily wide range of biological processes ranging from cell growth, adhesion and death to the enzymatic recycling of photosynthetically generated plant cell-wall polysaccharides, such as cellulose and xylan – the most abundant polymers on Earth. Characterizing the three-dimensional structures of carbohydrates and glycoproteins, and their interactions with other molecules, not least the ubiquitous solvent, water, are key starting points on the road towards the understanding of these processes.

The talk will introduce some of the milestones already passed along this road, driven by a combination of laser-based electronic and vibrational spectroscopy of mass-selected carbohydrate molecules and their molecular complexes conducted under molecular beam conditions, with *ab initio* computation. This approach has been revealed as a uniquely powerful means of characterizing carbohydrate conformations and the structures of their hydrated complexes; the hydrogen-bonded networks they support (or which support them); the factors which determine their conformational and structural preferences; the specificity of their interactions with other molecules; and the physical basis of their molecular recognition by proteins.

Plenary 3

The Optical Frequency Comb - a remarkable tool with many uses

John L. Hall

JILA, University of Colorado and NIST
Boulder CO 80309-0440
jan@HallStableLasers.com, jhall@jila.colorado.edu

The Optical Frequency Comb concept and technology exploded in 1999-2000 as the synthesis of advances in independent fields of Laser Stabilization, UltraFast Lasers, and NonLinear Optical Fibers. The Comb was developed first as a method for optical frequency measurement, and has enabled a new "industry" developing to check in the 16th digit for time-variation of physical "constants". The Comb methods also empower enhanced time-domain control, with broad applications in spectroscopy, metrology, and the extension of nonlinear optics to the XUV range and beyond. Combs should be a major help in frequency-based length metrology, whereby the incredible resolution is accessible ALONG WITH intrinsic resolution of the integer fringe question: two great applications will be next-generation interferometric planet-finder space missions, and cold-start dimensional metrology for tasks like layout of airplanes and accurate photolithography of large semiconductor wafers.

Plenary 4

Quantum Information Processing with Trapped Ca^+ Ions

- Multi-particle entanglement and quantum metrology –

Rainer Blatt

Institut für Experimentalphysik, Universität Innsbruck,
Technikerstraße 25, A-6020 Innsbruck, Austria,
and
Institut für Quantenoptik und Quanteninformation,
Österreichische Akademie der Wissenschaften,
Otto-Hittmair-Platz 1, A-6020 Innsbruck, Austria.
Rainer.Blatt@uibk.ac.at

Tel: +43-512-507-6350, Fax: +43-512-507-2952

Trapped strings of cold ions provide an ideal system for quantum information processing. The quantum information can be stored in individual ions and these qubits can be individually prepared; the corresponding quantum states can be manipulated and measured with nearly 100% detection efficiency. With a small ion-trap quantum computer based on two and three trapped Ca^+ ions as qubits we have generated genuine quantum states in a pre-programmed way. These states are of particular interest for the implementation of an ion quantum register: we have demonstrated selective read-out of single qubits and manipulation of inidvdual qubits of the register conditioned on the read-out results. Moreover, entangled states of up to eight particles were generated using an algorithmic procedure and the resulting states were analyzed using state tomography proving genuine multi-partite entanglement. With Bell states as a resource, entangled states are applied for teleportation and for improved precision measurements.

This work is supported by the Austrian Science Fund (FWF), by the European Commission (QGATES, CONQUEST) and in parts by ARDA and ARO.

Plenary 5

Cold Quantum Gases: when Atomic Physics meets Condensed Matter

Jean Dalibard
Laboratoire Kastler Brossel, Ecole Normale Supérieure,
24 rue Lhomond, 75005 Paris, France

A decade ago, when Bose-Einstein condensation was achieved in a cold atomic vapour, it came as a nice confirmation of the well established theory of the ideal gas. Since this initial discovery, the research on cold quantum gases has undergone a tremendous advance. It provides experimentalists with a wide variety of tools allowing one to study many-body and strongly correlated quantum systems, with the high control and precision achievable in atomic physics and quantum optics. Atomic motion in the periodic potential of an optical lattice simulates the physics of electrons in solid-state devices. Feshbach resonances are specific tools of atomic physics which enable one to adjust the sign and strength of the interaction between atoms. Quantized vortices in rotating gases lead to physical phenomena strongly connected with the Quantum Hall effect. The talk will review some recent advances in the domain, and show how these cold atomic assemblies can be considered as quantum simulators, mimicking the rich dynamics of condensed-matter systems.

Plenary 6

FEW-PHOTON MULTIPLE IONIZATION OF ATOMS BY INTENSE FEL RADIATION

R. Moshammer[1], L. Foucar[2], A. Rudenko[1], Th. Ergler[1], C.D. Schröter[1], K. Zrost[1],
S. Lüdemann[1], D. Fischer[3], J. Tietze[2], T. Jahnke[2], M. Schöffler[2], T. Weber[2,4],
R. Dörner2, T. Zouros[5], A. Dorn[1],T. Ferger[1], K.U. Kühnel[1], R. Treusch[4],
P. Radcliff[4], E. Plönjes[4], Y.H. Jiang[1], and J. Ullrich[1]

[1] *Max-Planck-Institut f̀ur Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*
[2] *Institut f̀ur Kernphysik, Universität Frankfurt, D 60486 Frankfurt, Germany*
[3] *Stockholm University, Stockholm, Sweden*
[4] *DESY, Notkestrasse 85, 22607 Hamburg, Germany*
[5] *University of Crete, Greece*
r.moshammer@mpi-hd.mpg.de

The investigation of few-electron ejection from atoms induced by interaction with light is a clean way to study the dynamics of many-body systems [1]. The simplest example of such process is double ionization by a single photon, which is nowadays considered to be well understood. In contrast, multi-photon double ionization, where about 50 optical photons are needed to release both electrons, has until now resisted any comprehensive theoretical description. Few-photon multiple ionization, i.e. the interaction of two or three photons with two or more electrons bridges the gap between these two regimes and, thus, is of decisive importance for advancing non-linear theories.

Especially intriguing is the so-called ‘direct’ or ‘non-sequential’ (NS) few-photon-induced few-electron emission in the wavelength range where one of the ionization steps can not be made with a single photon, whereas the sum of the photon energies is enough to overcome the total binding potential of all emitted electrons. Very recently NS two-photon double ionization of He with 42 eV high-harmonics [2] and with 44 eV free-electron laser (FEL) radiation [3] has been demonstrated.

Here we report on the experimental study of the few-photon multiple ionization of rare-gas atoms by intense FEL radiation with a dedicated ‘Reaction microscope’ [4]. Measurements were performed at the wavelengths of 44 nm (28.2 eV), 32 nm (38.7 eV) and 27 nm (45.9 eV) with the intensities of ~ 10^{12}-10^{14} W/cm^2. Analyzing the intensity-dependent rates of doubly charged Ne ions at 32 nm at low intensities ($I \leq 10^{13}$ W/cm^2), we observe a quadratic dependence, which indicates a dominance of the direct two-photon process. However, at higher intensities the yield curve becomes steeper, coming close to the I^3 dependence expected for the three-photon sequential ionization, which for the case of Ne at 32 nm is enhanced due to the intermediate resonant state [3]. Thus, we observe a transition between two different ionization mechanisms, which is also reflected in the measured momentum distributions of doubly charged Ne ions [5].

Signatures of NS processes were also observed for multiple ionization of Ar at 44 nm, and for the fragmentation of H_2 and D_2 molecules at 32 nm. A detailed analysis of these data, as well as of the latest results obtained at 27 nm is currently underway.

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INVITED TALKS

1a-1

QUANTUM CONTROL OF CHEMICAL REACTIONS AND FUNCTIONS

Leticia González

Institut für Chemie und Biochemie
Freie Universität Berlin, Takustrasse 3, D-14195 Berlin
leti@chemie.fu-berlin.de

This talk will address the problem of tracking the ultrafast dynamics of light induced reactions in real time and its possible manipulation. Using ultrashort laser pulses it is possible to follow carefully the movement of the nuclei. Furthermore, today's laser technology has made it possible to shape laser pulses in such a way that a particular nuclear motion can be artificially imprinted, leading to the so-called coherent control of molecular reactions.

Using ab initio potential energy surfaces and wave packet propagations, we will show how a sequence of laser pulses with appropriate frequencies and time delays can manipulate the formation of particular products. As an example, we will show recent results on the control of selective bond breaking in the organometallic complex $CH_3Co(CO)_4$ and in the halomethane CH_2ClBr. Besides structure, we will also show how functions can be also manipulated using laser pulses.

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1a-2

Quantum and mixed quantum/classical approaches to the control of ultrafast molecular wave packet interferences

C. Meier

Laboratoire Collisions, Agrégats et Réactivité, IRSAMC
Université Paul Sabatier, Toulouse

An important aspect of quantum dynamics in an environment is ultrafast vibrational relaxation. Additionally, if several initial vibrational states are excited coherently, the system-solute interaction not only leads to energy relaxation but also to decoherence. One way to study decoherence is considering interferences of moving wave packets.
Among others, we plan to consider the I_2 molecule, both free and in a dense rare gas environment. The excitation by femtosecond laser pulses and the subsequent relaxation dynamics is studied using quantum and mixed quantum/classical methods.

We first consider the interference of counterpropagating wave packets which create nodal structures that appear and disappear at a femtosecond timescale, and which have a spatial resolution defined by the de Broglie wavelength. Specifically, it is shown that these sub-picometric interference structures can be measured within a pump-probe setup by a thorough choice of laser parameters employed.
In a natural way, localised counterpropagating wave packets appear in weakly anharmoinc systems by the revival phenomena, albeit with fixed relative phases. Using a multiple pulse set up, a control of the relative phase should be possible, which in turn alters the fringes of the matter interferences. Additionally, further possibilies to actively control the quantum wave packet dynamics and their spatio-temporal nodal pattern will be addressed.

In a second part, we show the effect of random rare gas collisions onto the coherent wave packet motion. To this end, the quantum wave packet propagation is combined with a classical molecular dynamics simulation for the large number of degrees of freedom forming the environment . The coupling between classical and quantum degree of freedom is established via quantum trajectories, determined by the quantum flux associated with the moving wave packet. The possibility to include time-dependent external fields of arbitrary shapes allows for a direct comparison with experimentally measured pump-probe spectra.

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1a-3

DRESSED STATE TAILORING WITH ULTRASHORT LIGHT PULSES

Matthias Wollenhaupt

Universität Kassel, Institut für Physik und CINSaT, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany, E-mail: wollenha@physik.uni-kassel.de, phone: +49 561 804 4294

Modern elaborate quantum control strategies making use of tailored ultrashort light pulses are enormously successful to manipulate a great variety of physical and chemical properties of matter. However, in many cases the underlying physical processes are not very well understood - particularly when shaped resonant intense pulses are applied. This class of pulses is of general importance because resonant control scenarios will be the dominant pathways as shorter and shorter pulses with ultra broad spectra become available.

In this contribution the physical mechanism of quantum control using tailored intense resonant optimal pulses is investigated on model systems (atoms and small molecules [1-3]). Switching among different final electronic states is realized by manipulation of dressed state energies and dressed state population. Selective Population of Dressed States (SPODS) is a general approach to strong field control because specific implementations of SPODS by suitable pulse shapes comprise different physical mechanisms such as Photon Locking and Rapid Adiabatic Passage techniques.

Figure 1: Selective Population of Dressed States (SPODS) is directly mapped into the measured photoelectron spectra by variation of the phase ϕ. The maximum of the asymmetric photoelectron distribution alternates between 0.33 eV and 0.52 eV. These results are obtained at a laser energy of $W = 0.5 \mu J$. A section through the distribution along the energy axis at $\phi = 0.7\,\pi$ – indicated with the violet trajectory – yields the photoelectron spectrum (A) where the lower dressed state is selectively populated as depicted in the inset.

In the experiment different realizations of SPODS are demonstrated. High selectivity of the dressed state population, i.e. a switching efficiency of more than 90% is demonstrated (see Fig. 1). Because we achieve tunability of dressed state energies in the range of several hundred meV, our approach is attractive for control of chemical reactions. SPODS is ultrafast, i.e. proceeds within a few optical cycles. Therefore our strategy might be operative in the presence of decoherence processes as well.

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1b-1

Properties of Cluster Ions Probed by Mass Spectrometry, Laser Spectroscopy, Electron Diffraction and Quantum Chemistry

M. M. Kappes[1,2], O. Hampe[1], M. Neumaier[1], D. Schooss[1], A. Lechtken[1], M. Kordel[1], P. Weis[2], E. Oger[2], O. Ehrler[2], K. Matheis, C. Rensing and A. Glöss[2]

[1] *Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany;*
[2] *Institut für Physikalische Chemie, Universität Karlsruhe, 76128 Karlsruhe, Germany*

Clusters of refractory elements have been of interest for many years and for many reasons ranging from benchmarking quantum chemical calculations, through understanding heterogeneous catalysis, to providing appropriate building blocks for nanotechnology. A useful experimental approach continues to be cluster size-specific measurement under collisionless conditions – concentrating in particular on mass-selected ions. Methods for this have become increasingly sophisticated over the years. The starting situation more than 25 years ago was characterized by cluster beam source development coupled with mass spectrometric analysis of the resulting cluster abundances (e.g. “magic numbers”). Today, the field has advanced to the point that it is possible to rigorously determine molecular structures as well as many physical and chemical properties in the (free) cluster size range of up to 100 atoms. This is the consequence not only of experimental method development but also of significant advances in quantum chemistry.

The talk will concentrate on recent work from the group on boron (B_x^+, x<30), carbon (C_x^{2-}, x= 70, 76, 78 and 84) and gold clusters ($Au_x^{+/-}$, x=3-65) in various positive and negative charge states - examples chosen to illustrate the potential of present-day methods. Boron cluster cations were studied by ion mobility spectroscopy to yield collision cross sections which can in turn be interpreted by density functional calculations to allow structural assignment. With increasing particle size, boron cluster cations go from planar to stacked-ring geometries. Carbon cluster dianions have been studied using photoelectron- and photodissociation-spectroscopies. Together with measurements of the kinetics and energetics of bimolecular electron transfer reactions, these experiments yield insights into the size-dependence of electronic structure and Coulomb barrier heights in these model multianions. Gold cluster ions have been probed using a combination of ion mobility, laser spectroscopic methods and trapped ion electron diffraction. Together with calculations of ground and excited electronic states, these measurements have allowed structure determination for many cluster sizes. These structural inferences can be used to understand cluster size-dependent variations in the kinetics of simple radiative association reactions (e.g. $Au_x^+ + CO \rightarrow Au_xCO^+$).

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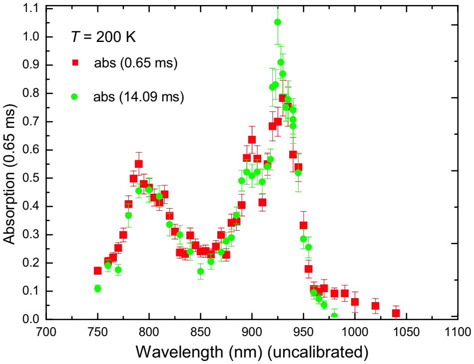
1b-2

Near-infrared spectroscopy on C_{60} anions

J.U. Andersen, University of Aarhus, DK-8000 Aarhus C, Denmark

The anions of C_{60} are of great interest for several reasons. The C_{60} molecule has very high symmetry (icosahedral) and the lowest unoccupied electronic level (t_{1u} symmetry) is triply degenerate, with orbitals analogous to p-states in an atom, and the orbitals are subject to Jahn-Teller splitting. Additional electrons couple mainly to quadrupole deformations of the C_{60} cage, and there is a close analogy to the coupling between single particle and collective excitations in heavy nuclei. Another interesting aspect is the connection to superconductivity of A_3C_{60} compounds (A= alkali metal) at fairly high temperatures. We have carried out spectroscopic studies of both C_{60}^{-} [1] and C_{60}^{2-} at the electrostatic storage ring ELISA in Aarhus. The anions have mostly been studied in liquid or solid solution where the charge is stabilised by neighbouring counter ions, but spectroscopy in the gas phase has obvious advantages. The photon absorption can be associated unambiguously with a single charge state, and the energy levels of the ion are unperturbed by interactions with a solvent. The electron-electron repulsion makes isolated anions with several additional electrons unstable and difficult to produce. For C_{60}, already the second additional electron is unbound but the detachment is hindered by the Coulomb barrier, just like emission of an alpha particle from a radioactive nucleus. The instability of the ions can be turned into an advantage because the decay dynamics gives information about the structure of the low-lying electronic levels [2]. The figure shows absorption spectra recorded at two different times after injection of C_{60}^{2-} ions into ELISA. At the longer time, the hottest ions have decayed so the average ion temperature is lower and the thermal population of the ground state is higher. The line at about 925 nm can therefore be identified as a transition from the ground state. The experiments are still in progress, with development of both the ion source and the laser facilities at ELISA.



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MOLECULAR DYNAMICS FOR FISSION PROCESSES

O. I. Obolensky, A. Lyalin, I. A. Solov'yov,
A. Yakubovich, E. Henriques, A. V. Solov'yov, W. Greiner

A.F. Ioffe Physical Technical Institute, 194021 St. Petersburg, Russia
Frankfurt Institute for Advanced Studies, 60438 Frankfurt am Main, Germany

Fission is a ubiquitous process playing important roles in many physical phenomena. In fission, the initial and final states of a system are separated by a potential barrier, the so-called fission barrier. The height and the shape of this barrier determine most of the experimental observables of the process, such as characteristic fission times and branching ratios between different fission channels.

We discuss relative advantages and disadvantages of two general approaches which are used for carrying out a molecular dynamics analysis of fission processes [1]. The goal of both approaches consists in finding the optimum fission pathway which minimizes the fission barrier. The optimum fission pathway frequently involves complicated rearrangements of the ionic structure including formation of intermediate metastable configurations [2] which makes this problem rather difficult.

The first approach to the molecular dynamics analysis is the conventional molecular dynamics simulations which emulate the evolution of a system with time [3,4]. This approach relies on the assumption that the system explores sufficiently large volumes of its phase space (thus covering sufficiently large areas of the potential energy surface) if a sufficiently large number of runs of the simulations are made and each run is sufficiently long. In order to shorten the required CPU time one usually assigns rather high initial temperatures to the system. In such a case, however, the system tends to fission along the shortest path rather than along the path with the lowest potential barrier. Therefore, one has to find the optimum balance between the reliability and the feasibility of simulations.

The second approach consists in a direct (manually- or algorithmically-driven) exploration of the potential energy surface of the system [5]. This approach allows one to perform a systematic analysis of the various fission scenarios, reducing the chance of an accidental omission of an important fission pathway. We review one of the possible algorithms for exploration of the potential energy surface [3,5] and give examples of its applications to fission processes in atomic clusters, bio- and macro-molecules.

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1b-4

Femtosecond optical spectroscopy of a single metal nanoparticle

Natalia Del Fatti, Otto Muskens, and Fabrice Vallée

LASIM, Université Lyon 1 - CNRS
43 Bd. du 11 Novembre 1918, 69622 Villeurbanne - France
email: delfatti@lasim.univ-lyon1.fr

The reduction of a material size to a nanometric scale drastically modifies its physical and chemical properties as compared to the parent bulk material. This is in particular the case in the optical domain for metallic nanostructures with apparition of new resonances, namely the surface plasmon resonances. They are at the origin of the large and growing interest for metal based optical nanomaterials, with many applications in new fields such as nanophotonics or plasmonics. In this context, confinement effects on the electronic and vibrational properties play central roles, as they determine most of the observed optical linear and nonlinear responses. With the advance of femtosecond laser sources, time-resolved optical spectroscopy has become an efficient and versatile tool to investigate the nonlinear optical response and the fundamental electronic and vibrational properties of nanomaterials. In particular, it constitutes a powerful tool for analyzing electron interactions processes and vibrational kinetics in nanoparticles embedded into a matrix [1].

Up to now most time-resolved optical investigations were performed on large ensembles of nanoparticles dispersed in a liquid or solid matrix, with the concomitant difficulty of nanoparticle size, shape and environment fluctuations. In the case of nanospheres, this has been circumvented by using high quality samples with weak size and shape dispersions and performing experiments in environment independent conditions [2]. However, precise investigation of the impact of the particle shape and environment on the electron response requires the development of femtosecond spectroscopy of single nanoparticles identified in-situ in size, shape and orientation on the substrate.

With the recent development of the far-field spatial modulation spectroscopy technique such characterization of a nanoparticle can now be performed optically [3]. We report here on coupling of this approach with a high sensitivity pump-probe time-resolved femtosecond setup. It permits to investigate the transient absorption of an identified single metal nanoparticle and, in particular, to obtain information on electron-lattice energy exchanges in a single nano-object [4,5]. Experiments were performed in silver nanospheres with size down to 20 nm. The measured nanoparticle size dependence of the extinction change kinetics is compared to theoretical models and to the ensemble response. Its application to other nanoparticle shapes will also be discussed.

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2a-1

Attosecond Physics

Ferenc Krausz
Max-Planck-Institut für Quantenoptik, Garching,
Ludwig-Maximilians-Universität München, Germany

Fundamental processes in atoms, molecules, as well as condensed matter are triggered or mediated by the motion of electrons inside or between atoms. Electronic dynamics on atomic length scales tends to unfold within tens to thousands of attoseconds (1 attosecond [as] = 10^{-18} s). Recent breakthroughs in laser science are now opening the door to watching and controlling these hitherto inaccessible microscopic dynamics.

The key to accessing the attosecond time domain is the control of the electric field of (visible) light, which varies its strength and direction within less than a femtosecond (1 femtosecond = 1000 attoseconds). Atoms exposed to a few oscillations cycles of intense laser light are able to emit a single extreme ultraviolet (xuv) burst lasting less than one femtosecond [1,2]. Full control of the evolution of the electromagnetic field in laser pulses comprising a few wave cycles [3] have recently allowed the reproducible generation and measurement of isolated sub-femtosecond xuv pulses [4], demonstrating the control of microscopic processes (electron motion and photon emission) on an attosecond time scale. These tools have enabled us to visualize the oscillating electric field of visible light with an attosecond "oscilloscope" [5], to control single-electron and probe multi-electron dynamics in atoms [6,7], molecules [8] and solids [9]. Recent experiments [10] hold promise for the development of an attosecond x-ray source, which may pave the way towards 4D electron imaging with sub-atomic resolution in space *and* time.

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2a-2

The other half of the story: attosecond time-resolved electron dynamic

Marc Vrakking
FOM-Institute AMOLF, Kruislaan 407,1098 SJ Amsterdam, The Netherlands

Femtosecond time-resolved experiments allow the real-time observation of atomic and molecular processes. Often however, these experiments tell only half the story: they show the motion of atoms moving under the influence of potential energy curves that result from a time-average over the motion of all electrons in the system. *Real-time* observation of these electrons requires recently developed attosecond laser techniques.

In my talk I will present results from recent experiments where isolated attosecond pulses and attosecond pulse trains are used to gain insight into electronic processes that occur in atoms and molecules on these ultrafast timescales. I will discuss experiments on the dissociative ionization of molecular hydrogen where electronic motion has been controlled on attosecond timescales, as well new experiments where attosecond pulse trains are used to develop a new type of interferometry, that may allow the reconstruction of atomic and molecular orbitals.

2a-3

ATTOSECOND METROLOGY IN THE SINGLE-CYCLE REGIME

G. Sansone, E. Benedetti, F. Calegari, C. Vozzi, S. Stagira, S. De Silvestri, M. Nisoli
National Laboratory for Ultrafast and Ultraintense Optical Science CNR-INFM
Department of Physics, Politecnico, Piazza L. daVinci 32, 20133 Milano, Italy
phone:+39 0223996057; fax: +39 02 23996126; e-mail: giuseppe.sansone@polimi.it
L. Avaldi, R. Flammini
CNR – IMIP Area della Ricerca di Roma 1, Monterotondo Scalo 00016, Italy
L. Poletto, P. Villoresi
Laboratory for Ultraviolet and X-Ray Optical Research CNR-INFM
D.E.I. - Università di Padova, Padova, Italy
C. Altucci, R. Velotta
CNISM-Dipartimento di Scienze Fisiche, Università di Napoli "Federico II", Napoli, Italy

The generation of attosecond pulses represents one of the frontier in the Ultrafast Optics for the possibility to influence, control and monitor the motion of electronic wave packet inside molecules and atoms. Complete temporal characterization is a fundamental step towards the application of attosecond pulses to time resolved studies.

In this work we report on the generation, compression and temporal characterization of isolated attosecond pulses down to the single cycle regime. Broadband spectra in the extreme ultraviolet have been generated focusing phase-stabilized few-optical-cycle driving pulses with a time dependent ellipticity in an Argon cell with static pressure. The infrared (IR) driving radiation and the low order harmonics generated in the gas cell have been filtered out using a 300 nm thick aluminum foil. The metallic filter also provides compensation of the intrinsic positive chirp of the attosecond pulse The high energy harmonic radiation and a portion of the IR field (streaking beam), with variable temporal delay with respect to the XUV pulse, have been spatially overlapped and focused on a second argon gas jet The energy spectra of the photoelectrons emitted by single XUV photon absorption and accelerated by the streaking beam, have been detected using a time-of flight (TOF) electron spectrometer. We have acquired photoelectron spectra as a function of the delay between the attosecond pulse and the IR streaking pulse. Applying an iterative procedure to these measurements, it is possible to retrieve the envelope and the temporal phase of the attosecond pulse [1]. Figure 1A and 1B show the experimental trace and the reconstructed pulse profile, respectively. The duration of the isolated pulse is 130 as and the temporal phase is almost flat.The duration is close to the Fourier limit of 110 as and corresponds to only 1.2 oscillation of the central frequency of the spectrum (36 eV) [2]. These results indicates the possibility of experiments for the determination of the CEP of the attosecond pulses.

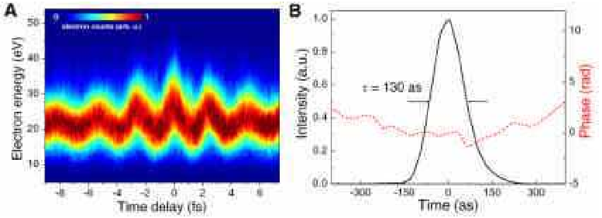

Fig. 1A. Photoelectron spectra acquired as a function of the delay between the IR and the XUV fields with an aluminum foil of 300 nm thickness.

Fig 1B. Reconstructed time profile of the attosecond pulse from the trace of Fig. 1A. The phase presents only residual oscillations indicating a good compensation of the intrinsic chirp of the attosecond pulse.

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2a-4

AUTOCORRELATION MEASUREMENT OF ATTOSECOND PULSES BY XUV TWO-PHOTON PROCESS

Yasuo Nabekawa, Toshihiko Shimizu, Hirokazu Hasegawa, and Katsumi Midorikawa

Laser Technology Laboratory, RIKEN
2-1 Hirosawa, Wako, Saitama 351-0198, Japan

The progress of chirped pulse amplification and femtosecond Ti:sapphire laser enables the study of the interaction of strong optical fields with atoms and molecules. A variety of interesting phenomena, including high-harmonic generation, high energy radiation/particles emission, and Coulomb explosion of molecules, have been investigated intensively. The underlying physics of these nonlinear optical phenomena have been emerging through the interaction with low-frequency optical radiations such as infrared or visible light; however, little has been understood concerning the interaction of *intense high-frequency radiation* such as xuv or soft x-ray. Great interest has been aroused recently in the interaction of intense high-frequency radiation with matters. Yet no one could observe it because of the lack of an intense coherent light source in this spectral region. The induced phenomena are expected to be much different from those caused by low frequency radiation because the electron quiver energy-the cycle averaged electron energy in the optical field-is proportional to a square of the wavelength. Photon energy higher than ionzation potentials of atoms and molecules also would differenciate mutliphoton ionization process from those observed with infrared or visible photons.

We have demonstrated nonlinear multiphoton process with intense xuv and soft x-ray pulses produced by phase-matched high-order harmonics. The observation of nonlinear optical process in the soft x-ray region has been a very attractive and challenging area of research in quantum electronics since the first obsrevation of second-harmonic generation and two-photon exciation in the visible region in 1961. Using two-photon double ionization in He, the temporal width of the 42-eV soft x-ray pulse was measured directly by an autocorrelation technique [1]. A train of attosecond pulses was also characterized by energy-resolved autocorrelation with photoelectrons produced through two-photon above threshold ionization (ATI) [2]. Although characterization of attosecond pluses is of great imporatnce for the progress of ultrafast optical science, most of reseaches owe their success to the indirect methods using two-color ATI [3, 4]. An autocorrelation signal given by the nonlinear interaction between optical fields and matter, on the other hand, directly reflects the shape of the pulse in the primary data, whether it is trainlike or isolated. Our methd using two-photon proecess is the naural extenstion of the well-developed method in the infrared or visible region.

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2b-1

Novel interactions in quantum gases

Tilman Pfau

5. Physikalisches Institut, Universität Stuttgart, Germany

Interactions in atomic quantum gases – i.e. cold collisions - make them a model system for many branches of physics including condensed matter, and nonlinear dynamics. So far all the impressive phenomena (like superfluidity, soliton and vortex formation, BEC-BCS crossover etc.) in atomic Bose and Fermi gases are caused by a contact interaction, originating from s-wave scattering off the van der Waals potential.

Here we report on our experiments on Bose Einstein condensation in a gas of chromium atoms [1] with a sizable magnetic dipolar interaction. We prove the anisotropic nature of the dipolar interaction by releasing the condensate from a cigar shaped trap and observe, in time of flight measurements, the change of the aspect-ratio for different in-trap orientations of the atomic dipoles [2]. One consequence of the anisotropic dipolar interaction is coupling between spin and motion, which we used for the first demonstration of demagnetization cooling of a gas of atoms [3], and which might lead to a quantum version of the Einstein de Haas effect [4].

We also report on our experiments on interacting ultracold Rydberg atoms excited from a Rb Bose-Einstein condensate or a thermal cloud. We observed a blockade of the Rydberg excitation due to the strong repulsive van der Waals interaction of Rydberg atoms in the 43 s state. We confirm the coherent collective nature of the excitation by the measurement of the scaling law for the excitation time [5]. We confirm the coherence of excitation also by reversing the excitation by a π phase-shift in the driving laser field.

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2b-2

Quantum Degenerate Gases of Metastable Helium-3 and Helium-4 Atoms

Wim Vassen

Laser Centre Vrije Universiteit, Amsterdam, the Netherlands

Bose-Einstein condensation (BEC) of metastable ^{4}He (^{4}He*) atoms has been observed for the first time in 2001 [1,2]. Since then research of ultracold ^{4}He* focused on determining ultracold collisional properties such as scattering length and two-body loss rate coefficients on the one hand and photo-association of (long-range) molecules on the other hand. In 2005, for the first time, atom bunching was observed for ^{4}He* bosonic atoms [3]. In Amsterdam we have observed BEC of ^{4}He* in 2005 and realized condensates containing more than 10^7 atoms [4]. Adding the fermionic isotope ^{3}He we have realized a degenerate Fermi gas (DFG) by sympathetic cooling of ^{3}He* by ^{4}He* [5]. Being able to create ultracold samples of either ^{4}He*, ^{3}He*, or a mixture of the two, we studied, in collaboration with the group of Chris Westbrook in Orsay, the analogue of the Hanbury Brown Twiss effect for ^{3}He* fermions and observed antibunching, as shown, together with bunching observed for ^{4}He* in the same apparatus, in Fig. 1 [6]. In my presentation I will discuss these experiments.

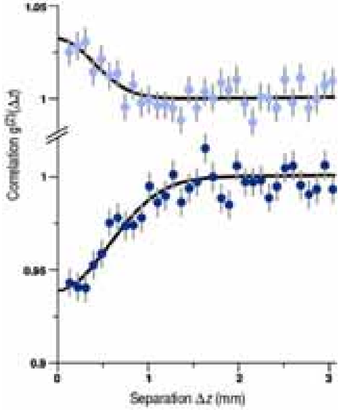

Fig. 1. Normalized probability of the joint detection of two atoms at two points separated by a distance Δz along the vertical z-axis, for ^{4}He (bosons) in the upper plot, and ^{3}He* (fermions) in the lower plot (from Ref. [6]).*

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SCATTERING LENGTH OF SPIN-POLARIZED HELIUM

Bogumił Jeziorski

Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland

The s-wave scattering length of metastable, spin-polarized helium has been determined for the first time in the BEC experiments performed in 2001. The experiments performed by Alain Aspect's (Orsay) and Claude Cohen-Tannoudji's (Paris) groups gave the values of 20 nm and 16 nm, respectively, with error bounds as large as 50% of the measured values. A more recent, 2004 experiment from the Paris group led to a value between 10.3 and 13.7 nm. Initial theoretical calculations were confirming these large values. Our group became interested in this problem in 2003. Using a combination of state-of-the-art electronic structure methods, we obtained a Born-Oppenheimer interaction potential for the lowest $^5\Sigma_g^+$ state of the helium dimer with an accuracy of the order of 0.01% at the minimum and even better at the inner and outer parts of the potential. By including also the adiabatic coupling of the nuclear and electronic motion, as well as an estimate of the leading relativistic and QED corrections, we predicted in 2005 a new theoretical value of the scattering length, equal to 7.64±0.20 nm, lying outside the error bounds of all previous experimental determinations based on the properties of Bose-Einstein condensate. Shortly after, Kim et al. (Paris group) measured the light induced frequency shifts in photoassociative spectra of metastable helium atoms and inferred the value of 7.2±0.6 nm for the s-wave scattering length, in full agreement with our prediction. In a subsequent development, Moal et al. (Paris group) carried out a two-photon photoassociation experiment and determined very accurately the energy of the least-bound, v=14 state of the metastable helium dimer. Their result of 91.35±0.06 MHz was used to scale the inner part of our ab initio potential, which led to a new "experimental" value of 7.512±0.005 nm for the scattering length. This value turns out to be in a slight disagreement with the most recent ab initio calculation from our group which takes higher relativistic effects into account. The possible origin of this disagreement will be discussed. It will also be shown that the very accurately measured value of the energy of the v=14 state provides a very stringent test for the relativistic theory of interatomic interactions.

Signatures of Efimov's effect in ultracold gases

Thorsten Köhler

Department of Physics, University of Oxford, Clarendon Laboratory,
Parks Road, Oxford, OX1 3PU, United Kingdom

Abstract

Based on the approach of Ref. [1], we present numerically exact calculations of resonance enhanced three-body recombination in ultracold ^{133}Cs Bose gases. We discuss associated atom-loss-rate constants at low magnetic-field strengths in comparison with recent experiments [2] on Efimov's effect [3] and interpret these measurements in terms of their relation to similar studies on helium trimers in molecular beams [4, 5]. We show how, as yet unobserved, excited Efimov-trimer states might be detected in ultracold gases of ^{85}Rb, as well as ^{133}Cs at high fields in the vicinity of 800 G. This involves schemes for the association of such exotic molecules using magnetic-field sweeps in optical lattices with three atoms per site [6].

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3a-1

Conical Intersections and Photostability of the Building Blocks of Life

Wolfgang Domcke
Department of Chemistry, Technical University of Munich, Germany
Andrzej L. Sobolewski
Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

It is nowadays well established that conical intersections of electronic potential-energy surfaces are ubiquitous in polyatomic molecules and that they play a decisive role in photochemistry [1-3]. This talk addresses the ab initio calculation of potential-energy surfaces of excited electronic states of fundamental biomolecules, in particular the reaction paths leading to conical intersections. Time-dependent quantum wave-packet calculations have been performed which confirm the ultrafast time scale of the photophysical dynamics at conical intersections. Indole and phenol serve as models for the investigation of the photochemistry of aromatic amino acids (tryptophan and tyrosine). Adenine is considered as an example of the DNA bases. The calculations reveal the role of hitherto uncharacterized low-lying dark excited electronic states of $^1\pi\sigma^*$ character, which intersect both the $^1\pi\pi^*$ excited singlet states as well as the electronic ground state [4]. The resulting conical intersections provide a pathway for the ultrafast radiationless deactivation of the UV absorbing excited states. For the guanine-cytosine and adenine-thymine Watson-Crick base pairs, an additional mechanism of ultrafast excited-state deactivation has been identified [5, 6] which involves proton transfer driven by electron transfer. A novel and specific picture of the ultrafast excited-state deactivation in biomolecules emerges: the energy deposited by an UV photon in the molecule is first transferred to a hydrogen-bonded proton within about 50 fs and subsequently dissipated into the vibrations of the surrounding heavier atoms. Preliminary results indicate that this picture also applies for hydrogen bonds in peptides [7]. These findings suggest that electron-driven proton-transfer processes play an universal role in the photochemistry of biomolecules and biopolymers (proteins and DNA). The ultrafast photochemistry of hydrogen bonds may be the origin of the exceptional photostability of these compounds, which has lead to their selection at the very beginning of the biological evolution.

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3a-2

Probing the secondary structures of short peptide chains in the gas phase: IR / UV double resonance studies

E Gloaguen, F. Pagliarulo, F. Piuzzi, V. Brenner, I. Dimicoli and M. Mons

Laboratoire Francis Perrin, URA CEA-CNRS 2453,
Service des Photons, Atomes et Molécules,
CEA Saclay, Bât 522, Gif-sur-Yvette Cedex, France

A bottom-up approach involving conformer-specific IR studies of short peptide sequences enables us to map the intramolecular interactions that shape the peptide backbone, in particular those H-bonds that are responsible for stability and formation of secondary structures in proteins, like turns or helices.

The combination of laser-desorption of solid samples coupled to the efficient cooling in a supersonic expansion makes it possible to isolate in the gas phase the lowest conformations of the energy landscape of small flexible biomolecules. The low temperature achieved enables spectroscopists to record UV spectra in which the contribution of each conformer populated can be distinguished and the corresponding conformation identified using IR/UV double resonance spectroscopy. Data collected are directly comparable to the best quantum chemistry calculations on these species and therefore constitute a severe test for the theoretical methods used.

It will be shown how investigation of sequences with an increasing number of building blocks permits to deduce the robust structural trends of a peptide backbone:

i) local conformational preference of the backbone in one-residue chains,

ii) the competition between a succession of local conformational preferences and overall folded structures in longer chains (capped dipeptides), in particular with the formation of beta-turns, the secondary structures responsible for chain reversals in proteins,

iii) the role of the conformation of the residues (L or D chirality) within the chain on the type of structure formed and, finally,

iv) evidence for the spontaneous helical folding (short 3-10 helix) of three-residue chains will be presented.

3a-3

IR and UV Spectroscopy of cold, biomolecular ions

Thomas R. Rizzo

Laboratoire de chimie physique moléculaire, Ecole Polytechique Fédérale de
Lausanne, Station 6, CH-1015 Lausanne

The spectroscopic study of small neutral biological molecules in supersonic free jets has provided a wealth of information on their energy landscapes and represents an important means to test the reliability of structure calculations. In such studies, the spectral simplification afforded by the cooling in a supersonic expansion is essential for being able to extract useful information. Many, if not most, biological molecules exist in the form of closed-shell molecular ions in solution, however, and one would like to have the same degree of spectral simplification for such species as for neutrals. Toward this end, we have constructed a tandem mass spectrometer with a linear 22-pole ion trap that can be cooled down to ~6K [1]. Ions produced by nanospray are mass-selected, injected into the trap and cooled through collisions with helium. We then irradiate the cold ions with different combinations of UV and IR laser pulses and measure spectra by detecting fragments that are produced after photon absorption as a function of the laser frequency.

This talk will focus on electronic and vibrational spectroscopy of cold, protonated amino acids [1], small protonated peptides as well small clusters of these species with a controlled number of solvent molecules [2]. The almost complete absence of hot-bands in the electronic spectra demonstrate that the trapped ions attain a vibrational temperature of ~10K. Features in the spectra arising from distinct conformations of the molecules clearly appear, and we characterize these different conformers by using IR-UV double-resonance to measure vibrational spectra. When combined with calculations, these spectra provide insights into the driving forces that determine the gas-phase conformation.

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3b-1

OPTICAL CAVITY QED

Gerhard Rempe

Max-Planck Institute for Quantum Optics
Hans-Kopfermann-Str. 1, D-85748 Garching, Germany

This year sees the 20th anniversary of the first experiment demonstrating the strong coupling between single Rydberg atoms and single microwave photons. At that time, the investigation of light-matter interaction at the single-particle level was considered purely academic. Today, fundamentally new applications are on the horizon, in particular in the optical domain where laser cooling and trapping techniques for atoms can be implemented. New light forces have been discovered, enabling one to store atoms for such a long time that genuine quantum protocols can be realized with just one single atom. The first example of such a protocol concerns the realization of a source of single photons with realtime control of its performance. The bit stream of photons delivered by such a single-photon server is useful for many applications, e.g. in quantum information science. A second experiment concerns the deterministic entanglement of an atom with a flying photon, with information stored in magnetic states of the atom and the polarization state of the photon. Subsequent mapping of the atomic state onto a second photon makes possible to produce entangled photons on demand. The experimental demonstration of such a novel scheme is an important step towards the production of highly entangled many-photon quantum states and scalable quantum networks of atom-cavity systems. The fascinating possibilities opened up by cavity quantum electrodynamics continue to keep the field young and exciting.

3b-2

Single Photons from Strongly Coupled Atom-Cavity Systems

Axel Kuhn
University of Oxford

A plethora of new experiments, e.g. in quantum information science [1], rely on deterministically controlled light-matter interactions at the single-atom and single-photon level. This can be achieved with a single atom coupled to an optical cavity. Therefore many efforts are made to govern atom-cavity coupling, and to trap and cool single atoms in micro cavities.

Here, it is shown that the controlled energy exchange between an atom and the quantized light field of the cavity allows generating single photons on demand [2-4]. An atom coupled to a high-finesse optical cavity is exposed to classical laser pulses that trigger the single-photon emissions. The photons are produced in an adiabatically driven Raman transition, with the vacuum field of the cavity acting as stimulating field. Antibunching is found in the intensity correlation of the light, showing that single atoms emit photons one-by-one [2]. Two-photon interference effects [5], with pairs of photons impinging simultaneously on a beam splitter [6-8], reveal that the photons are nearly indistinguishable, which is essential in optical quantum computing [9] and cavity-mediated entanglement and teleportation schemes [10,11]. The interference effects are studied in a time-resolved manner, which allows an unprecedented insight into the structure and phase variations of the photons. In particular, long photons of different frequencies give rise to a quantum beat of high visibility in the two-photon correlation function, with the beat amplitude being a measure for the coherence properties. Most remarkably, simultaneous photodetections are not observed, so that a temporal filter allows one to obtain perfect two-photon coalescence in any case.

Furthermore, a major step towards a network of addressable atoms located in different cavities has been taken. A dipole-trapping and cavity-cooling scheme is used to cool atoms in all directions, and it is shown that this scheme can be used for capturing and storing individual atoms in a cavity for almost one minute [12]. To deterministically address these atoms by the cavity, a standing-wave dipole-force trap [13] is used to adjust their position with respect to the cavity mode. In this way, single atoms are repeatedly moved into and out of the region of strong atom-cavity coupling with a sub-micron precision [14]. This paves the way to permanent atom-cavity coupling, which is essential in cavity-based quantum information science.

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3b-3

QED THEORY OF HEAVY IONS AND ATOMS

V.M. Shabaev

Department of Physics, St.Petersburg State University, Oulianovskaya 1,
Petrodvorets, 198504 St.Petersburg, Russia

Quantum electrodynamic (QED) theory of highly charged few-electron ions is reviewed. Theoretical predictions for the Lamb shift, the hyperfine splitting, and the bound-electron g-factor are compared with available experimental data. Special attention is focused on tests of quantum electrodynamics at strong fields and on determination of the fundamental constans. Calculation of the full gauge-invariant set of the one-loop QED corrections to the parity nonconserving 6s-7s transition amplitude in neutral cesium is also discussed.

4a-1

Anion resonances, threshold phenomena, and chemical change revealed by electron-scattering

Michael Allan, Bogdan C. Ibănescu and Olivier May

Department of Chemistry, University of Fribourg, Fribourg, Switzerland

The talk will report on recent findings concerning the mechanisms of chemical and physical change induced by free electrons. A series of molecules containing the hydroxyl group will be treated, motivated by the importance of this functional group in biological materials.

The specific molecules will include formic acid and its hydrogen-bound dimer, a series of alcohols including methanol, ethanol, cyclopentanol, tetrahydrofuran-3-ol, *cis*- and *trans*-cyclopentane-1,2-diols and other molecules. The processes treated will be dissociative electron attachment and vibrational excitation mediated by dipole-bound resonances, σ^* and π^* resonances, and Feshbach resonances with double occupation of Rydberg-like orbitals.

Scattering theory treating the detailed reaction dynamics is not yet available for these polyatomic molecules. Model compounds where detailed theory is available, in particular hydrogen halides [1] and water [2], will therefore be discussed first and the phenomena encountered and understood in these simple systems will then be transferred qualitatively to the larger molecules.

The relevant phenomena are the changing of nature of the anion potential surfaces from valence to dipole-bound as a function of internuclear distances and the ensuing vibrational Feshbach resonances, the vibronic coupling between σ^* and π^* resonances leading to symmetry-lowering and dramatic reduction of activation barriers, and the dynamics of dissociation of the electronic Feshbach resonances.

The experimental results will include the study of resonances in formic acid by means of vibrational excitation by electron impact, the observation of the surprisingly large capacity of the formic acid dimer (held together by hydrogen bonds) to quasithermalize incident electrons, explained by a rapid electron-induced intra-complex proton transfer, and recent results on the dissociative electron attachment to larger alcohols [5], revealing both σ^* shape resonance and Feshbach resonance bands, large H/D isotope effects, interesting fragmentation patterns, and state and site selectivity in the Feshbach resonance regime.

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4a-2

Theory of electron collisions with polar molecules

Roman Čurík[1] and David Field[2]

[1]J.Heyrovský Institute of Physical Chemistry, Dolejškova 3, Prague 8, Czech Republic
[2]Institute for Physics and Astronomy, Aarhus University, DK-8000 Aarhus, Denmark

The phenomenon of low energy rotationally inelastic scattering by electrons was first observed in Randell *et al* 1993 and data on a variety of molecules may be found for example in Field *et al* 2001. These results are of fundamental theoretical interest and also have numerous potential applications in atmospheric, interstellar and man-made plasmas. We developed a theory for the interaction of electrons with polar species, extending methods in Mittleman *et al* 1965 and Greene *et al* 1985. In our work we show how state-to-state rotationally inelastic cross-sections may be derived from experimental cold electron scattering data for polar molecules, using H_2O as an example. Fig. 1 shows state-to-state inelastic cross sections extracted from the experimental data.

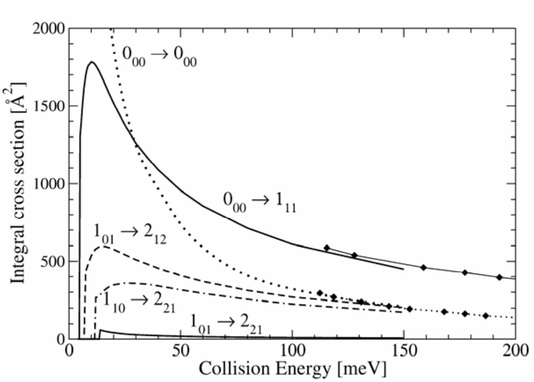

Figure 1: Selected state-to-state integral cross-sections for rotational excitation of the H_2O molecule determined from experimental data. Full curves represent results for para-H_2O and dashed for ortho-H_2O.The dotted curve represents elastic scattering for para-H_2O in its lowest rotational state. Curves with diamonds show the results of R-matrix calculations in Faure *et al* 2004.

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4a-3

Synthesis of amino acids by low-energy electrons in molecular ices

A. Lafosse,[1] M. Bertin,[1] I. Martin,[2] E. Illenberger,[2] and R. Azria[1]

[1] Laboratoire des Collisions Atomiques et Moléculaires, CNRS-Université Paris-Sud (UMR 8625, FR LUMAT), Bât. 351, Université Paris Sud, F-91405 Orsay Cedex, France

[2] Institut für Chemie – Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, D-14195 Berlin, Germany

lafosse@lcam.u-psud.fr

Reactions in pure condensed material (ices frozen at ~20-40 K) initiated by low-energy electrons have attracted considerable interest within the last few years due to their potential to induce specific chemical reactions[1,2]. Recently the ability of low-energy electrons to initiate complex chemical reactions in mixed ices has been demonstrated[3,4].

In particular the synthesis of the simplest amino acid, the glycine, in its zwitterionic form ($^{+}NH_3CH_2COO^{-}$) in binary molecular films of ammonia (NH_3) and acetic acid (CH_3COOH) deposited at 25 K was demonstrated by means of High Resolution Electron Energy Loss Spectroscopy (HREELS).[4] Glycine formation results from the electron irradiation alone without any need for thermal activation. Glycine identification has been recently confirmed by comparison of HREELS spectra obtained after electron irradiation of the NH_3/CH_3COOH condensed films with vibrational energy loss spectra of vapor glycine[5].

The mechanisms involved in this electron induced synthesis is quite complex, since in the explored energy range (0-25 eV) electrons induce dissociations leading to the formation of negative ions[6,7], positive ions[8] and radicals[9]. Probable mechanisms will be discussed considering (i) the electron energy and dose used to irradiate the mixed ices and (ii) the role played by carbon dioxide CO_2 as reaction intermediate in the synthesis process, since CO_2 is produced by electron irradiation of pure films of acetic acid[2]. For that purpose the chemical modifications induced in binary condensed films of CO_2-NH_3 (1:1) by low-energy electron irradiation have been studied. This mixture undergoes important chemical modifications after electron irradiation above 9 eV. The obtained vibrational spectra lead us to conclude in favour of the formation of the carbamic acid rather than formamide $HCONH_2$.

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4a-4

Structural aspects of the radiolysis of proteins and peptides: the example of disulfide bonds

Chantal Houée-Levin[1]

LCP, UMR 8000, F-91405 Orsay Chantal.houee-levin@lcp.u-psud.fr

Radiolysis is extensively used for studies of free radical reactions on biopolymers. Radiolysis provided a wealth of data that allowed the understanding of the effect of ionising radiation and of the chemical basis of disease, *i. e.* oxidative stress. Although the main lines of the redox reactions of proteins are understood, some uncertainties remain, that can have important consequences when they take place in living organisms. One of the main systems that should be understood is the disulfide/dithiol interconversion, because it intervenes in the control of genes and thus in the induction or development of diseases such as cancer or AIDS.

It is known that this system is very sensitive to one-electron transfers. Gamma and pulse radiolysis studies have shown that generally the disulfide bonds can be converted in dithiols and vice-versa. Thus if one considers that in living cells enzymes can restore the equilibrium concentrations of both forms, the disulfide/dithiol system can be considered as a protection against ionising radiation or oxidative stress. However we have recently shown that these reactions are modulated by the protein structure and environment. Moreover, the adjacent carbon-sulfur bonds are sensitive and can be broken, which leads to degraded forms of proteins.

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4b-1

Rydberg excitation and plasma formation in an ultracold atomic environment

Jan M. Rost

Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

The long range interaction of ultracold Rydberg atoms in an ensemble has attracted considerable attraction recently. This includes particularly the effect of Rydberg excitation blockade [1–3] since it might become relevant in addressing single atoms which is necessary for the realization of quantum computation [4].

A theoretical quantum description of many interacting atoms, even if they have only two levels, is prohibitively expensive [5]. In [2] a mean field model has been formulated to describe the experiment published in the same paper.

However, the special two-step excitation scheme of the Rydberg atoms used in the other two key experiments [1, 3] allows one to reduce the atomic excitation process to classical rate equations. Given this approximation, one can easily take into account the full interaction among a large ensemble of cold atoms. Our results are in good agreement with those of [3], identifying a sub-possonian distribution of Rydberg atoms as a consequence of the blockade effect.

Moreover, we have made another, surprising observation: under the conditions of excitation as used in the experiments [1, 3], *antiblockade* may occur, that is, an increased Rydberg excitation despite the increasing interaction between the atoms in the ensemble [6].

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4b-2

DIPOLE BLOCKADE IN HIGH-RESOLUTION LASER EXCITATION OF RYDBERG STATES

Pierre Pillet

Laboratoire Aimé Cotton, CNRS
Bât. 505, Univ Paris-Sud, 91405 Orsay cedex, France

Rydberg atoms have long been known to have huge polarizabilities leading to exaggerated collisional properties of room temperature atoms, in particular, large cross sections and long interaction times. These properties have stimulated great interest in the possibility to control the strong long-range interactions between cold atoms [1,2], which could be particularly exciting for quantum information applications. One interesting process is the possibility of the dipole blockade in the Rydberg excitation of atoms, due to the dipole-dipole interaction shifting the Rydberg energy from its isolated atomic value. The use of the dipole blockade of the excitation has been proposed as a very efficient realization of a scalable quantum logic gate [3]. In a large ensemble of atoms, the first excited Rydberg atoms shift the resonance for their non-excited neighbors and prevent their excitation with a narrow-bandwidth laser. A partial, or local, blockade of the Rydberg excitation is expected in a high resolution spectroscopy. If the volume of the laser excitation is small enough, no two-atom collective excitation can occur, producing an atomic ensemble in a singly excited collective state.

Two different configurations for laser excitation of states, *np*, have been studied in the case of cesium. A first evidence of the dipole blockade consists in adding a static electric field, inducing a permanent dipole for each Rydberg atom with high principal quantum number ($40 < n < 120$) by mixing the p and *d* characters in the *p* Stark level. A second approach considers Förster resonances corresponding to the resonant energy transfer of the $np + np \rightarrow ns + (n+1)s$ reaction. Here the dipole – dipole interaction is tuned on and off by adding a small electric field with relatively low *n*, smaller than 42 [4]. The effects due to saturation in laser excitation, to Penning ionization result of cold Rydberg collisions or to the presence of eventual spurious ions can perturb the blockade. They are carefully analyzed. For both configurations, efficient dipole blockade has been demonstrated.

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4b-3

Coherent phenomena in ultracold Rydberg gases

M. Weidemüller *
Physics Institute, Albert-Ludwig University Freiburg, 79104 Freiburg, Germany
m.weidemueller@physik.uni-freiburg.de

Due to the long-range character of the interaction between highly excited atoms, the dynamics of an ultracold gas of Rydberg atoms is entirely determined by van-der-Waals and dipole-dipole interactions. One outstanding property is the tunability of the strength and the character of the interactions with static electric fields. This allows one to explore the transition from a weakly coupled two-body system to a strongly coupled many-body system. The long-range interaction leads to many-body entanglement and has possible applications in quantum computing.

In a recent series of experiments we studied coherent phenomena in an ultracold gas of Rydberg atoms under the influence of dipolar interactions. The Rydberg gas is formed in in a magneto-optical trap via cw two-photon excitation of Rb atoms into states with principal quantum number 30…100 using cw lasers at 780 nm and 480 nm [1]. Our recent results include coherent Rabi oscillations between ground and Rydberg states and the observation of the dipole blockade in a mesoscopic sample [2,3], stimulated rapid adiabatic passage with 90% transfer efficiency into Rydberg states [4], and studies of the many-body character of resonant energy transfer processes [5]. Our experiments also reveal the role of interaction-induced mechanical forces [6]. In my lecture I will present an overview over recent developments in the field with special emphasis on the experiments in Freiburg.

* Work performed in collaboration with M. Reetz-Lamour, T. Amthor, K. Singer, J. Deiglmayr, S. Westermann, J. Denskat, A.L. de Oliveira, L.G. Marcassa.

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5a-1

Controlling the rotational motion of asymmetric top molecules by laser pulses

HENRIK STAPELFELDT

Department of Chemistry, University of Aarhus, Denmark

While the vast majority of previous studies on laser induced alignment of small molecules dealt with linear systems, interest is now shifting to asymmetric tops due to both the new physics involved and the broad range of applications. However, controlling the rotational motion of asymmetric tops represents, in general, a much harder task because they are characterized by three axes with different moments of inertia and different polarizability components.

This talk will discuss recent studies on laser alignment of asymmetric tops. First, we show how the alignment dynamics induced by a single linearly polarized short laser pulse can be controlled by the fluence. When the fluence is increased the complex non-periodic revival structure of an asymmetric top approaches a simple periodic rotation around a single axis. Second, we introduce a new method for 3-dimensional (3D) alignment control by combining two linearly polarized pulses laser pulses, one short and one long compared to the molecular rotational periods. The long pulse strongly aligns the most polarizable molecular axis along its polarization axis while the orthogonally polarized short pulse sets the molecule in to controlled rotation about the axis aligned. As a result strong 3D alignment occurs immediately after the short pulse and is repeated periodically reflecting the revolution about the axis aligned. Our method opens new directions for field-free 3D alignment and for controlling internal rotations of molecules.

5a-2

NEW METHODS FOR THE PRODUCTION AND DETECTION OF SPIN-POLARIZED HYDROGEN

T. Peter Rakitzis

Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, 71110 Heraklion-Crete, Greece, and Department of Physics, University of Crete, P.O. 2208, 71003 Voutes-Heraklion, Greece

Two methods for the production of polarized atoms, based on molecular photodissociation, are presented. One method involves the polarization of the electronic angular momenta of the photofragments, by exciting to specific molecular electronic states, and by taking advantage of the correlation of molecular electronic states to separated (polarized) atomic states [1]. The second, complementary, method polarizes the rotational polarization of the molecule with a pulsed laser, without hyperfine resolution; the ensuing hyperfine quantum beats produce nuclear polarizations that can approach 100% in selected cases, and at specific time delays. Photodissociation at the maximum nuclear polarization "freezes" the polarization in the nuclei [2,3]. The combination of these two techniques allow the production of highly polarized atoms, at very high pulsed-densities which can approach the density of the parent molecule (well in excess of $10^{16}/\text{cm}^3$), and can be produced on the nanosecond timescale. These techniques are demonstrated for the cases of spin-polarized hydrogen, chlorine, and bromine.
In addition, a new pulsed-laser method for the detection of spin-polarized hydrogen is presented, using polarized fluorescence of Lyman-alpha radiation [4,5]. Together, these techniques allow the production and detection of spin-polarized hydrogen nanosecond timescales, so that studies can be performed under singe-collision conditions.

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Kinematically Complete Study of Dissociative Ionization of D_2 by Ion Impact

G. Laurent[1,2], J. Fernández[2], S. Legendre[1], M. Tarisien[1], L. Adoui[1], A. Cassimi[1], X. Fléchard[3], F. Frémont[1], B. Gervais[1], E. Giglio[1], J. P. Grandin[1], and F. Martín[2]

[1]Centre Interdisciplinaire de Recherche Ions Lasers (CIRIL)—CEA-CNRS-ENSICaen, rue Claude Bloch, BP 5133, F-14070 Caen cedex 5, France
[2]Departamento de Química C-9, Universidad Autónoma de Madrid, 28049 Madrid, Spain
[3]LPC-Caen, 6 Bd du Maréchal Juin, F-14050 Caen cedex, France

Ionization of the simplest H_2 molecule by the impact of photons [1,2], electrons [3,4], and ions [5,6] has been the subject of extensive experimental and theoretical investigations for almost three decades. With the advent of kinematically complete collision experiments, in which the full momentum vector of all charged particles is determined, it is now possible to investigate these processes with unprecedented detail and precision. In contrast with photoionization, in which a well-defined amount of energy is absorbed by the target (the photon energy), the energy absorbed by H_2 in a collision with a fast charged projectile follows a distribution with practically no upper limit. Thus all processes capable of ionizing the molecule are energetically allowed and can, in principle, occur simultaneously. It also means that ionization can involve one or all electrons of the molecule. In this talk we present a kinematically complete experimental study of the collision between 13.6 MeV/u S^{15+} ions and D_2 molecules. We detect in coincidence all ejected ions and electrons in the whole energy range accessible in the collision. The experiment allows us to unravel the competing mechanisms leading to dissociative ionization of D_2. The measurements are supported by theoretical calculations in which the motion of all electrons and nuclei as well as correlations and interferences between them are described from first principles [7].

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5b-2

Large hot atomic gasses as ideal quantum systems for quantum information

Klaus Mølmer
Lundbeck Foundation Theoretical Center for Quantu System Research
Department of Physics and Astronomy
University of Aarhus
DK 8000 Aarhus C.m Denmark
Moelmer@phys.au.dk

Large samples of atoms have collective degrees of freedom associated with their internal electronic state that can be monitored and manipulated with light fields at the quantum level.

We discus the features that make hot atomic gasses ideal for the study of very sensitive quantum phenomena such as quantum squeezing, entanglement, and teleportation, and we describe our collective variable formalism, that allows analytical and simple numerical treatments of atomic losses, light absorption, and measurement back action.

Our quantum description of collective atomic properties follows the spirit of classical parameter estimation, discussed in seminal works by Gauss as early as 1792. This spirit was revived and an effective formalism for the classical problem, the so-called Kalman filter, was derived in 1960.

5b-3

QUANTUM TELEPORTATION BETWEEN LIGHT AND MATTER

J. F. Sherson[1,2,*], H. Krauter[1], R. K. Olsson[1], B. Julsgaard[1], K. Hammerer[3], J.I. Cirac[3], and E.S. Polzik[1]

[1]Niels Bohr Institute, Copenhagen University, Blegdamsvej 17, Copenhagen Ø, Denmark.
[2]Department ofPhysics and Astronomy, University of Aarhus, Aarhus, 8000, Denmark.
[3]Max Planck Institute for Quantum Optics, Hans-Kopfermann-Str. 1, Garching, D-85748, Germany.

In this talk I will discuss the first experimental demonstration of interspecies teleportation between an atomic and a photonic object[1]. The state of a mesoscopic light pulse containing up to 300 photons is transferred onto the collective state of an atomic ensemble of 10^{12} Cesium atoms. This is an important step towards e.g. distributed quantum networks in which the exchange of information between "flying" and long lived "stationary" systems is essential.

The teleportation is enabled by the entanglement created by sending an auxiliary light pulse through the atomic sample. This is created by a quantum Faraday-type interaction in which the polarization state of the light pulse is rotated conditioned on the atomic spin state and simultaneously the atomic spin state is rotated based on the light polarization state.

An essential parameter in such experiments is the teleportation distance. In our realization it was 0.5 meters – representing an improvement by a factor 10^5 compared to previous teleportation experiments involving atomic objects. The teleportation distance is in practice limited by the entanglement distance. Since our entanglement is light-mediated it is scalability to much larger distances should be feasible.

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*: current address: QUANTUM, Joh. Gutenberg University, Mainz, Germany, sherson@uni-mainz.de

6a-1

Realization and Application of Frequency Combs

Thomas Udem, Akira Ozawa, Christoph Gohle, Jens Rauschenberger, Ronald Holzwarth, Maximilian Herrmann, Elisabeth Peters, Birgitta Bernhardt, and Theodor W. Hänsch

Max-Planck-Institut für Quantenoptik
Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany

Since 1997, the cross-fertilization of precision spectroscopy and ultrafast science has led to several spectacular accomplishments. The advent of femtosecond laser optical frequency combs has revolutionized the measurement of optical frequencies [1] and enabled optical atomic clocks [2]. A femtosecond frequency comb is a simple and compact tool that allows the phase coherent connection of the radio frequency domain (below 100 GHz) with the optical domain (above 200 THz). A large variety of narrow optical transitions, such as the 1S-2S two-photon resonance in atomic hydrogen [3], has been measured with this technology allowing to test fundamental physics and the determination of fundamental constants with high precision. The same comb techniques are employed to control the carrier-envelope phase and therefore the waveform of ultrafast laser pulses, which permitted the generation of single attosecond pulses [4], and have been used in a recently demonstrated "oscilloscope" for light waves [5].

Thus far femtosecond laser optical frequency combs are produced by pulse trains from infrared mode locked lasers. Coherent radiation up into the X-ray region may be produced by higher order harmonic generation (HHG) when focusing intense pulses into a gas. The standard technique to achieve the required high intensities of ($> 10^{13}$W/cm^2) effectively concentrates the available time averaged laser power into a small number of ultrashort pulses per second. This limits the pulse repetition rates for HHG to typically a few kHz. In order to exploit the mode structure for high resolution spectroscopy, a larger mode spacing appears to be necessary. Using an external buildup cavity we have recently succeeded to produce HHG's with unamplified pulses of a $\sim$ 100 MHz femtosecond oscillator [7]. The method is similar to resonantly enhanced second harmonic generation that has been in use for many years.

Such a laser system could enable new high precision tests for fundamental physical theories such as Quantum Electrodynamics (QED). For example the 1S-2S transition of singly charged helium can be probed with the 13th harmonic of a Ti:Sapphire laser at 60 nm. Hydrogen like ^{4}He is an even simpler atom than hydrogen as it shows no hyperfine structure. The QED contributions to the energy levels scale as Z^4 with the nuclear charge Z. Even more interesting are higher order contributions which makes helium more sensitive for this kind of test. Hydrogen like helium is charged and can be readily trapped and sympathetically laser cooled. Additionally one can envision many other applications of such a quasi-continuous compact and coherent XUV source, including XUV holography, microscopy, nano lithography or even X-ray atomic clocks.

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Measuring the electron's electric dipole moment with heavy, polar molecules.

J.J. Hudson, D. Kara, H.T. Ashworth, M.R. Tarbutt, B.E. Sauer, E.A. Hinds

Centre for Cold Matter, The Blackett Laboratory,
Imperial College London, London SW7 2BW

Measurement of the electric dipole moment of the electron (e-edm) provides a very sensitive probe for physics beyond the Standard Model [1]. Such a measurement explores CP-violating physics at the tera-eV level, possibly shedding light on the origin of the thus-far-unexplained matter-antimatter asymmetry of the universe [2].

Precision spectroscopy of cold, heavy, polar molecules allows us to measure the electron's interactions at the atto-eV level [3,4]. I will outline our experimental technique, paying particular attention to diagnostic techniques we have developed recently. These diagnostics employ velocity-resolved Stark- and Zeeman-spectroscopy and Ramsey- and Zeeman-interferometery to produce detailed maps of the electric, magnetic and radio-frequency fields inside our apparatus. Such maps are crucial for understanding and eliminating possible sources of systematic error.

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6a-3

ON A VARIATION OF THE PROTON-ELECTRON MASS RATIO

W. Ubachs

Laser Centre Vrije Universiteit, Amsterdam

Recently the finding of an indication for a *decrease* of the proton-to-electron mass ratio $\mu=m_p/m_e$ by 0.002% in the past 12 billion years was reported [1]. We will discuss the methods that led to that result and put it in perspective. Laser spectroscopy on molecular hydrogen, using a narrow-band and tunable extreme ultraviolet laser system at the Laser Centre Vrije Universiteit Amsterdam, results in transition wavelengths of spectral lines in the B-X Lyman and C-X Werner band systems at an accuracy of (4 - 10) x 10^{-8}, depending on the wavelength region. This corresponds to an absolute accuracy of 0.000004 - 0.000010 nm. A database of 233 accurately calibrated H_2 lines is produced for future reference and comparison with astronomical observations. Recent observations of the same spectroscopic features in cold hydrogen clouds at redshifts z=2.5947325 and z=3.0248970 in the line of sight of two quasar light sources (Q 0405-443 and Q 0347-383) resulted in 76 reliably determined transition wavelengths of H_2 lines at accuracies in the range 2 x 10^{-7} to 10^{-6}. Those observations were performed with the Ultraviolet and Visible Echelle Spectrograph at the Very Large Telescope of the European Southern Observatory at Paranal, Chile. A third ingredient in the analysis is the calculation of an improved set of sensitivity coefficients K_i, a parameter associated with each spectral line, representing the dependence of the transition wavelength on a possible variation of the proton-to-electron mass ratio μ. The new model for calculation of the sensitivity coefficients is based on a Dunham representation of ground state and excited state level energies. Moreover, the model includes adiabatic corrections to electronic energies as well as local perturbation effects between B and C levels.

A statistical analysis of the data yields an indication for a variation of the proton-to-electron mass ratio of $\Delta\mu/\mu = (2.45 \pm 0.59) \times 10^{-5}$ for a weighted fit and $\Delta\mu/\mu = (1.98 \pm 0.58 \times 10^{-5}$ for an unweighted fit. This result has a statistical significance of 3.5 σ. Mass-variations as discussed relate to *inertial* or kinematic masses, rather than gravitational masses. The observed decrease in μ corresponds to a rate of change of $d\ln \mu/dt = -2 \times 10^{-15}$ per year, if a linear variation with time is assumed. Experiments for detecting a possible variation of μ in the modern epoch via ultra-precision experiments on H_2 quadrupole transitions are proposed.

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6a-4

Matter-Antimatter Chemistry with Antiprotons

E. Lodi Rizzini, L. Venturelli, N. Zurlo

Dipartimento di Chimica e Fisica per l'Ingegneria e i Materiali, Università di Brescia,
25133 Brescia, Italy

A chemical reaction between the building-block antiatomic nucleus, the antiproton (pbar), and the hydrogen molecular ion (H_2^+) has been observed by the ATHENA collaboration at the Antiproton Decelerator at CERN [1]. The oppositely charged pair interacts via the long-range Coulomb force in the environment of a nested Penning trap which was built to produce antihydrogen [2], as it routinely did from 2002 to 2004. The presence of H_2^+ ions was essentially serendipitous, as we believe that the positrons injected into the trap to produce antihydrogen could have ionized some H_2 molecules from the residual gas.

The final result of the low energy collision of the pair is the creation of an antiproton-proton bound state, known as antiprotonic hydrogen or protonium (Pn), together with the formation of a hydrogen atom. The protonium produced by this reaction is metastable, having a lifetime against annihilation of about 1 μs, as it is formed in a highly excited state ($n \approx 70$ and $l < 10$). With respect to the older experiments in molecular hydrogen (H_2), the new method will make possible higher rates in a volume of the order of some mm^3. Moreover, this small volume is well suited for laser irradiation, with further enhancement of the protonium mean lifetime, thanks also to the absence of the collisional de-excitation (Stark mixing) due to the Ultra High Vacuum environment.

Finally, a clear effect of the H_2^+ temperature before the interaction has been observed, and it is worth noticing that protonium production occurs at temperatures up to thousands kelvin.

This result can be considered as a first milestone towards protonium laser-spectroscopy experiments, leading to values of the antiproton properties relative to those of the proton, and so to a new class of CPT-invariance tests. A further, more futuristic application of this work could consist in using the protonium production like a tool to investigate the properties of different molecular ions species.

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Ab initio quantum defect theory

R. Guérout[‡], H. Oueslati[†‡], Ch. Jungen[‡] and M. Telmini[†]

[‡] Laboratoire Aimé Cotton du CNRS, Bâtiment 505,
Université de Paris-Sud, F-91405 Orsay, France
[†] LSAMA Department of Physics, Faculty of Sciences of Tunis,
University of Tunis El Manar, 2092 Tunis Tunisia

Multichannel quantum defect theory is well established as a theoretical tool to aid the analysis of complex spectra involving electronically highly excited states of molecules, and it has also proven useful for the description of the non-adiabatic fragmentation of electronically highly excited species (ionization and/or dissociation including resonance effects). However, it is often difficult to determine the relevant non-diagonal quantum defect or reaction matrices in instances where a large number of interacting channels needs to be taken into account. Such instances occur when many partial waves become mixed by the molecular field, when electronic and nuclear spin effects are observable, when configuration interaction between singly and doubly excited channels is important, or when several nuclear degrees of freedom are present such as in polyatomic molecules. Standard quantum chemical codes are limited to low excited states, typically $n \leq 5$ (n effective principal quantum number).

In this contribution we shall describe our efforts to devise calculational schemes that allow reaction matrices in the discrete as well as in the continuum ranges to be calculated directly *ab initio*. Our aim is to take advantage of existing quantum chemical computer codes and to combine them with scattering theory (quantum defect theory). Several approaches have been implemented which are all inspired by the R-matrix concept which divides the configuration space into an inner 'reaction' or 'core' region where multi-electron interactions dominate, and an outer 'asymptotic' region where long range fields (Coulomb and/or multipole and polarization contributions) dominate. We describe the electronic motion in the asymptotic zone in spheroidal coordinates such as to be able to account for strong long range dipole fields. The inner and outer regions are separated by an ellipsoid (R-matrix radius, 'hard' wall) or by an artificial wall potential (AWP, 'soft wall').

Several applications will be described (H_2, NO, N_2, N_2^-, CaF, H_2O) where spectroscopic and dynamical problems have been solved with the help of the present approach.

6b-2

INTERSTELLAR POLYCYCLIC AROMATIC HYDROCARBONS: FROM SPACE TO THE LABORATORY

C. Joblin

CESR, CNRS – Université Toulouse III, Observatoire Midi-Pyrénées
9 Av. du Colonel Roche, 31028 Toulouse cedex 04, France

The question of the carriers of the Aromatic Infrared Bands (AIBs) is very intriguing for the astrochemist and the chemical physicist. The AIBs are major spectral features of interstellar matter located between 3.3 and 12.7 µm and observed in emission in many astronomical environments irradiated by UV photons. Polycyclic Aromatic Hydrocarbons (PAHs) are the best candidates to account for these bands but despite a wealth of observational data, no individual molecule could be identified so far. The exact nature of interstellar PAHs has therefore to be explored by considering the formation mechanism of these species, the processing by UV photons and the reactivity with gas-phase species. This is one of the topics addressed by the Molecular Universe European network.

Spectro-imagery performed with infrared and sub-millimeter space observatories provides a unique tool to probe the evolution of the AIB carriers. Studies show that the carriers are produced by the destruction/processing of very small grains that are also strong emitters in the mid-IR. These nanograins could be PAH clusters or PAH-iron complexes. On the laboratory side, one of the challenges is hence to try to reproduce the physical conditions that prevail in interstellar space: a cold environment (10-50 K), absence of collisions on long timescales and presence of stellar far-UV photons. PIRENEA, “Piège à Ions pour la Recherche et l'Etude de Nouvelles Espèces Astrochimiques”, is an experimental set-up which has been developed according to these specifications. Using the trapping, and the mass spectrometry analysis of an ion cyclotron resonance (ICR) cell that is connected to cryogenic shields, novel studies can be performed on processes which occur on long timescales and which are of interstellar relevance: IR radiative cooling, photodissociation in low energy channels, radiative association. Recent results obtained on the photophysical and chemical evolution of carbon macromolecules and nanograins of interstellar interest will be presented.

6b-3

Biomolecules studied by High resolution laser spectroscopy: State of the art.

W. Leo Meerts

Molecular- and Biophysics Group, Institute for Molecules and Materials,
Radboud University Nijmegen, P.O. Box 9010, 6500 GL Nijmegen, The Netherlands.

The conformations of a molecule play a crucial role in molecular recognition processes, which are the basis for all selective biochemical reactions. Even small biomolecules have a structure with several conformers of partly comparable energies. Nevertheless, under physiological conditions, generally only a few conformers show up. This is a surprising and important observation, because the reactivity and functionality of biologically active substances is governed by their structure.

Especially the interaction of those molecules with surrounding molecules most importantly water is determined by their structure. The controlled complexation by a small number of water molecules and the subsequent mapping of the conformational landscape after each solvation step should result in a deeper understanding of how and why biomolecules change their molecular shape when they are dipped into a water bowl.

High Resolution UV Laser spectroscopy [1, 2] is an excellent tool to obtain detailed structural information on large molecules and their hydrogen bonded clusters. The experimental technique which allows us to obtain rotationally resolved Ultra Violet spectra with a resolution of typically 10 MHz will be discussed.

From these rotationally resolved spectra we can deduce not only the relevant structural information, but in addition the direction of the electric dipole moment from the intensities and the lifetimes of the electronically excited states from the line widths. The latter can be used to investigate radiative and nonradiative relaxation channels in these molecules.

We have applied the method of Genetic Algorithm [3] in the analysis of these complex spectra. This has proven to be a very powerful tool which can be used for routine like analyses but also turned out to be very valuable in an automatic assignment of entangled spectra.

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COINCIDENCE STUDIES OF PHOTOIONIZATION PROCESSES

P. Bolognesi and L. Avaldi

CNR-IMIP, Area della Ricerca di Roma 1, CP10, 00016 Monterotondo Scalo, ITALY

In the last years several types of coincidence techniques, which involve the simultaneous detection of up to four-charged particles, have provided valuable information on single and double ionization of atoms and molecules by synchrotron radiation.

Recent results on photodouble ionization, PDI, of atoms and molecules and inner shell photoionization of molecules obtained at Elettra storage ring, Trieste, will be reviewed.

The possibility to measure the basic quantities, i.e. the amplitudes and their relative phase, which determine the fully differential cross section of the PDI of He via a combination of experiments with linearly and circularly polarized radiation as well as the observation of “dynamic nodes” in the measured circular dichroism in He will be discussed.

It will be also shown how a set of three different types of electron-electron and electron-ion coincidence experiments can provide unique information on inner shell ionization and decay in diatomic molecules.

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Double Photoionization of Small Molecules and Related Phenomena*

A. Belkacem
Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720
Email: abelkacem@lbl.gov

Understanding correlated interactions among electronic and nuclear components of complex systems and ultimately their control gives rise to the exciting possibility to control matter at the atomic level. This involves breaking and rearranging intra- or intermolecular bonds. Often we are interested in the atomic position changes during a transformation; however, it is what the valence electrons are doing that determines the chemistry. In this work we study photo-double ionization of simple diatomic and polyatomic molecules to investigate the interplay between nuclear and electronic motion that happens on a femtosecond time scale. For example double excitation of hydrogen molecules followed by autoionization; we find that at some ion kinetic energies (which classically could be associated with bond length distances) the autoionization pathways interfere leading to symmetry breakup. In this talk I will focus primarily on double photoionization of the simplest polyatomic systems acetylene (C_2H_2) and ethylene (C_2H_4). In the acetylene study we investigate the K-shell photoionization and the dynamics of the following breakup pathways by measuring the momenta of the positively charged ions in coincidence with Auger electrons. The photoionization and the subsequent Auger process lead to the formation of the doubly charged $C_2H_2^{++}$ ion that dissociates into two or more fragments. We observe two clearly separated Auger electron peaks correlated with different kinetic energies taken by the fragments. The result of this analysis in the 2-D plot (Auger energy – kinetic energy of ions) shows that the isomerization to vinylidene is associated with a very sharp peak around 255 eV Auger energy and 4.5 eV ion kinetic energy. This gives a clear insight on the isomerization process. Following the emission of the 255 eV Auger electron {$C_2H_2^+ \rightarrow C_2H_2^{2+} + e_A$ (255 eV) } the di-cation ends up in the lower laying states $^1\Sigma_g^+$, $^1\Delta_g$ and $^3\Sigma_g^-$. The di-cation is trapped behind a high (3-4 eV) and wide barrier preventing it from directly dissociating along the C-C bond or C-H bond. The dissociation appears to be achieved after an isomerization to vinylidene first followed by dissociation along the C-C bond forming $C^+ + CH_2^+$ fragments. In contrast, neutral ethylene has a planar geometry while in the di-cation ground state the two CH_2 radicals form a 90° with respect to each other. Thus a direct double ionization from the neutral molecules ground state does not yield a stable $C_2H_4^{2+}$ di-cation while a two step process consisting of an K-shell ionization followed by an Auger relaxation appears to very efficiently yielding stable $C_2H_4^{2+}$. This may be an indication that the first ionization "launches" a nuclear motion and the nuclear motion is of the same order of magnitude as the Auger process itself.

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* Work done in collaboration with the group of Pr. R. Doerner at the university of Frankfurt, the group of Pr. C.L. Cocke at Kansas State University and Pr. A. Landers at Auburn University.

UNRAVELING MODE-SPECIFIC REACTIVITY BY PRODUCT PAIR-CORRELATION MEASUREMENTS

Kopin Liu

Institute of Atomic and Molecular Sciences (IAMS),
Academia Sinica, P. O. Box 23-166, Taipei, Taiwan 10617.
Email: kpliu@gate.sinica.edu.tw

In this talk I will highlight some of our recent studies on mode-specific behaviors in the reaction of atomic chlorine with methane. The experiments were performed under crossed-beam conditions with a time-sliced, ion velocity-imaging detection scheme [1]. An OPO/OPA was exploited to prepare the stretch-excited methane, and a heated pulsed valve was used in a separate experiment for bending and/or torsional excitations of the reagent [2]. The results will then contrast to the ground-state reaction with equivalent amount of total energy [3,4]. Contrary to the general belief, we found that both types of vibrational excitation do not enhance the reaction rate more than the translational factor - thus, none mode-specific behaviors in total reactivity. However, in terms of pair-correlated angular and state distributions, the stretch-excited reaction is very different from the ground-state reaction, whereas the bend-excited methane behaves nearly identical to the latter. A new method [5] will also be introduced on how to determine, effectively and reliably, the fraction of molecules being excited in a molecular beam by laser - a crucial quantity in deducing any quantitative vibration effect from measurements.

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7a-4

Effect of the geometric phase on chemical reaction dynamics

Stuart C. Althorpe
Department of Chemistry, University of Cambridge
Lensfield Road, Cambridge, CB2 1EW, UK.

If a molecular system follows a path which encircles a conical intersection (an electronic degeneracy), then the electronic wave function changes sign. This sign-change is an example of the geometric (or Berry) phase (GP). There has been much debate recently about how the GP can affect a reaction mechanism which loops around a conical intersection. It is known that, in bound systems, the GP changes the nodal structure of the nuclear wave function, causing shifts in the energy levels. Hence one might expect comparable changes to the nuclear wave function in a reactive system. However, recent studies[1] on the hydrogen-exchange reaction (which is the simplest reaction with a conical intersection) showed that, although GP effects are present in individual partial wave contributions to the wave function, these effects cancel out completely in the cross sections. Recently, we demonstrated[2-4] that these cancellations and other effects of the GP on the reaction observables are a consequence of the fact that classes of paths that loop different numbers of times around the conical intersection can be separated in the Feynman sum-over-paths[5]. We explain how these paths can be separated from the computed wave function of a chemical reaction, and show that this separability leads, amongst other things, to the cancellation of GP effects in the cross sections of the hydrogen-exchange reaction.

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Evidence for Efimov Quantum States in Experiments with Ultracold Cesium Gases

Hanns-Christoph Nägerl

Institut für Experimentalphysik und Forschungszentrum Quantenphysik, Universität Innsbruck, Technikerstrasse 25, 6020 Innsbruck, Austria.

Three interacting particles form a system which is well known for its complex physical behavior. A landmark theoretical result in few-body quantum physics is Efimov's prediction of a universal set of weakly bound trimer states appearing for three identical bosons with a resonant pairwise interaction [1]. While Efimov's scenario has attracted great interest in many areas of physics, experimental evidence was missing so far. In our talk we report the observation of an Efimov resonance in an ultracold thermal gas of Cs atoms [2]. For Cs atoms the binding energy of a weakly bound dimer state can be magnetically tuned near a Feshbach resonance, giving access to the regime of resonant two-body interaction which can be either attractive or repulsive. The Efimov resonance occurs in the range of large attractive two-body interaction and arises from the coupling of three free atoms to an Efimov trimer. We observe its signature as a giant three-body recombination loss when the strength of the two-body interaction is tuned. In addition, we find a scattering resonance in ultracold collisions between atoms and weakly bound dimer molecules as the dimer binding energy is tuned. It is likely that this resonance arises from the coupling of the dimer and an atom to an Efimov trimer, thus providing a direct link between the weakly bound dimer state and the appearance of Efimov states.

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7b-2

DECELERATION AND TRAPPING OF NEUTRAL POLAR MOLECULES

Sebastiaan Y.T. van de Meerakker

Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, 14195 Berlin, Germany

Over the last years our group has been developing methods to get improved control over the absolute velocity and over the velocity spread of molecules in a molecular beam. These methods rely on the, quantum state specific, force that polar molecules experience in inhomogeneous electric fields. This force is rather weak, but nevertheless suffices to achieve complete control over the molecular motion, using techniques akin to those used for the control of charged particles. This has been explicitly demonstrated by the construction of two types of linear accelerators/decelerators, a buncher, traps, and a storage ring for neutral polar molecules [1]. With the Stark decelerator, a part of a molecular beam can be selected and transferred to any arbitrary velocity, producing bunches of state-selected molecules with a computer-controlled velocity and with longitudinal temperatures as low as a few mK.

We will report on the deceleration and electrostatic trapping of ground state OH and OD radicals. Depending on details of the trap loading sequence, typically 10^5 OH or OD radicals in the $X\,^2\Pi_{3/2}, v = 0, J = 3/2$ state are trapped at a density of $10^7 - 10^8$ cm^{-3} and at a temperature in the 50-500 mK range [2]. The blackbody radiation limited trap lifetime is determined to be 2.8 s and 7.1 s for the OH and OD radical, respectively [3]. The long interaction time afforded by the trap is exploited to measure the radiative lifetime of the long-lived first vibrationally excited state of the OH radical [4]. The trap loading has been optimized using evolutionary strategies [5], and using a new trap geometry that is better matched to the geometry of the Stark decelerator.

Recently, we have performed the first scattering experiments using a Stark decelerated beam of polar molecules. A beam of ground-state OH ($X\,^2\Pi_{3/2}, v = 0, J = 3/2, f$) radicals is decelerated or accelerated, and scattered with a beam of Xenon under 90 degrees, allowing to measure the energy dependence of the cross-sections for inelastic scattering to higher rotational states around the energetic thresholds [6].

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Trapping Rydberg atoms and molecules using electric fields

E. Vliegen and F. Merkt

Laboratorium für Physikalische Chemie, ETH Zurich, Switzerland

In recent years considerable efforts have been invested in producing slow, cold samples of atoms and molecules in the gas phase [1]. Supersonic gas beams are a convenient starting point to create such samples because the particles in these beams are already translationally and internally cold. However, the particles travel with a high velocity in the laboratory frame. Therefore to bring such cold particles to rest in this frame, they must be decelerated.

I shall present a method to slow down and subsequently trap Rydberg particles in a supersonic beam using inhomogeneous electric fields. The deceleration mechanism relies on the large dipole moments ($\frac{3}{2}ea_0n^2$) that Rydberg particles exhibit as a result of the linear Stark effect [2, 3]. At n values between 20 and 30 the dipole moments are more than three orders of magnitude larger than those typically found in dipolar molecules. These large dipole moments can be exploited to apply forces on these particles accelerating them on the order of up to 10^8 m/s^2. The deceleration path length is therefore only a few mm [4, 5] and it is possible to create very deep electrostatic traps. Measurements on atomic hydrogen will be presented in which deceleration to zero velocity in the laboratory frame and subsequent trapping for 100s of μs was achieved.

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1a-4 (Mo4-4)

COHERENTLY CONTROLLED ADIABATIC PASSAGE TO MULTI-CHANNEL CONTINUUM STRUCTURE

Ioannis Thanopulos* and Moshe Shapiro

Department of Chemistry, University of British Columbia, Vancouver B.C., Canada

*E-mail: ioannis@chem.ubc.ca

We present the merging of Coherent Control (CC) and Adiabatic Passage (AP) and the type of problems that can be solved using the recently developed ``Coherently Controlled Adiabatic Passage'' (CCAP) method [1].

We start by discussing the essence of CC as the guiding of a quantum system to arrive at a given final state via a number of different quantum pathways.

The guiding is done by ``tailor-made" external laser fields. We show that selectivity in a host of physical and chemical processes can be achieved by controlling the interference between such quantum pathways. We then discuss the AP process, in which a system is navigated adiabatically along a single quantum pathway, resulting in a complete population transfer between two energy eigenstates. The merging of the two techniques (CCAP) is shown to achieve both selectivity and completeness, demonstrated in a series of applications involving bound-states.

We lastly present a solution to the ``Multi-Channel Quantum Control'' problem, where the CCAP is successfully applied for first time to a system including continuum structures. Selective and complete population transfer from an initial bound state to M energetically degenerate continuum channels is achieved under loss-free conditions. The control is affected in an adiabatic fashion proceeding via N bound intermediate states. In a realistic situation, where presence of real loss is inevitable, we further demonstrate that the control efficiency remains significant. We illustrate the viability of the method by computationally controlling the multi-channel photodissociation of methyl-iodide [2,3].

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1a-5 (Mo4-16)

NEW WAY TO INDUCE AND CONTROL ELEMENTARY CHEMICAL TRANSFORMATIONS ON A GAS-SOLID INTERPHASE BY MEANS OF RESONANT LASER RADIATION

V. V. Petrunin

Physics and Chemistry Department, University of Southern Denmark
5230 Odense M, Denmark

We will briefly review different approaches used in laser chemistry. By considering them under a specific angle and using basic theoretical arguments, we will point out that one particular possibility to conduct laser-induced chemical transformations is left unexplored.

It will be shown how this theoretical prediction can be realized experimentally. In contrast to the majority of photochemical studies dealing with molecular fragmentations, our recent experiment [1] reports a highly endothermic associative chemical reaction, in which only a small fraction of the excitation energy being lost to heat, whereas the rest is used to establish new chemical bonds. We will present several experimental observations justifying the interpretation of the phenomenon and show how microscopic amount of the outcome of the reaction can be produced.

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3a-4 (Tu3-4)

ON MAGNETORECEPTION MECHANISMS IN BIRDS

Ilia A. Solov'yov[1], Danielle Chandler[2], Klaus Schulten[2] and Walter Greiner[1]

[1]Frankfurt Institute for Advanced Studies, Max-von-Laue str. 1
60438 Frankfurt am Main, Germany

[2]Department of Physics, University of Illinois at Urbana-Champaign, and
Beckman Institute for Advanced Science and Technology.
E-mail: ilia@fias.uni-frankfurt.de

The ability of some animals, most notably migratory birds, to sense magnetic fields is still poorly understood. Two, likely co-existing, mechanisms underlying animal magnetoreception are discussed.

It has been suggested [1, 2] that animal magnetoreception is mediated by the blue light receptor protein cryptochrome, which is known to be localized in the retinas of migratory birds. Cryptochromes are a class of photoreceptor signaling proteins which are found in a wide variety of organisms and which primarily perform regulatory functions, such as the entrainment of circadian rhythm in mammals and the inhibition of hypocotyl growth in plants. Recent experiments have shown that the activity of cryptochrome-1 in *Arabidopsis thaliana* is enhanced by the presence of a weak external magnetic field, confirming the ability of cryptochrome to mediate magnetic field responses. Cryptochrome's signaling is tied to the photoreduction of an internally bound chromophore, flavin adenine dinucleotide (FAD). The spin chemistry of this photoreduction process, which involves electron transfer from a chain of three tryptophans, can be modulated by the presence of a magnetic field through the so-called radical pair mechanism based on Zeeman and hyperfine coupling. We present calculations showing that the radical pair mechanism in cryptochrome can produce an increase in the protein's signaling activity of approximately 10% for magnetic fields on the order of 5 Gauss, which is consistent with experimental results. These calculations, in view of the similarity between bird and plant cryptochromes, provide further support for a cryptochrome-based model of avian magnetoreception.

An alternative avian magnetoreception mechanism is based on the interaction of two iron minerals (magnetite and maghemite) which were experimentally found in subcellular compartments within sensory dendrites of the upper beak of several bird species [3]. The iron minerals in the beak form platelets of crystalline maghemite and assemblies of magnetite nanoparticles. We develop a theoretical model [4] to quantitatively describe the interaction between the iron-mineral containing particles. We demonstrate that depending on the external magnetic field the external pull or push to the magnetite assemblies, which are connected to the cell membrane, may reach a value of 0.2 pN. This might be principally sufficient to excite specific mechanoreceptive membrane channels leading to different nerve signals and causing a certain orientational behavior of the bird.

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3b-4 (We4-2)

INDIVIDUAL ADDRESSING AND ERROR RESISTANT SINGLE QUBIT GATES WITH TRAPPED YB^+ IONS

A. Braun, V. Elman, M. Johanning, W. Neuhauser, N. Timoney, C. Weiß,
Chr. Wunderlich

Universität Siegen, 57068, Siegen, Germany

Recently it has been shown that the simulation of one quantum system by means of observing the dynamics of another suitably tailored quantum system can be experimentally far less demanding than universal quantum computation. A system of pair-wise coupled spins described by a Heisenberg model, or a variant thereof, is particularly useful for quantum simulations that in turn are relevant, for instance, for condensed matter physics. We work on the implementation of a pseudo-spin many-body system that will serve as a well controlled prototype system and will allow for the exploration of quantum simulations: in a particular type of ion trap individual atomic ions interact via an adjustable pseudo-spin-spin coupling and, in addition, each spin is individually accessible, thus providing us with an "ion spin molecule" [1].
An important milestone towards realizing such ion spin molecules is the individual addressing of a particular spin employing a spatially varying magnetic field. We demonstrate for the first time individual addressing of ions using radio frequency radiation. Yb^+ ions are confined in a linear Paul trap and laser cooled such that they form a linear Coulomb crystal. Then, an rf-optical double resonance experiment is performed: The ions are optically pumped into the $|m_j|=3/2$ Zeeman states of the electronic metastable state $^2D_{3/2}$. Coherent transitions between the $|m_j|= 3/2$ and $|m_j|=1/2$ states are induced by rf radiation and the population of the $|m_j|=1/2$ states is monitored using an optical transition. Thus individual addressing of trapped ions in frequency space is demonstrated for the first time.

Another line of work with trapped Yb^+ ions is the implementation of error-resistant single qubit gates. In particular, we demonstrate for the first time single qubit gates with trapped ions that have been developed using optimal control theory [2] and are robust against experimental imperfections over a wide range of parameters. It is shown that errors caused by an inaccurate setting of either frequency, amplitude, or duration of the field driving a qubit transition, or a combination of these errors are tolerable (in terms of a desired accuracy, or error probability per gate) when a suitable shaped pulse is applied instead of, for instance, a single rectangular $\pi/2$-pulse [3].
Multi-qubit gates (involving two or more qubits) are usually synthesized by applying a sequence of such elementary unitary operations on a collection of qubits. Thus an essential prerequisite for fault-tolerant, scalable quantum computation with trapped ions is demonstrated here.

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3b-5 (We3-5)

A Scheme for Cavity Cooling of Internal and External Degrees of Freedom of Molecules.

P.W.H. Pinkse[1], G. Morigi[2], M. Kowalewski[3], R. de Vivie-Riedle[3]
[1] Max-Planck-Institut-für Quantenoptik, Hans-Kopfermannstr. 1,
D-85748 München, Germany
[2] Departament de Fisica, Universitat Autonoma de Barcelona,
E-08193 Bellaterra, Spain
[3] Department Chemie, LMU, Butenandtstr. 11, D-81377 München, Germany.

Ultracold molecules are of interest for the study of cold chemistry, cold collisions, astrochemistry and quantum information processing. Their preparation, in particular of ultracold ground state molecules, however, is still challenging. Adapted versions of laser cooling, which try to optimize optical pumping into the molecular ground state, have been proposed [1], but their efficiency is limited by the absence of closed transitions in molecules. A more viable optical avenue seems the use of cavities for cooling, which would avoid the leakage by open transitions. For instance, efficient cavity cooling of the external degrees of freedom has been proposed [2] and demonstrated for atoms [3].

In this contribution we propose to cool the internal and external degrees of freedom of molecules by suitably tailored Raman processes, where absorption of photons from a laser beams is followed by emission into the cavity resonances. On average, this removes rovibrational and translational excitations. The method relies on the enhancement of emission along resonances of a resonator, while the laser, driving the molecules, is sequentially set to different frequencies corresponding to anti-Stokes lines, in order to empty the higher excited rovibrational states of the molecules.

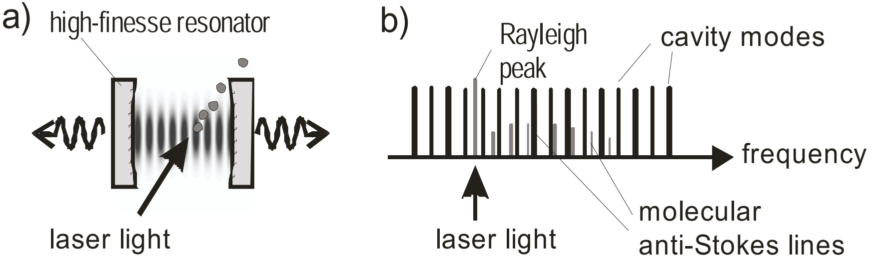

Fig. a) Schematic of the cooling setup. b) Sketch of the involved frequencies. The cavity defines a comb of resonances at which photon emission into the cavity is enhanced. The grey bars symbolize the molecular lines, which in OH extend over several 10 nm. The laser sequentially addresses several anti-Stokes lines.

The cooling efficiency is investigated numerically for the case of the OH radical, using ab initio data and taking into account the rovibrational dependence of the Raman scattering into the cavity modes.

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Zeeman deceleration of neutral ground state atoms

S. D. Hogan, N. Vanhaecke, M. Andrist, U. Meier, D. Sprecher, B. H. Meier
and F. Merkt

Laboratorium für Physikalische Chemie,
ETH Zurich, Switzerland

The development of general methods with which to control the translational motion of atoms and molecules in the gas phase is of particular interest in high resolution spectroscopy and studies of cold reactive collisions. Several of these techniques start from cold samples formed in supersonic expansions and aim at stopping them in the laboratory frame. So far interest has centred on the deceleration and manipulation of atoms and molecules produced in such sources using electric field gradients. The techniques employed include multi-stage Stark deceleration of polar molecules [1], optical Stark deceleration [2], and Rydberg Stark deceleration [3,4]. With the construction, in our laboratory, of a multi-stage Zeeman decelerator for neutral ground state radicals, the possibility to manipulate a wider range of species has been demonstrated [5].

The Zeeman decelerator is composed of a series of co-axial solenoids through which a pulsed gas beam propagates. By switching the current in each solenoid to generate a pulsed magnetic field as the gas pulse enters we can take advantage of the linear Zeeman interaction of a ground state atom or molecule with unpaired electrons to decelerate the gas pulse in a manner analogous to that employed in a multi-stage Stark decelerator [1]. The pulse sequences which we generate, in numerical particle trajectory simulations, and apply to the coils are completely programable and permit us to implement the concepts of phase stability as in the Stark decelerator and charged particle accelerators [6].

The results of a recent series of experiments in which we have decelerated ground state atomic hydrogen with the Zeeman decelerator will be presented. In these experiments magnetic fields of 1-2 T were pulsed in each coil for tens of microseconds, with rise and fall times as short as 5 μs. We have characterised the decelerated part of the gas pulse and studied the effect of zero field time windows, in which electron spin flips can occur, on the deceleration process.

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4b-5 (We3-15)

Mesoscopic Physics with Ultracold Atoms: From Confined Scattering to Rydberg Atoms in Magnetic Traps

P. Schmelcher

Physikalisches Institut, Universität Heidelberg, Philosophenweg 12, 69120 Heidelberg, Germany and Theoretische Chemie, Institut für Physikalische Chemie, Universität Heidelberg, INF 229, 69120 Heidelberg, Germany

E-mail:peter.schmelcher@pci.uni-heidelberg.de

Mesoscopic physics of ultracold atoms is discussed at hand of two different examples. We demonstrate that scattering strongly interacting particles in three dimensions (3D) can be suppressed at low energies in a quasi-one dimensional (1D) confinement. A wave-packet dynamical simulation of the collisional process is performed in harmonic cylindrical confinement by employing a fully 3D screened Coulomb interaction. An almost lossless total transmission is observed. The underlying mechanism is the interference of the s- and p-wave scattering contributions with large s- and p-wave scattering lengths being a necessary prerequisite. This low-dimensional quantum scattering effect might be probed in gases of "strongly" interacting ultracold atoms in elongated traps or in impurity scattering in strongly confined quantum wire-based electronic devices [1].

Ultracold Rydberg atoms exposed to magnetic traps such as the quadrupole field and the Ioffe-Pritchard trap are studied subsequently. A general Hamiltonian which describes the quantum dynamics of an atom in an arbitrary linear magnetic field configuration is derived. The coupled center of mass and electronic motion is solved by incorporating an adiabatic separation of the dynamics. We provide the adiabatic energy surfaces and discuss under which conditions trapped center of mass states can be achieved for Rydberg atoms. Energies and wavefunctions of the corresponding quantum hybrid states are studied thereby entering a new regime where both the external and internal motion are coupled and quantized leading to e.g. ring states. By analyzing the properties of the resulting combined motion we demonstrate that the extension of the electronic wavefunction can exceed that of the center of mass motion in a Ioffe-Pritchard trap. Such atoms cannot be considered as being point-like [2,3].

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5a-4 (We1-7)

Laser induced molecular alignment of ethylene

A. Rouzée, S. Guérin, B. Lavorel, and O. Faucher

Institut Carnot de Bourgogne, UMR 5209 CNRS - Université de Bourgogne, BP
47870, 21078 Dijon cedex, France

Molecular orientation and alignment play a key role in strong field-molecule interactions, chemical reactions, and gas-phase solid interactions. For example, in chemistry, the product of a reaction can be maximized by aligning molecules, or in gas-phase solid interaction, stereodynamic effects on surface adsorption processes can be studied by guiding molecules [1]. To investigate the effects of molecular alignment on these processes, it is necessary to control the rotational degrees of freedom of the molecules. The last years, it has been established that strong non-resonant laser pulses of duration $\tau >> \hbar /B$, with B the rotational constant of the molecule, align molecules during the interaction with the field, while impulsive pulses ($\tau << \hbar /B$) yield to post-pulse transient alignment revivals [2]. These effects have been studied both theoretically and experimentally, principally in linear molecules. However, lot of applications implies asymmetric top molecules. It is necessary therefore to implement experiments in order to control their rotational motions.

Here, we show that a single elliptically polarized laser pulse with appropriate ellipticity allows to align the three axes of an asymmetric top molecule. We present a theoretical model where we define the ellipticity that maximizes simultaneously the alignment of two molecular axes, and therefore the 3-D alignment. Experimentally, field free 3-D molecular alignment has been probed using the optical kerr effect in a molecular jet of ethylene. One-dimensional alignment experiments have been first conducted with linearly polarized laser pulses in order to estimate peak intensity and temperature. Then, using elliptically polarized laser pulses, we have induced and measured three-dimensional alignment of ethylene.

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5b-4 (We3-29)

COLLECTIVE EXCITATIONS AND INSTABILITY OF AN OPTICAL LATTICE DUE TO UNBALANCED PUMPING

P. Domokos[1], J. K. Asbóth[1,2], H. Ritsch[2]

[1]Research Institute of Solid State Physics and Optics, Hungarian Academy of Sciences, H-1525 Budapest P.O. Box 49, Hungary
[2]Institut für Theoretische Physik, Universität Innsbruck, Technikerstr. 25, A-6020 Innsbruck, Austria

Optical lattices (OL) are perfectly periodic arrays of particles trapped by the standing wave interference pattern of several laser beams. They have important applications as model systems for solid state physics as well as for quantum information science. The back-action of the trapped particles on the trap light is carefully avoided in most OL experiments. However, it is known to give rise to intriguing phenomena in related systems, e.g., cavity cooling, mirror cooling, and optical binding. For OL's this back-action has been predicted [1] and observed [2, 3] to reduce the lattice constant d compared to the naive expectation.

We will consider the effects of optical back-action in one-dimensional OL's, brought about by tuning a hitherto neglected parameter: the relative intensity of the lattice beams. Introducing an asymmetry in the trap not only enhances the reduction of the lattice constant, but, more importantly, alters the *interaction* between the trapped particles mediated by the light. The asymmetry gives rise to traveling density waves even in the presence of arbitrarily strong viscous damping [6]. This is directly related to the wavelike excitations in other crystals driven far from equilibrium, such as arrays of vortices in a type-II superconductor [4], and trains of water drops dragged by oil [5]. These waves arise resonantly at specific values of the asymmetry, and destabilize the lattice at a critical asymmetry that decreases sharply as the lattice size is increased.

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6b-4 (Mo5-1)

VACUUM ULTRAVIOLET PHOTODISSOCIATION IMAGING OF HeH$^+$ USING INTENSE FREE ELECTRON LASER PULSES

H. B. Pedersen[1], S. Altevogt[1], B. Jordon-Thaden[1], O. Heber[2], M. L. Rappaport[2],
D. Schwalm[1], J. Ullrich[1], D. Zajfman[1,2], R. Treusch[3], N, Guerassimova[3], M. Martins[4],
J.-T Hoeft[4], M. Wellhöfer[4], and A. Wolf[1]

[1]Max-Planck-Institut für Kernphysik, D-69117 Heidelberg, Germany
[2]Department of Particle Physics, Weizmann Institute of Science, Rehovot, Israel
[3]HASYLAB at DESY, Hamburg, Germany
[4]Institut für Experimentalphysik, Universität Hamburg, Germany

The new Free Electron LASer in Hamburg (FLASH) [1] delivers unprecedented intense light pulses in the VUV and soft X-ray regime that, combined with fast ion beam techniques, allows the regime of valence shell excitation so far inaccessible for molecular ions to be explored by 3D momentum imaging of photofragments. These excitations are of importance in astrophysically occurring radiation fields [2,3] and the fragment momenta reflect the dynamics of the excited quantum chemical system, thus providing a sensitive probe of molecular theory.

We report a first benchmark crossed-beams photodissociation experiment with FLASH, where the photofragment geometry and absolute photodissociation cross section were measured at 38.7 eV excitation energy (32 nm) for HeH$^+$ on the channel H$^+$ + He(1*snl*). HeH$^+$ is a benchmark case as the ionic analogue of H_2; its excited states have only been addressed theoretically [4] while being of potentially high importance in both astrophysical environments [2,3] and in neutrino mass measurements [5].

The experiment used a novel ion beam infrastructure installed for this purpose at the plane grating monochromator beam line (PG2) [6] at FLASH, performing three-dimensional event-by-event fragment imaging of cold molecular ions in a crossed beams geometry with ~100 HeH$^+$ ions in the interaction region for each FLASH pulse.

The absolute photodissociation cross section at 32 nm into the He-fragment channel was determined to $1.4 \cdot 10^{-18}$ cm^2 with a systematic error of ~50 %. The measured energy release spectrum of HeH$^+$ showed a remarkably large fraction of ~50 % in highly excited states of $n \geq 3$. The angular distributions showed an unexpected dominance of fragmentation transverse to the photon polarization, originating from excitation into curves of $^1\Pi$ symmetry. In contrast, theoretical studies [4] and astrophysical models of the early universe [2] and planetary nebulae [3] have so far emphasized parallel transitions via the low-lying excited states of $^1\Sigma$ symmetry.

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6b-5 (Mo5-5)

Single Photon-Induced Symmetry Breaking of H_2 Dissociation

F. Martín[1], J. Fernández[1], T. Havermeier[2], L. Foucar[2], Th. Weber[2],
K. Kreidi[2], M. Schöffler[2], L. Schmidt[2], T. Jahnke[2], O. Jagutzki[2], A. Czasch[2],
E. P. Benis[3], T. Osipov[4], A. L. Landers[5], A. Belkacem[4], M. H. Prior[4],
H. Schmidt-Böcking[2], C. L. Cocke[3], R. Dörner[2]

[1] Departamento de Química, C-9, Universidad Autónoma de Madrid, 28049 Madrid, Spain.
[2] Institut für Kernphysik, University Frankfurt, Max von Laue Strasse 1, D-60438 Frankfurt, Germany.
[3] Department of Physics, Kansas State University, Cardwell Hall, Manhattan, KS 66506, USA.
[4] Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA.
[5] Department of Physics, Auburn University, Auburn, AL 36849, USA.

The indistinguishableness of the two protons in the dissociating H_2^+ molecule prohibits the electron to prefer one nucleus for the generation of the neutral hydrogen. In this contribution a method is shown to break this symmetry via the population of doubly excited states. In March 2005 an experiment was performed at the Advanced Light Source in Berkeley to observe the dissociating channels in hydrogen and deuterium molecules. The COLTRIMS method allows a kinematically complete measurement so that a map of all appearing states could be obtained.

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7b-4 (Th3-11)

Many-Body Dynamics of Repulsively Bound Pairs of Particles in a Periodic Potential

David Petrosyan,[1,2] Bernd Schmidt,[1] James R. Anglin,[1] and Michael Fleischhauer[1]

[1]Fachbereich Physik, Technische Universität Kaiserslautern, D-67663 Kaiserslautern, Germany
[2]Institute of Electronic Structure & Laser, FORTH, 71110 Heraklion, Crete, Greece

Recently, Winkler *et al.* [Nature 441, 853 (2006)] have observed repulsively bound atom pairs in an optical lattice. In a tight-binding periodic potential described by the Bose-Hubbard model, when the on-site repulsion between the particles exceeds their inter-site tunneling rate, such “dimers” are well localized at single sites and are stable over the time scale on which the energy dissipation is negligible. We derive an effective many-body Hamiltonian for a lattice loaded with dimers only, and discuss its implications for dynamics of the system. We show that strong on-site repulsion and nearest-neighbor attraction favor clusters of dimers with minimum surface area and uniform, commensurate filling, representing thus incompressible “droplets” of a lattice liquid.

7b-5 (We3-6)

CREATION OF AN ULTRACOLD MIXTURE OF FERMIONIC LITHIUM AND POTASSIUM

F.M. Spiegelhalder[1], E. Wille[1,2], G. Kerner[1], D. Naik[1], A. Trenkwalder[1], C. Aiello[1],
R. Chulia Jordan[1], G. Hendl[1], F. Schreck[1] and R. Grimm[1,2]

[1]Institut für Quantenoptik und Quanteninformation
Österreichische Akademie der Wissenschaften
Innsbruck, Austria

[2]Institut für Experimentalphysik
Leopold-Franzens-Universität
Innsbruck, Austria

Degenerate mixtures of fermionic ^{6}Li and ^{40}K provide a new, intriguing many-body quantum system, which enables the study of strongly interacting Fermi gases consisting of atoms with unequal masses. In our experiment, cold atoms from a magneto-optical trap are transferred into a crossed-beam optical dipole trap realized with a 100 W near-infrared laser. The sample is cooled down evaporatively to quantum degeneracy by lowering the trapping potential. The broad Feshbach resonance in ^{6}Li at a magnetic field of B = 834 G allows for precise tuning of the scattering length *a*. At a field of B = 764 G, we obtained a molecular $^6Li_2$ BEC (Fig. 1). At the same field we observe sympathetic cooling of bosonic ^{39}K and fermionic ^{40}K. By simultaneous absorption imaging of each atomic species at the end of each experimental cycle, we could verify the creation of ultracold mixtures of ^{6}Li-^{39}K and ^{6}Li-^{40}K. The next step will be to find inter-species Feshbach resonances at which we want to study strongly interacting gases and the formation of heteronuclear molecules.

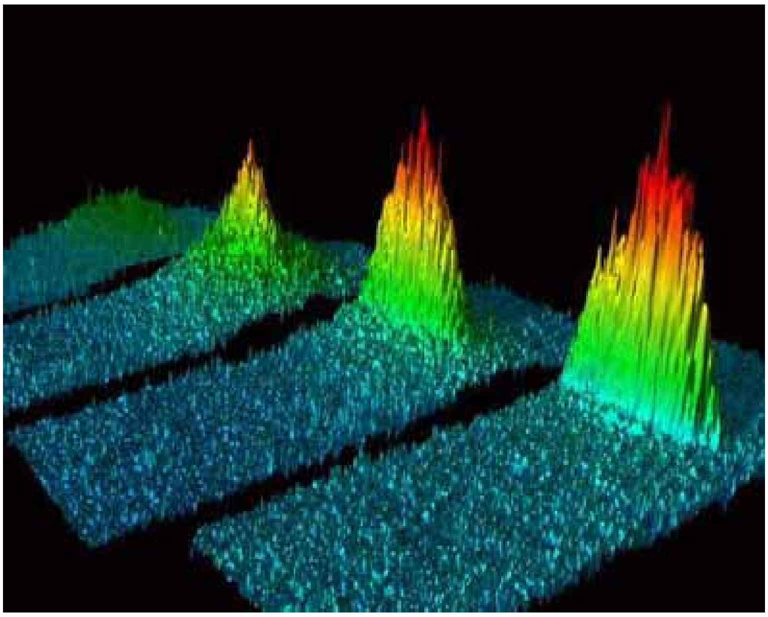

Fig. 1. Formation of a molecular BEC of about $5*10^5$ $^6Li_2$: the four time-of-flight images show the formation of a condensate peak in the centre of the initial thermal distribution.

8a-1 (Mo1-8)

Attosecond Ionization Dynamics

P. Johnsson[1,2], J. Mauritsson[1,3], T. Remetter[1], K. J. Schafer[3] and A. L'Huillier[1]

[1] Department of Physics, Lund University, P. O. Box 118, SE-221 00 Lund, Sweden
[2] *Now at:* FOM-Institute AMOLF, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands
[3] Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001, USA

In the interaction between light and matter, the central energy and bandwidth of the radiation, in relation to the energy structure of the studied atoms or molecules, are important parameters. Extreme ultraviolet attosecond pulses, produced through high-order harmonic generation[1,2], have during the last years been increasingly used for such studies, particularly in combination with intense infrared (IR) fields, for time-resolved studies of strong field processes[3-6]. Attosecond experiments have so far utilized pulses with high central energies, in excess of the ionization potentials of the studied species. When these pulses interact with matter they induce single-photon ionization, creating electron wave packets with a significant initial energy.

In the work presented here, we generated attosecond pulse trains in xenon, with individual pulse durations of 370 as. Their central energy was 23 eV, which is above the ionization potential of argon (15.8 eV), but below that of helium (24.6 eV). These pulses were brought to interact with the target gas in the presence of a strong IR laser pulse, and the ion yield was measured as a function of the phase of the IR field at the time of arrival of the pulse. For helium, where the central energy of the pulses is below the ionization threshold, we find a significant enhancement of the ion yield when the IR field is present. In addition, the ion yield exhibits a sub-cycle modulation as a function of the IR phase. Theoretical calculations based on the integration of the time-dependent Schrödinger equation suggest that the observed results originate in the creation of bound electron wave packets by the attosecond pulses, which subsequently ionize.

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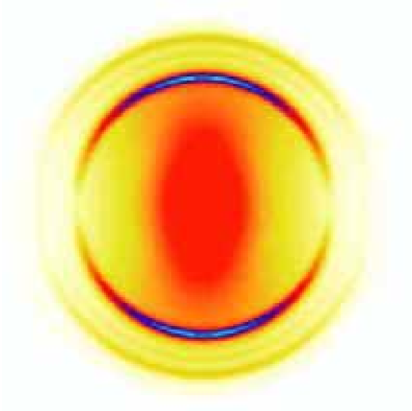
8a-2 (Mo5-27)

A FEMTOSECOND IMAGING STOPWATCH FOR THE BOND BREAKAGE OF A POLYATOMIC MOLECULE

R. de Nalda[1], J.G. Izquierdo[2], J. Durá[2], L. Bañares[2]

[1]Instituto de Química Física Rocasolano, Consejo Superior de Investigaciones Científicas, Serrano 119, 28006 Madrid, Spain
[2]Facultad de Ciencias Químicas, Universidad Complutense de Madrid, Avda. Complutense s/n, 28040 Madrid, Spain

We demonstrate that the combination of velocity map imaging and femtosecond pump-probe technology for the observation of ground-state neutral fragments allows the measurement of the reaction times of several well-defined channels in the bond breakage of a polyatomic molecule. By using resonant detection, we have been able to clock the C-I bond rupture of methyl iodide, CH_3I, from the *A* band, which involves non-adiabatic dynamics yielding ground-state $I(^2P_{3/2})$ and spin-orbit excited $I^*(^2P_{1/2})$ and ground and vibrationally excited CH_3 fragments. The reaction times found for the different channels are directly related with the non-adiabatic dynamics of this multidimensional photodissociation reaction. Once the wave packet is formed in the $^3Q_0$ potential surface, the dynamics is probed by a time-delayed femtosecond pulse. Results obtained with both resonant and non-resonant probing will be presented and discussed in relation to the observation of transition states.



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Contact: r.nalda@iqfr.csic.es, lbanares@quim.ucm.es

8a-3 (Tu2-34)

Visualizing and Controling Ultrafast Wave-Packet Interference in Diatomic Molecules

Hiroyuki Katsuki[1,2], Hisashi Chiba[1,2], Kenji Ohmori[1,2], Christoph Meier[3], and Bertrand Girard[3]

[1]Institute for Molecular Science, Myodaiji, Okazaki 444-8585 Japan
[2] CREST, Japan Science and Technology Agency, Kawaguchi, Saitama 332-0012, Japan
[3] LCAR –IRSAMC, CNRS, Université Paul Sabatier–Toulouse 3, France.

Inteference of matter waves has been a focus topic in the quantum world, playing important roles in the studies on the quantum-classical boundary, quantum computations, quantum cryptography and so on. Here we demonstrate unprecedently high-resolution measurements and control of the interference of vibrational wave packets created in diatomic molecules.

Recently we have observed transient interference of two counter-propagating vibrational wave-packets generated around the half-revival period on the *B*-state potential of the iodine molecule (I_2) [1]. 'Quantum ripples' appeared periodically only when the two wave packets cross each other, and their structures were measured successfully with a few picometers and ~100fs spatiotemporal resolutions (see Fig. 1).

In this talk, we also present 'active' control of these quantum ripples; the control has been carried out with a pair of fs laser pulses whose relative phase is locked with our highly-stable interferometer called an "attosecond phase modulator (APM)" [2, 3]. Two counter propagating wave packets are prepared by setting the delay τ between the phase-locked twin pulses to around $1.5T_{vib}$, where T_{vib} is a classical vibrational period of I_2. Depending on the relative phase between the twin pulses, the spatiotemporal pattern of the ripples, which we call "quantum fabric", changes drastically. To the best of our knowledge, this is one of the finest manipulations within the molecules ever performed.

Moreover, we have utilized these experimental techniques to read and write amplitude and phase information of the vibrational eigenstates within the wave packets.

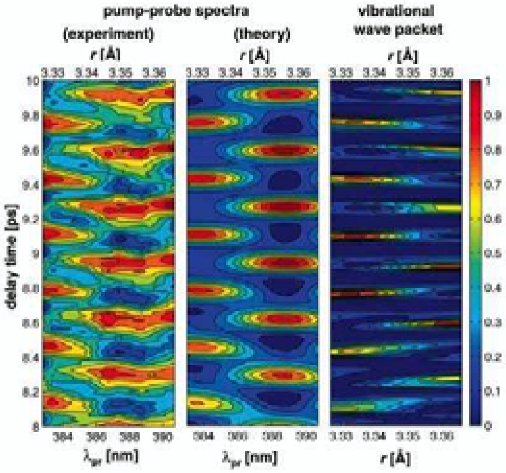

Fig. 1: (left) observed interferometric structure by pump-probe spectroscopy. (center) theoretical simulation.
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8a-4 (Tu2-6)

MAPPING THE VIBRATION OF FAST MOLECULES WITH ULTRASHORT LASER PULSES

C R Calvert[*], J McKenna[*], D S Murphy[*], W A Bryan[†], E M L English[†], J Wood[†],
I C E Turcu[δ], J F McCann[*], W R Newell[†] and I D Williams[*].

[*] School of Mathematics and Physics, Queen's University Belfast, Belfast, UK
[†] Department of Physics and Astronomy, University College London, London, UK
[δ] Central Laser Facility, CCLRC Rutherford Appleton Laboratory, Chilton, UK

Dynamical studies of bound vibrational motion in the fastest moving molecular systems [1,2] have recently become possible due to state of the art advancements in laser pulse technology. Using ultrashort intense field laser pulses in a 'pump-probe' arrangement, we have initiated and probed coherent wavepacket motion of the deuterium molecular ion (D_2^+) on a sub-vibrational timescale. In our experiment the nuclear wavepacket is initiated in a coherent superposition of vibrational states and consequently we observe the dephasing of these vibrational components with subsequent re-phasing (the so-called 'Quantum Revival') occurring at later times.

At this meeting we will present unambiguous observations of vibrational wavepacket revivals in D_2^+ imaged via both the photo-dissociation and Coulomb explosion channels. We will also show how Fourier transform analysis provides a measure of vibrational population and how this population may be manipulated [3] in order to obtain state selective control of vibrational motion.

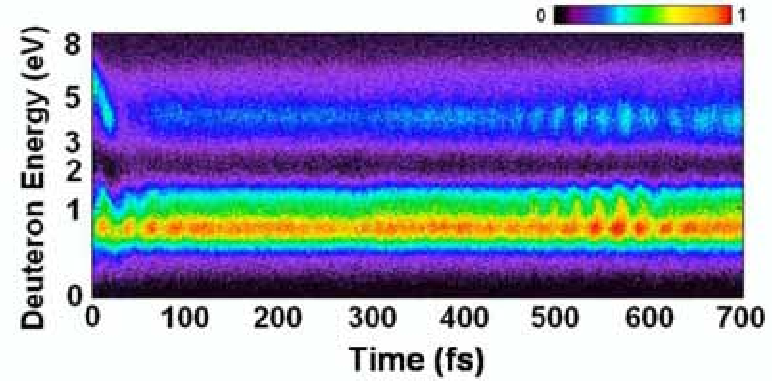

Figure 1:
Deuteron yield as a function of wavepacket evolution time. High energy fragments arise from Coulomb explosion events and low energy fragments are from photodissociation. Both of these imaging channels are enhanced at large internuclear separation for the D_2^+ molecule. Thus the notable modulation in the 500 – 600 fs region signifies a quantum revival wherein the individual vibrational components rephase and the vibrational wavepacket executes semi-classical motion.

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Email: c.calvert@qub.ac.uk

8a-5 (Mo3-19)

Femtosecond laser induced fusion of gas phase fullerenes

K.Hansen[1*], M.Kjellberg[1], A.V.Bulgakov[2], E.E.B.Campbell[1]

1. Dept. of Physics, Göteborg University, SE-41296 Göteborg, Sweden
2. Institute of Thermophysics, SB-RAS, 1 Lavrentyev Ave. 630090 Novosibirsk, Russia
* email: klavs@physics.gu.se

van der Waals bound clusters of fullerenes have been observed to undergo intra-cluster fusion when exposed to femtosecond laser light [1,2,3,4]. The fusion is followed by fragmentation with loss of C_2 units, demonstrating both the fullerene nature of the products and the large thermal energy of the fusion product. Fusion is absent when the clusters are exposed to a nanosecond laser pulse, where the decay channel is instead loss of intact fullerene molecules.

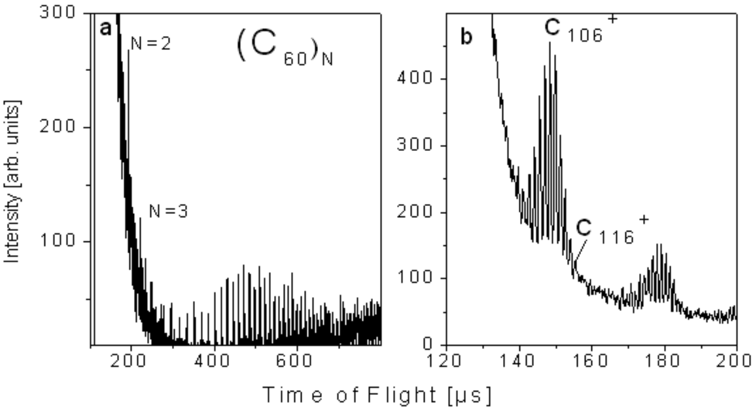

Fig.1 (a) Time-of-flight mass spectrum obtained by single-photon ionisation of $(C_{60})_N$ clusters from a gas aggregation source. (b) Part of ion time-of-flight mass spectrum from an identical cluster distribution ionized with 200 fs laser pulses providing evidence for intra-cluster molecular fusion.

Fusion-fragmentation products of precursors up to $(C_{60})_5$ and $(C_{70})_5$ have been observed but only as singly charged species. These facts suggest that the fusion process involve timescales similar to the ones found for the quasi-thermal electron emission from fs-heated fullerenes, of several hundred femtoseconds. This has been confirmed with pump-probe experiments where the total fragment yield was measured [2].

The degree of post-fusion fragmentation is fairly invariant to source conditions and laser fluence. The number of C_2 units lost from the fusion products grows linearly with the precursor size and reaches 30 for $(C_{60})_5$. The shape of the dimer fusion product distribution can be understood in terms of the fusion barrier which provides the high mass (low energy) cutoff and, for the low mass (high energy) cutoff, as the tendency for more highly charged and hotter van der Waals bound clusters to *fission*[3,4].

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8a-6 (We2-8)

BEYOND MEAN FIELD: USING LASER PULSES TO PROBE PAIR CORRELATIONS IN CONDENSATES

J. Mur-Petit,[1] * P. Naidon,[2] E. Luc-Koenig,[1] and F. Masnou-Seeuws[1]

[1] *Laboratoire Aimé Cotton, CNRS and Univ. Paris-Sud, 91405 Orsay, France*

[2] *Atomic Physics Division, NIST, Gaithersburg, Maryland 20899-8423, USA*

The formation of molecular condensates from atomic condensates by means of optical or magnetic Feshbach resonances is a topic of growing interest [1,2]. The theoretical methods required by these processes need to account for the correlations in the system, which is *beyond the validity of the mean-field approximation.*

Following the ideas of Ref. [3], we have developed a method that takes into account two-body correlations in such situations [4]. In particular, we have shown that a sudden switch-on of a photoassociation laser onto an atomic sample shall give rise to *correlated* pairs of “hot” atoms leaving the trap [5]. This leads to an *increase* in the correlation for the equal-time detection of two atoms with opposite momenta:

$$^{(2)}(\boldsymbol{k},-\boldsymbol{k};\ ) = \frac{\langle \hat{a}^{\dagger}_{\boldsymbol{k}}(\ )\hat{a}^{\dagger}_{-\boldsymbol{k}}(\ )\hat{a}_{-\boldsymbol{k}}(\ )\hat{a}_{\boldsymbol{k}}(\ )\rangle}{\langle \hat{a}^{\dagger}_{\boldsymbol{k}}(\ )\hat{a}_{\boldsymbol{k}}(\ )\rangle\langle \hat{a}^{\dagger}_{-\boldsymbol{k}}(\ )\hat{a}_{-\boldsymbol{k}}(\ )\rangle} > 2\,.$$

We analyze the detection of these correlations with time-of-flight measurements as in the experiments with metastable helium by the group of Chris Westbrook [6].

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[*] Also at Institut Francilien de Recherche sur les Atomes Froids (IFRAF).

E-mail: jordi.mur@lac.u-psud.fr

8b-1 (Mo3-8)

ELECTRON SPIN RELAXATION IN ALKALI SAMPLES ON THE SURFACE OF HELIUM NANODROPLETS

Johann Nagl, Gerald Auböck, Carlo Callegari, and Wolfgang E. Ernst

Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria
Email: wolfgang.ernst@tugraz.at

Helium nanodroplets formed in a supersonic expansion of high pressure gas from a low temperature source (10 to 20K) represent finite size superfluid samples with 0.4 K internal temperature. Using a helium backing pressure around 100 bar, nanodroplets of average size $N=10^4$ atoms are generated. In a molecular beam apparatus, the droplets pass through a pick-up cell containing a gas at low pressure, where each droplet is doped with a statistical number of atoms or molecules. Most degrees of freedom of these dopants are immediately cooled to 0.4 K, and the released energy leads to evaporation of a corresponding number of helium atoms from the droplet. The cold environment can be used to cool individual molecules for a spectroscopic study of their lowest energy configuration, to produce weakly bound molecular complexes, or study cold collisions between different dopant species residing in the same droplet. In the analysis of condensed matter samples, electron spin resonance is a common experimental technique. ESR spectroscopy could become a versatile tool to investigate oligomers formed on He droplets after an examination of spin lifetimes and the development of a detection method for spin states. This paper reports the first magnetic study of any species in or on helium droplets as well as approximate relaxation times for electron spin states of potassium atoms and molecules on helium droplets.

Alkali atoms were one of the first chromophores ever attached to a helium droplet, and are unique in that they do not become solvated inside the droplet, but instead remain in a dimple on its surface. Further, because of the smaller binding energy released into the droplet, it is the high spin complexes (triplet dimers, quartet trimers) which preferentially survive the formation process [1]. We now investigated their electronic spin in the low-symmetry environment offered by the surface of a droplet. In a first step, we have measured magnetic dichroism spectra of potassium atoms residing on the surface of He nanodroplets 1) to estimate the spin-relaxation time; 2) to demonstrate that a spin-polarized sample can be easily created and that optical detection is a viable technique for ESR in He droplets. Laser induced fluorescence was used to probe the K 4p←4s atomic transition and the $1^3\Pi_g \leftarrow 1^3\Sigma_u$ band of K_2. A magnetic field of 2.9 kG was applied and the laser beam polarization continuously varied with a Pockels cell from σ^- through π to σ^+. By measuring the circular dichroism, the populations of Zeeman sublevels were probed. No dichroism was observed for the atomic potassium sample on helium droplets, indicating that the sublevels have not thermalized and putting a lower limit to the spin relaxation time of 1.9 ms [2], based on the geometrical conditions in the molecular beam apparatus.

Dichroism spectra of K_2 molecules on helium droplets showed a different behavior. Their analysis yields a population of Zeeman sublevels close to thermal equilibrium with the helium droplet. Geometric considerations put an upper limit of ~40 μs to the spin relaxation time in this case [2].

Further to the exploration of spin lifetimes whose different values will have to be explained on the basis of the interaction of the alkali atoms and molecules with the helium environment, the optical saturation of the spectra was measured and will be used for the preparation of spin polarized samples on cold droplets.

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8b-2 (Mo3-15)

Resonances in Transition Metal Complexes by TDDFT calculations

P. Decleva, G. Fronzoni and M. Stener

Universita' di Trieste
Dipartimento di Scienze Chimiche,Via Giorgieri, 1
I-34127 Trieste, Italy

Time Dependent Density Functional Theory (TDDFT) has been shown to be a powerful and accurate description of photoionization processes, including interchannel coupling, in small systems [1,2]. A new direct algorithm for the solution of the equations in complex molecules has been presented [3], which eliminates convergence problems which hinder application of the classical SCF approach to large systems, and a parallel implementation is being developed. Applications to the description of resonances, both shape and autoionization, in organometallic systems [4] will be presented, together with a discussion of chemical effects on the position and strength of the resonances.

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8b-3 (Mo3-2)

NON-METALLIC BEHAVIOR OF C_{60} ELECTRON SHELL

M. Ya. Amusia[1, 2] and A. S. Baltenkov[3]

[1]Racah Institute of Physics, the Hebrew University, Jerusalem 91904, Israel
[2]Ioffe Physical-Technical Institute, St.-Petersburg 194021, Russia
[3]Arifov Institute of Electronics, Tashkent, 700125, Uzbekistan

The dynamical and static dipole polarizabilities of the C_{60} molecule have been calculated on the basis of the experimental data on the cross section of the fullerene photoabsorption [1]. It has been shown that the fullerene shell in the static electric field behaves most likely as a set of separate carbon atoms, rather than as a conducting sphere [2].

We demonstrate that by studying photoabsorption cross-section of a mesoscopic object one can conclude whether its electron system forms a "conductor" or "dielectric". Of course, these notions characterize the ability of the object to conduct electricity and are applicable, only to macroscopic bodies. However, for mesoscopic objects that include many atoms, the feature of conductivity can also become meaningful starting from the certain number of constituent atoms. This makes sensible the question whether a mesoscopic system behaves as a conductor, i.e. whether its electrons can move freely under the action of an external electric field.

As a feature that characterizes a conductor we use a quite natural definition that a static external electric field cannot penetrate inside a conducting body. As an object of investigation and as a particular example of the mesoscopic system, in this talk we choose the fullerene C_{60} molecule. We calculate the effective electric field $\mathbf{E}_{eff}(\omega)$ that is at the fullerene center when the external electric field $\mathbf{E}(\omega)$ with frequency ω is applied to C_{60}. The modification of the external field comes from the effect of the dynamic dipole polarizability $\alpha_d(\omega)$ of the fullerene C_{60} that is expressed via its total photoionization cross-section $\sigma(\omega)$. We calculate the frequency dependence of the ratio $\eta(\omega) \equiv \mathbf{E}_{eff}(\omega)/\mathbf{E}(\omega)$ and then investigate whether $\eta(0)$ is equal to zero or not.

The equality of the ratio $\eta(\omega)$ to zero in the static limit $\omega \to 0$ is the critical condition being general for a conducting body with any form. In the case of the fullerene C_{60} this ratio is $\eta(0) \approx 2$, i.e. C_{60} is not a hollow metallic sphere at all.
For the nonzero frequencies of radiation ω the metallic sphere stops to be an ideal screen for the incidental radiation and the alternating electric field penetrates into the conducting sphere. However, as is shown in the talk, the frequency dependence of the ratio of the fields $\eta(\omega)$ at the center of the C_{60} molecule and outside it has nothing to do with $\eta(\omega)$ for the conducting sphere [2], which is additional evidence that the C_{60} shell is strongly non-metallic.

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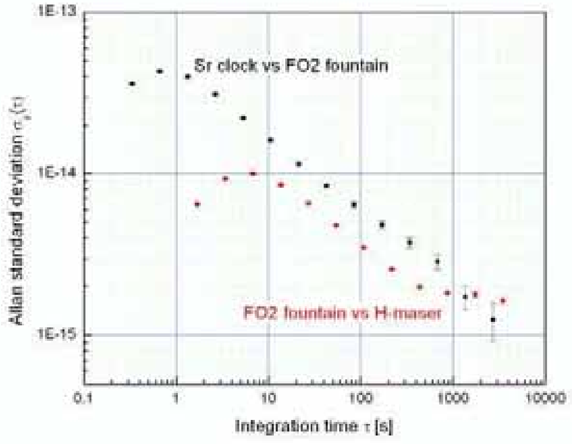
8b-4 (We5-18)

^{87}Sr OPTICAL LATTICE CLOCK USING SPIN-POLARIZED ATOMS

X. Baillard, M. Fouché, R. Le Targat, P. Westergaard, A. Lecallier, F. Chapelet,
S. Bize, P. Rosenbusch, M. Abgrall, P. Laurent, Y. Lecoq, G.D. Rovera, A. Clairon,
P. Lemonde
LNE-SYRTE, Observatoire de Paris, 61 Avenue de l'Observatoire, 75014 Paris,
France

B. Lipphardt, G. Grosche, H. Schnatz
Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig,
Germany

We present a new accuracy evaluation of the LNE-SYRTE optical lattice clock with ^{87}Sr atoms. The interrogation is now achieved with spin-polarized atoms in the (F=9/2, m_F=9/2) or (F=9/2, m_F=-9/2) Zeeman sub-state. Using a pi-polarized clock laser, we alternate cycles where the 9/2 → 9/2 and -9/2 → -9/2 transitions are probed, strongly decreasing the uncertainty on the magnetic field effects for this measurement. The frequency measurement was made thanks to a femtosecond frequency comb based on a fiber laser, and referenced to the three atomic fountains FO1, FO2 and FOM at LNE-SYRTE. The resulting accuracy of the Sr clock is in the low 10^{-15} range. An experimental standard Allan deviation is plotted on the figure. The stability of the measurement at 1s is 5.10^{-14}, with roughly equal contribution of the Sr clock and of the fountain.
We also made a measurement of the frequency for the ^{88}Sr bosonic isotope, using a static magnetic field to allow the transition. The evaluation of the systematic effects and a comparison with the fermionic isotope will also be discussed.



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8b-5 (Th3-3)

Photoionization microscopy: experiment and simulations.

A. Ollagnier[1], F. Lépine[1], M-A. Lebeault[1], F. Robicheaux[2], M.J.J. Vrakking[3] and C. Bordas[1]

[1] Université Lyon 1 ; CNRS ; LASIM UMR 5579, 43 boulevard du 11 novembre 1918, F-69622 Villeurbanne Cedex, France.
[2] Department of Physics 206 Allison Lab Auburn University, AL 36849-5311
[3]FOM-Institute AMOLF, Kruislaan 407,1098 SJ Amsterdam, The Netherlands

In the 80's Kondratovich, Ostrovsky and Demkov ([1],[2]) proposed an experiment in which the two dimensional flux of electron produced in a photoionization process in the presence of a static electric field is measured with a position sensitive detector placed at a macroscopic distance, perpendicularly to the electric field. They noticed that this electron current is a direct measurement of the square modulus of the transverse component of the electronic wavefunction. This experiment is named "photoionization microscopy" as it provides an image that is a macroscopic projection of the electronic wave function which properties are determined by the short distance motion of the electron around the nucleus.

The first photoionization microscope has been built recently and first experimental results were obtained on Xe atoms ([3],[4]). Ionization with one and two photons was performed and electrons were detected using a state-of-the-art imaging spectrometer. A typical image shows two main structures explained by the topology of electron trajectories. These results have demonstrated that this asymptotic measurement allows one to distinguish between "indirect" electrons scattered by the ionic core and "direct" electrons with trajectories mainly influenced by the electric field. Even more spectacular is the interference pattern observed for both contributions and the smooth evolution of the number of fringes when the ionization wavelength varies. Surprisingly, the structure of the ionization continuum only affects the angular distribution.

These results can be understood intuitively in terms of interferences between several trajectories followed by the electron in order to reach a given position on the detector. A hydrogenic semiclassical model has been able to describe the main features of the experimental results ([5]). However, a complete quantum description of the photoionization microscopy experiment is needed and requires a more refined theoretical description taking into account the effect of the electric field, ionic core, electronic core and ionization process. There, we have recently performed calculations based on wavepacket propagation using a split-operator code. It allows us to study electron dynamics for different atoms and to get a better insight into the relation between interference patterns and electronic motion. In this contribution we will discuss comparisons between experimental results and calculations as well as predictions for photoionization microscopy experiments on hydrogen and non-hygrodenic atoms.

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8b-6 (Th2-62)

FLUORESCENCE OF HELIUM DOUBLY EXCITED STATES BELOW $N = 2$ IN HOMOGENEOUS ELECTRIC FIELD

Andrej Mihelič* and Matjaž Žitnik

Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

We study the Stark effect on doubly excited states of the helium atom below the $N = 2$ ionization threshold in high electric fields. The *ab initio* photoionization and total inelastic photon scattering cross sections for field strengths up to 100 kV/cm are calculated and compared to the ion yield [1] and the recent VUV fluorescence yield measurements [2,3]. The method of complex scaling is used, for incident photons with the polarization vector **P** both parallel and perpendicular to the externally applied electric field **F**. Radiation damping due to coupling of the atom to the radiation field is taken into account [4], which may be seen to be crucial for those states that decay predominantly by fluorescence. The present results are the first *ab initio* calculations of the photoionization cross sections that explain in detail the measured signal for the parallel experimental setup (**P** $\parallel$ **F**), and the first predictions for the perpendicular experimental geometry (**P** $\perp$ **F**). Furthermore, the total inelastic scattering cross sections in strong fields are calculated for the first time for both linearly independent polarizations.

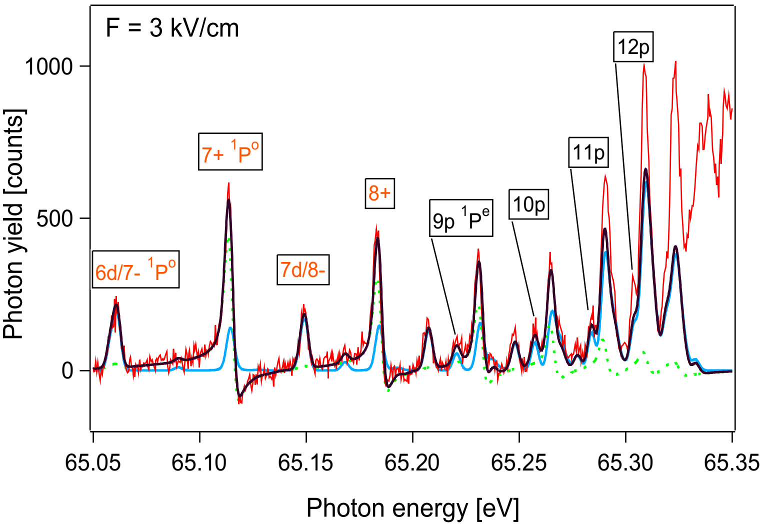

Figure: The calculated and measured [3] fluorescence yield. The dashed line is the admixture of the (calculated) photoionization signal due to the fluorescence generated by collisions of charged particles with the experimental equipment.

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* Electronic address: andrej.mihelic@ijs.si

POSTERS

Monday 7/5

1. Attosecond Physics

Mo1-1

Attosecond real-time observation of electron tunnelling and multi-electron dynamics in atoms

M. Schultze[2],M. Uiberacker[1,2], Th. Uphues[3], A.J. Verhoef[2], V. Yakovlev[1], M.F. Kling[4], J. Rauschenberger[1,2], N.M. Kabachnik[3,6], H. Schröder[2], M. Lezius[2], K.L. Kompa[2], H.-G. Muller[4], M.J.J. Vrakking[4], S. Hendel[3], U. Kleineberg[1], U. Heinzmann[3], M. Drescher[5] & F. Krausz[1,2,7].

[1] Department für Physik, Ludwig-Maximilians-Universität, Am Coulombwall 1, D-85748 Garching, Germany
[2] Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany.
[3] Fakultät für Physik, Universität Bielefeld, Universitätsstrasse 25, D-33615 Bielefeld, Germany
[4] FOM-Instituut voor Atoom- en Molecuulfysica (AMOLF), Kruislaan 407, 1098 SJ Amsterdam, The Netherlands
[5] Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, D-22671 Hamburg, Germany
[6] Institute of Nuclear Physics, Moscow State University, Moscow 119992, Russia
[7] Vienna University of Technology, Gusshausstr. 27, A-1040 Wien, Austria

Atoms exposed to intense light lose one or more electrons and become ions. In strong fields, the process was predicted to occur via tunnelling through the binding potential suppressed by the light field near the peaks of its oscillations. Here we report the first real-time observation of this most elementary step in strong-field interactions: light-induced electron tunnelling. The process is found to deplete atomic bound states in sharp steps lasting several hundred attoseconds.

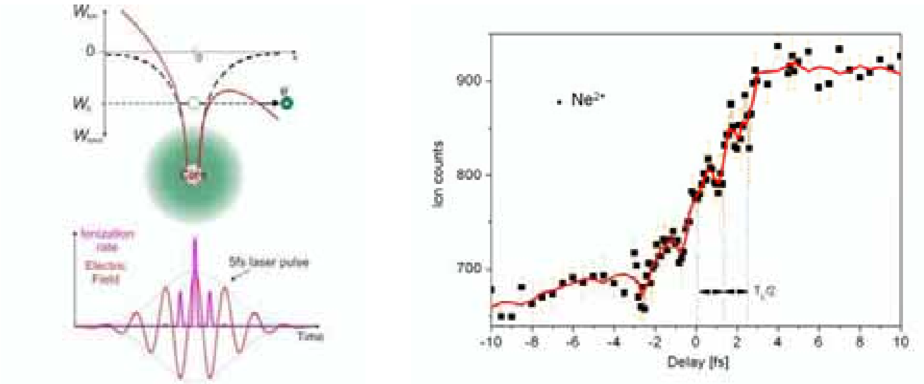

Fig. 1 Under the influence of a strong laser field electrons can escape the binding potential via tunnelling through the coulomb barrier. The ionization rate is therefore modulated with the half period of the driving laser (left panel). The total ion yield shows this modulation as stepwise structure as can be seen clearly in our data(right panel).

The observed sub-femtosecond ionization steps provide a powerful means of probing the transient population of short-lived valence electronic states in excited atoms or molecules, offering direct, time-domain access to a wide range of multi-electron dynamics unfolding on an attosecond to femtosecond time scale. The utility of attosecond tunnelling is demonstrated by capturing multi-electron excitation (shake-up) and relaxation (cascaded Auger decay) processes with sub-femtosecond resolution in proof-of-principle attosecond tunnelling experiments in neon and xenon. Electrons are found to escape from their atomic binding potential within several sub-femtosecond time intervals near the oscillation peaks of the ionizing few-cycle near-infrared laser field. The results of our pump-probe measurements[1] are in good agreement with the predictions of the theory Keldysh[2,3] put forward four decades ago.

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Mo1-2

The route to intense attosecond pulses using high power lasers

R. Hörlein[1,2], Y. Nomura[1], S. Rykovanov[1], M. Geissler[3], P. Tzallas[4],
S. Karsch[1], Zs. Major[1], J. Osterhoff[1], D. Charalambidis[4,5], F. Krausz[1,2], and G. D. Tsakiris[1]

[1]*Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany*
[2]*Department für Physik, Ludwig-Maximilians-Universität München, D-85748, Garching, Germany*
[3]*Department of Physics and Astronomy, Queen´s University, Belfast BT7 1NN, UK*
[4]*Foundation for Research and Technology – Hellas, Institute of Electronic Structure and Laser, GR-71003 Heraklion (Crete), Greece*
[5]*Department of Physics, University of Crete, P.O. Box 2208, GR71003 Heraklion (Crete), Greece*

While the method of attosecond pulse generation from rarefied has been demonstrated and applied in numerous experiments [1,2,3] it is also limited in the number of XUV photons it can generate. This limits the scope of experiments that can be preformed with such sources. The generation of harmonics from solid targets using high power laser systems constitutes an alternate route towards the generation of attosecond pulses in the XUV and SXR range that are expected to be intense enough to perform for example XUV pump-XUV probe experiments. Given the rapid technological advancements in the laser technology, tabletop lasers based on the Optical Parametric Chirped Pulse Amplification (OPCPA) technique delivering several tens of TW power with kHz repetition rate that would be ideally suited for such applications appear to be within our reach[4].

Motivated by these prospects, we have studied the harmonic generation process from solid surfaces both numerically and experimentally. The results of 1D particle-in-cell (PIC) simulations indicate that it is quite feasible that surface harmonics generated at laser intensities of 10^{20} W/cm^2 can produce a train of or even single attosecond pulses in the 20 - 70 eV spectral range with duration of ~80 as and efficiency of a few percent [5]. More elaborate simulations using a 3D-PIC code not only corroborate these findings but also show that the XUV light reflected from the few-cycle-driven relativistic surface posess an excellent spatial coherence [6]. We will also present the results of a series of experiments towards the spectral, spatial and temporal characterization of harmonics generated from solid fused silica targets using the ATLAS 45-fs 25-TW laser system at the MPQ.

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Mo1-3

Towards intense isolated attosecond pulses

P. Tzallas[1], E. Skantzakis[1,2], C. Kalpouzos[1], E. P. Benis[1], A. Bonarou[1], G. D. Tsakiris[3]
and D. Charalambidis[1,2]

[1]*Foundation for Research and Technology - Hellas, Institute of Electronic Structure & Laser, PO Box 1527, GR711 10 Heraklion (Crete), Greece*
[2]*Department of Physics, Univ. of Crete, PO Box 2208, GR71003 Heraklion (Crete), Greece*
[3]*Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany*

Real time studies of several fundamental ultra fast processes, such as electron-electron interactions in all states of matter, require intense XUV radiation pulses with attosecond (asec) pulse duration. Persistent efforts accompanied by sophisticated developments in ultra short pulse engineering have recently led to the breakthrough of the atto-science. Attosecond pulse trains made of XUV frequency combs of properly phased odd harmonic superpositions [1], as well as isolated attosecond pulses, formed by coherent continua emitted during half an optical cycle [2], have been demonstrated in a number of laboratories around the world. While attosecond pulse trains are generated through the interaction of many optical cycle infrared (IR) pulses with noble gas targets, a process that has led to intense XUV emission [3], the generation of isolated attosecond pulses is based, so far, on few cycle IR pulses, leading to limited XUV intensities. Tuneable isolated asec pulse generation has been lately attained exploiting the strong dependence of the harmonic yield on the ellipticity of the driving laser field, using a few cycle driving pulse with modulated ellipticity [4]. However, attosecond scale XUV-pump- XUV-probe type of dynamical studies would substantially benefit from the availability of intense isolated asec pulses that could induce a two-XUV-photon process.

Here we present an alternative experimental approach, permitting the generation of intense isolated attosecond XUV radiation bursts, starting from many cycle IR pulses. Through an interferometrically controlled ellipticity modulation of many cycle IR pulses we can control the dynamics of the electron wavepacket of the non-linearly driven medium, as to revisit only once per laser pulse the parent ion, where by recombining emit a coherent XUV continuum. Using this technique we demonstrate continuum XUV generation induced by 50fs driving pulses. The method opens up excellent perspectives for intense single attosecond pulse generation, as it is applicable for any high peak power many cycle laser system.

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Mo1-4

SPATIOTEMPORAL EFFECTS IN ATTOSECOND PULSE TRAINS METROLOGY

E.P. Benis[1], J. Kruse[1,2], P. Tzallas[1], E. Skantzakis[1,2], G.D.Tsakiris[3] and D. Charalambidis[1,2]

[1]Foundation for Research and Technology – Hellas, Institute of Electronic Structure and Laser, P.O. Box 1527, GR-71110 Heraklion, Greece
[2]Dept. of Physics, Univ. of Crete, PO Box 2208, GR71003 Heraklion, Greece
[3]Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany

The strong dependence of the harmonic phases on the intensity of the driving field requires a detailed modeling including both the harmonics production and their propagation in the gas medium as well [1]. Aside from the establishment of the semi-classical approach as an adequate model for the production of the harmonics [2,3], such studies revealed the conditions for good phase matching, i.e., conditions where the phases of the harmonics are locked resulting in a superposition with ultra short duration. Many researchers, based on experimental findings, adopted a simplified picture of the process, in which the harmonic phases are manifested by the semi-classical model while the good phase matching conditions are met by ruling out one of the two contributing paths for the harmonics production according to the semi-classical model [4].

However, in this simplified picture spatiotemporal effects arising from the strong dependence of the harmonic phases on the intensity of the driving field are often neglected. Utilizing the above simplified picture it has been shown that spatiotemporal effects could play a considerable role in pulse duration measurements resulting in a broadening of the pulse duration [5,6]. This effect would be prominent in methods that use spatiotemporally averaged pulse durations like those based on 2nd order autocorrelation [7,8]. However, in approaches that measure spatiotemporally averaged spectral phases, like those using XUV-IR cross-correlation [4], the same effect would result in an underestimation of the pulse duration.

Here, the importance of spatiotemporal effects in attosecond metrology will be emphasized with certain examples, while preliminary experimental data from our current comparative studies between the two aforementioned measuring approaches will also be shown.

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Mo1-5

SINGLE ATTOSECOND PULSES FROM SURFACE HARMONICS USING POLARIZATION GATING TECHNIQUE

S.G. Rykovanov, M. Geissler, J. Meyer-ter-Vehn,
and G. D. Tsakiris

Max-Planck Institute for Quantum Optics, Hans-Kopfermannstr. 1,
D-85748 Garching, Germany

E-mail: sergey.rykovanov@mpq.mpg.de

Over the last few years there has been a considerable interest in high-order harmonics generation from solid surfaces as it may pave the route towards intense single attosecond x-ray pulses (AXP) [1]. These pulses will be a powerful tool in x-ray spectroscopy, plasma diagnostics etc. To obtain such pulses one needs few-cycle laser radiation with intensity exceeding the relativistic limit $(I_{rel}\lambda(\mu m)^2=1.37\cdot{}^{18}10 W/cm^2)$. However, it appears to be possible to use longer pulses for generation of single AXP. This possibility is based on polarization gating technique and was proposed for surface harmonics in [2]. In this talk we would like to present a more detailed study of polarization gating technique based on 1D and 3D PIC simulations.

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Mo1-6

Full temporal reconstruction of lower order harmonic superpositions

E. Skatzakis[1,2], P. Tzallas[1], , E. Papalazarou[1,2], C. Kalpouzos[1], A. Bonarou[1], E. P. Benis[1],
G. D. Tsakiris[3] and D. Charalambidis,[1,2]

[1]*Foundation for Research and Technology - Hellas, Institute of Electronic Structure & Laser, PO Box 1527, GR711 10 Heraklion (Crete), Greece*
[2] *Department of Physics, Univ. of Crete, PO Box 2208, GR71003 Heraklion (Crete), Greece*
[3]*Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany*

The retrieval of the spectral phase-amplitude distribution in the high frequency spectral domain is the key parameter for the precise reconstruction of radiation pulses with ultra-short duration. For the reconstruction of the temporal profile of a harmonic field E_q or a superposition of harmonic fields $\sum_{q} E_q$, the reference phase can be q-times the phase of a Fourier transform limited (FTL) fundamental laser field, q being the order of each harmonic of the superposition. This reference phase appears in ω_q vs qω interaction schemes, like those utilized in the technique known as phase sensitive coherent control of photoionization products [1]. A cross-correlation approach, based on this principle, i.e., on ω_q vs qω ionization of atoms that allows for the full spectral phase distribution (between the harmonics and within the bandwidth of each harmonic) retrieval of ultra-short harmonic pulses, was proposed recently [2]. A modified “all optical” version in which harmonic generation is measured instead of ionization has been successfully implement in fully characterizing arbitrary temporal waveforms of third harmonic fields [3].

In this work the cross-correlation measurements are performed utilizing a transmission grating interferometer [4]. Examples of phase retrieval and pulse reconstruction are given for lower order harmonics and low order harmonic superpositions of a Ti:Sapph laser, generated in Xe gas. The harmonic spectral amplitude distributions are extracted from their field autocorrelation. The measured pulse durations are found to be in agreement to that expected from lowest order perturbation theory both for un-stretched and chirped pulses. This proof of principle experiment reveals the appropriateness of the method, apart from spatial effects [5], for the full retrieval of spectral phase/amplitude distributions of harmonic superposition and thus for the complete temporal reconstruction of attosecond pulses [6] and pulse trains [7].

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Mo1-7

ATTOSECOND ELECTRON PULSES FROM INTERFERENCE OF ABOVE-THRESHOLD DE BROGLIE WAVES

Sándor Varró and Győző Farkas

Research Institute for Solid State Physics and Optics
H-1525 Budapest, PO Box 49, Hungary
E-mail: varro@sunsev.kfki.hu

It is shown that the above-threshold electron de Broglie waves, generated by an intense laser pulse at a metal surface, are combined to yield attosecond electron pulses. This interference of the de Broglie waves is an analogon of the superposition of high harmonics, usually generated from rare gas atoms, resulting in the appearance of attosecond light pulses, as was first proposed by one of the authors [1]. Our model is based on the Floquet analysis of the inelastic electron scattering on the oscillating double-layer potential generated by the incoming laser field at the metal surface [2]. This model has already been succesfully used to interpret the experimental results on very high order surface photoelecric effect in the near infrared [3] and in the far infrared [4] regime. Owing to the inherent kinematic dispersion, the propagation of attosecond de Broglie waves in vacuum is very different from that of attosecond light pulses. The clean attosecond structure at the immediate vicinity of the matal surface is largely spoiled due to the propagation, but it partially recovers at certain distances from the surface. On the basis of the existence of a plateau in the electron spectrum [5], [6], [7], we conjecture that a similar effect of interference of de Broglie waves may exist in the case of the widely studied above-threshold ionization of atoms.

Acknowledgement

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Mo1-8

Attosecond Ionization Dynamics

P. Johnsson[1,2], J. Mauritsson[1,3], T. Remetter[1], K. J. Schafer[3] and A. L'Huillier[1]

[1] Department of Physics, Lund University, P. O. Box 118, SE-221 00 Lund, Sweden
[2] *Now at:* FOM-Institute AMOLF, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands
[3] Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001, USA

In the interaction between light and matter, the central energy and bandwidth of the radiation, in relation to the energy structure of the studied atoms or molecules, are important parameters. Extreme ultraviolet attosecond pulses, produced through high-order harmonic generation[1,2], have during the last years been increasingly used for such studies, particularly in combination with intense infrared (IR) fields, for time-resolved studies of strong field processes[3-6]. Attosecond experiments have so far utilized pulses with high central energies, in excess of the ionization potentials of the studied species. When these pulses interact with matter they induce single-photon ionization, creating electron wave packets with a significant initial energy.

In the work presented here, we generated attosecond pulse trains in xenon, with individual pulse durations of 370 as. Their central energy was 23 eV, which is above the ionization potential of argon (15.8 eV), but below that of helium (24.6 eV). These pulses were brought to interact with the target gas in the presence of a strong IR laser pulse, and the ion yield was measured as a function of the phase of the IR field at the time of arrival of the pulse. For helium, where the central energy of the pulses is below the ionization threshold, we find a significant enhancement of the ion yield when the IR field is present. In addition, the ion yield exhibits a sub-cycle modulation as a function of the IR phase. Theoretical calculations based on the integration of the time-dependent Schrödinger equation suggest that the observed results originate in the creation of bound electron wave packets by the attosecond pulses, which subsequently ionize.

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Mo1-9

THEORETICAL STUDY OF ATOMIC PHOTOIONIZATION BY ATTOSECOND XUV PULSES IN A STRONG LASER FIELD

A.K. Kazansky[1,2] and N.M. Kabachnik[1,3]

[1] Faculty of Physics, Bielefeld University, Bielefeld, Germany
[2] Fock Institute of Physics, State University of St Petersburg, St Petersburg, Russia
[3] Institute of Nuclear Physics, Moscow State University, Moscow, Russia

A theoretical description of atomic photoionization by attosecond pulses in the presence of the intense laser pulse is suggested. It is based on the numerical solving of a non-stationary Schroedinger equation for an active electron which includes, on equal footing, the realistic atomic potential and the electric fields of both pulses. We also include in our study *polarization* of the atomic states by the IR pulse and caused by it *relaxation* of the one-electron potential. A particular calculations of double differential cross sections (DDCS) (energy and angular distributions of photoelectrons) have been done for photoionization of Ar (3s) electrons by 90 eV and 40 eV XUV 250 as pulses in the presence of 5fs IR pulse of a powerful (10^{13} W/cm^2) laser with a carrier wavelength 800 nm. The parameters of the both pulses have been chosen in accordance with recent attosecond experiments [1,2]. We have suggested also a comparatively simple method of calculation of the DDCS based on the strong field approximation (SFA) [3]. The method involves an expansion of the initial XUV pulse in a sequence of very short pulses ("pulselets") with duration much less than the period of the IR laser. The electrons are ejected by these pulselets coherently and the electron pulse is formed by constructive interference of the electron wave packets emitted by each pulselet. The method provides a convenient possibility of analyzing the ultra-short pulse since it is mathematically sufficiently flexible and computationally fast in order to be used in a fitting procedure. On the other hand it is physically transparent and permits to analyze the contribution of different parts of the pulse taking into account their coherent properties and dephasing introduced by the laser field. The energy spectra and angular distributions of photoelectrons calculated by solving the non-stationary Schroedinger equation are compared with those obtained using the SFA model.. The agreement is excellent for large energy of photoelectrons. When the energy is small and/or the intensity of the IR laser is large, the rescattering of electrons by the ionic core affects the cross section considerably making the SFA inadequate. In this case, the interference fringes associated with the photon absorption by the scattered electron are predicted. The role of the orbital polarization by the strong field and the potential relaxation is shown to increase with the intensity of the IR pulse. Possible generalization of the approach will be discussed.

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Mo1-10

MECHANISMS FOR EFFICIENT PRODUCTION OF SINGLE ATTOSECOND PULSE: BREMSSTRAHLUNG VERSUS RECOMBINATION

M. Yu. Emelin, A. A. Gonoskov, M. Yu. Ryabikin and A. M. Sergeev

Institute of Applied Physics, RAS
46 Ulyanov Street, 603950, Nizhny Novgorod, Russia
e-mail: emelin@ufp.appl.sci-nnov.ru

High-order harmonic generation (HHG) in intense laser-gas interactions provides a very useful method for attosecond pulse production. The generation of light pulses as short as 130 attoseconds [1] (isolated pulse) and 170 attoseconds [2] (pulse train) in the HHG process have been reported recently. Increasing the attosecond pulse energy is of great interest for future applications.

If a rapidly increasing electric field in a few-cycle driving pulse exceeds the critical value, atoms are ionized during a short time within one optical cycle. The free-electron wave packet then moves as a single whole and, upon return to a parent ion, gives rise to a burst of radiation due to the classical bremsstrahlung mechanism. Unlike in the commonly treated high-harmonic regime, in which only a part of the electron wave packet is emitted each half-cycle of the driving field, in the case of quick bound-state depletion high-harmonic radiation is not produced via continuum-bound transitions (recombination leading to cut-off law [3]) but via continuum-continuum transitions (bremsstrahlung). This mechanism is of potential use for a single attosecond pulse production, and, as we have shown recently, an efficiency of this process can be enhanced by orders of magnitude [4] and an attosecond pulse duration can be shorten to $\tau \sim 20$ as [5] if pre-excited atomic states are used.

In this work we discuss the possibilities for increasing the energy of single attosecond pulses. We present the results of three-dimensional numerical simulation of a single attosecond pulse production at atom ionization by intense femtosecond laser pulse. Furthermore, by an example of a free-electron wave packet encountering partly ionized hydrogen atom we study the contribution of above-mentioned mechanisms to the radiation spectrum for different relative amplitudes of bound and free states. On the basis of these calculations we compare bremsstrahlung with recombination radiation as two possible mechanisms for single attosecond pulse generation and show that the first one can lead to significant increasing of the energy of a single attosecond pulse compared with the second one.

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Mo1-11

SUPER INTENSE LASER FIELD ON SURFACE WITH FORMING THE ATTO-SECOND LASER PLASMA AND NEW LASER SPECTROSCOPY OF NUCLEAR ISOMERS

Alexander V. Glushkov

Odessa University, P.O.Box 24a, Odessa-9, 65009, Ukraine-Russia

It is well known that using super short light pulses changes principally a character of interaction of a laser radiation with substance [1]. For laser intensities more than 10^{15} Wt/cm^2 electrons get energy of 100-1000eV and it is realized a process of forming the femto-second laser plasma.(FLP). We consider possibilities of governing by processes, which are taken a place in the FLP in nano-structured porous materials (NSPM; Si). NSPM consist of the separated clusters set with the fractal structure. The key mechanism of the hot electrons generation in plasma is provided by oscillation of electron on the border "plasma-vacuum" or resonant absorption of laser radiation. One may wait for the sharp increasing the hot electrons generation and X-ray radiation. For large laser intensity it is observed a new type of the hydrodynamic ablation with the explosion character. Experimental estimates show that a velocity of the plasma flying of the strongly porous samples Si ($I \sim 3x10^{16}$W/cm^2) is $\sim 10^8$cm·s^{-1}, that is ~ to energy 2±1 MeV [2]. We carried out the modelling of FLP forming in the porous materials on the basis of the energy balance equations, the Greens function method and S-matrix formalism [2]. Special attention is devoted to the modelling the system: NSPM with clusters, on surface of which there is a great number of bonds with H and OH groups. In a case of D-and OD group's one can wait for realization of the cluster explosion process and reaction $D+D \rightarrow \alpha + n$ (3,8MeV). In the high density plasma there is possible an excitation of the low lying isomers (level energy less 20 keV) by means of the channels: photo excitement by own X-ray plasma radiation etc. We carried out some estimates of the stable and long lived nuclei low lying isomers characteristics (energy, decay channels etc.) [3].

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POSTERS

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2. Advanced Radiation and Particle Sources

Mo2-1

A BRIGHT ULTRACOLD ATOMS - BASED ELECTRON SOURCE

G. Taban, M.P. Reijnders, S.B. van der Geer, O.J. Luiten, and E.J.D. Vredenbregt

Department of Applied Physics, Eindhoven University of Technology,
PO Box 513, 5600 MB Eindhoven, The Netherlands

An important application of pulsed electron sources is Ultrafast Electron Diffraction [1]. In this technique, used e.g. in chemistry, biology and condensed matter physics, one can observe processes that take place at the microscopic level with sub-ps resolution. To reach the holy grail of UED, single-shot diffraction images of biologically relevant molecules, electron bunches of 1pC charge, 100fs length and 10nm coherence length are required. Conventional pulsed electron sources cannot fulfil these requirements, but according to the simulations reported in [2] and [3] a new type of source can.

The new source combines the use of magneto-optical atom trapping with fast high voltage technology. We start by cooling and trapping rubidium atoms, followed by ionisation just above threshold, leading to an ultracold plasma. Another possibility is to excite the atoms into a high Rydberg level, from which they spontaneously evolve into an ultracold plasma. Applying a fast high voltage pulse, electron bunches can be extracted. In an initial study [2] it has been shown that this type of source can provide a very high brightness. Depending on the initial particle distribution, the reduced brightness can be in the order of $1\text{x}10^9$ A/(rad^{2}m^{2}V), which is orders of magnitude higher than what established technology such as an electron photogun can provide.

Here we report the first experiments toward realisation of the source. A simple accelerator structure consists of four bars surrounding a MOT, on which an 800V pulsed voltage with a rise time of 1μs is applied. An MCP together with a phosphor screen and a CCD camera are used as detection system. The bunch size obtained from the phosphor screen is fitted with a Gaussian distribution, from which the electron temperature is extracted. For small extracted charges, the electron temperature is found to have an upper limit of 500K, the measurement being limited by stray magnetic fields due to the low electron energy (10eV). We have also extracted a pulsed ion beam by reversing the sign of the accelerating voltage. Since ions are heavier, they obtain higher energy and are less influenced by the magnetic fields. The temperature in this case is found to be <60K, indeed orders of magnitude lower than 50,000K found in conventional sources.

To improve this setup, namely to reduce the stray magnetic fields influence, minimize the influence of the space-charge, and create a cylindrically symmetric electric field, a new fast high voltage switch and a new accelerating structure were developed and installed. They will provide a 30kV pulse in 30ns, which is closer to our goal.

Because the properties of the electron beams depend on the initial properties of the ultracold plasma, in particular its temperature, understanding the plasma dynamics is very valuable. The new setup also allows for fundamental studies of such properties.

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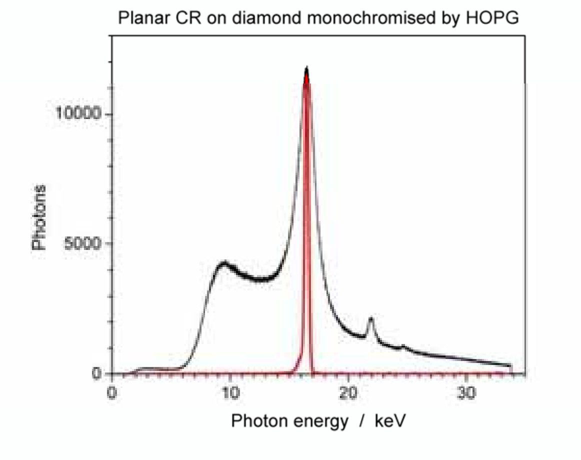
Mo2-2

AN INTENSE CHANNELING RADIATION X-RAY SOURCE

W. Wagner*, B. Azadegan and J. Pawelke

Forschungszentrum Dresden-Rossendorf, Institute of Radiation Physics

Already in the first publications about channeling radiation (CR) [1], it has been declared as a unique quasi-monochromatic photon source. Numerous investigations devoted to the fundamental properties of CR have been carried out up to now at research centers all around the world. New perspectives for the application of CR as a non-conventional intense tunable X-ray source opened with the construction of brilliant superconducting cw electron sources [2].
At the Radiation source ELBE [3], systematic measurements of planar electron CR have been performed on diamond crystals. A water-cooled radiation production target has been constructed. The crystal alignment with respect to the beam axis is performed by means of an inventive remotely controlled goniometer.
Intense CR from 14.6 MeV electrons channeled along the (110) plane of a 150 μm thick diamond crystal has for the first time been produced at average beam currents of up to 100 μA. On-line monitoring the of CR X-rays at primary counting rates of the order of 10^{11} photons per second and per 10% band width was realised by the use of a Compton spectrometer [4]. Applying X-ray diffraction on a HOPG crystal, monochromatisation of CR and bremsstrahlung-background reduction has been investigated [5].



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* Email-address : w.wagner@fzd.de

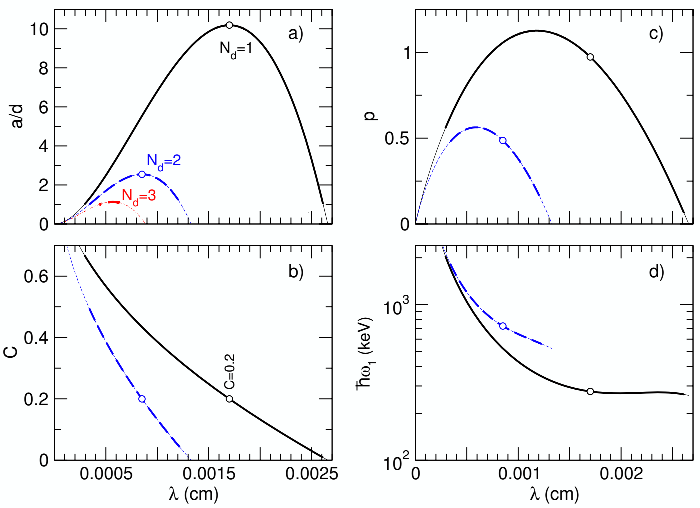
Mo2-3

On the possibility of a crystalline “undulator” for low-energy electrons

A.V. Korol, M. Tabrizi, A.V. Solov’yov, W. Greiner

Frankfurt Institute for Advanced Studies, Johann Wolfgang Göthe-Universität,
Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

The feasibility to generate monochromatic radiation of the undulator type in the gamma region of the spectrum by means of planar channeling of 50 GeV electrons in the periodically bent Si(111) crystal has been recently proven [1] within the framework of the PECU project [2]. In the present work we demonstrate the possibility of a crystalline undulator for low-energy electrons ($E \sim 1$ GeV). We carried out numerical analysis of Si and C electron-based undulator for $E = 855$ MeV and 2 GeV. The figure illustrates the dependences of undulator amplitude a (scaled by interplanar distance d), parameter C, the undulator parameter p and the photon energy on undulator period λ for a 855 MeV electron channeling in a periodically bent C(111) crystal. The curves correspond to different numbers of undulator periods N_d within the dechanneling length (indicated in graph (a)). The results show that such crystalline undulator is feasible for low energy electrons.



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Mo2-4

ULTRASHORT TUNABLE UV PULSES FROM SELF-FOCUSING OF FEW-CYCLE PULSES IN ARGON AND APPLICATION FOR PUMP-PROBE SPECTROSCOPY

W. Fuß, K. Kosma, W.E. Schmid, S.A. Trushin

Max-Planck-Institut für Quantenoptik, D-85741 Garching, Germany

Focusing of 800-nm pulses with various durations (τ = 6-20 fs) and low energy (0.2-1 mJ) into a long (>1 m) cell with atmospheric-pressure argon gives rise to a spectrum with a very broad pedestal. With the shortest pulses it reaches as far as 200 nm and to nearly 2 µm, whereas its width is narrower with 45-fs pulses. With the 45-fs pulses, the spectrum is also broadened by increasing the focal length from 1 to 2 m. Larger spectral widths are also obtained by increasing the pulse energy, but only up to an optimum above which multiple filamentation seems to occur. Lower Ar partial pressure in mixtures with He permits higher optimum energies. The width seems to grow (though not proportionally) with L/τ, where L is the length of the filament. It is discussed what terminates the filaments.

The shortest-wavelength cutoff is found, if the input pulses have no chirp. Whereas with long pulses, much of the short-wavelength radiation is found in the form of conical emission, with the 10-fs pulse the blue and UV wavelengths are concentrated on the axis.

Third-harmonic radiation at 270 nm is detected besides the continuum only if the Ar partial pressure is low; raising this pressure does not much affect the third harmonic but broadens and raises the continuum until it covers also the range of 270 nm. An isolated third harmonic is produced with much better efficiency (0.1-0.2%), if the 10-fs pulses are focused through a short (18 mm) cell (with pinholes) filled with Ar (250 mbar) with He or vacuum outside.

From the supercontinuum we cut out spectral parts (width 9 nm) from 270-320 nm and compressed the pulses by a pair of CaF_2 prisms (which serves both as a monochromator and a compressor) to 30 fs. The pulse durations were determined by cross correlation with the fundamental in an ionization experiment, involving 1 UV + 3-5 IR photons to ionize Xe. The total path length of the UV beam was 2.5 m in air and a few mm in the prisms and a window. The duration is probably limited by third-order dispersion in air and CaF_2. Shorter pulses are expected with a vacuum beam line, and first results with such a setup will be reported.

To demonstrate the applicability as a tunable short-pulse pump source in pump-probe experiments, we used these pulses to study the wavelength-dependent dynamics of $Cr(CO)_6$. As compared with a previous investigation at 270 nm [1], we could resolve faster steps and higher-frequency coherent oscillations in the intact molecule and the dissociation product $Cr(CO)_5$, which helped to assign the detailed path.

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Mo2-5

CRYSTALLINE UNDULATOR BASED GAMMA-LASER: CURRENT SATUS AND PROSPECTS

Andriy Kostyuk[1,2], Andrei Korol[1,3], Andrey Solov'yov[1,4], Walter Greiner[1]

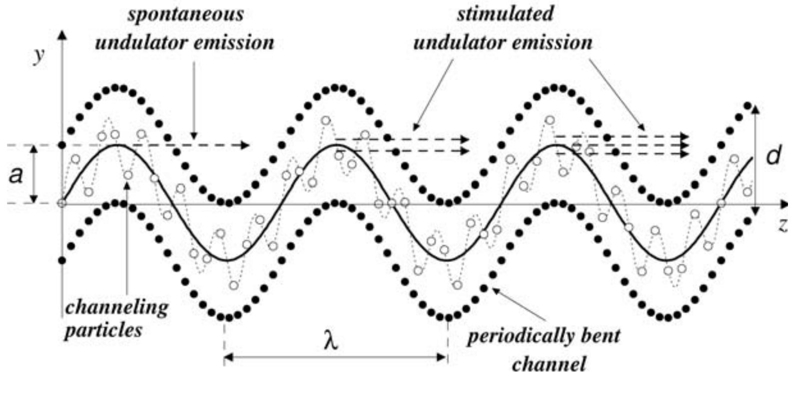
[1] Frankfurt Institute for Advanced Studies, Johann Wolfgang Goethe-Universität,
Frankfurt am Main, Germany
[2] Bogolyubov Institute for Theoretical Physics, Kyiv, Ukraine
[3] St. Petersburg Maritime Technical University, Russia
[4] Ioffe Physical-Technical Institute, St. Petersburg, Russia

The feasibility of gamma-rays generation by means of *spontaneous* emission from ultra-relativistic positrons due to their planar channeling through a periodically bent crystal (crystalline undulator) was demonstrated several years ago (see [1] and references therein). In these papers the possibility of *stimulated* emission within the MeV range (i.e. on the feasibility of crystalline undulator based gamma-laser) was considered within quantum formalism.

However for a high energy ($E > 10^2$ MeV) particle the emission of comparatively low energy photons (i.e., when $\hbar\omega/E \ll 1$) can be treated classically. In the current work we present classical formalism to describe the stimulated emission in a crystalline undulator. We demonstrate that the classical approach also leads to an adequate and somewhat more detailed picture.

The proposed presentation will be concentrated on the details of the description of the *stimulated* gamma-ray emission. In particular, the following points will be addressed:

- the conditions under which the emission stimulation is possible;
- the physical limits on the gamma-laser parameters;
- the estimates of the optimum parameters of the undulator and the beam.



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Mo2-6

LASER-COOLED ION SOURCE

M.P. Reijnders, S.B. van der Geer, G. Taban, O.J. Luiten, P.H.A. Mutsaers,
and E.J.D. Vredenbregt

Eindhoven University of Technology,
P.O. Box 513, 5600 MB Eindhoven, The Netherlands

Focused Ion Beams (FIB) are widely used in the semiconductor industry for milling, sputtering and imaging applications. In particular it is used for quality control of wafers, by using a combination of a FIB and an electron microscope to make cross-sectional inspections of wafers. In addition, FIBs are used for mask repair through gas-assisted etching.

The speed of these processes, as well as the minimum feature size are determined in essence by the quality of the ion source. The current industry standard ion-source is the liquid-metal ion (LMI) source, which allows a smallest focal spot size of several tens of nanometres. The fast developments in the semiconductor industry will require in a few years time ion beam milling capabilities at the 1nm level. A new source is proposed based on creating very cold ion beams by near-threshold photo-ionization of a laser-cooled and trapped atomic gas[1]. Fundamental limits for the reduced brightness and energy spread in terms of neutral particle flux and temperature are investigated, which show that 1 nm focus can be achieved. Experiments are underway.

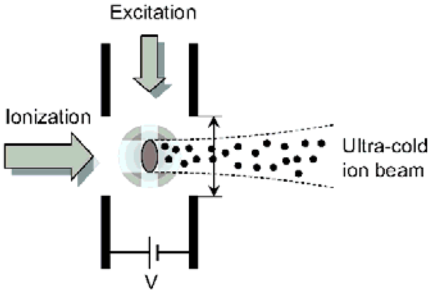

Figure 1: Schematic overview of the proposed setup for the generation of ultra-cold ion beams.

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Mo2-7

Colliding Laser Produced Plasmas as Atomic, Molecular and Cluster Sources: A Progress Report

P. Hough, C. McLoughin, J.P. Mosnier, J. Costello

National Centre for Plasma Science and Technology and School of Physical Sciences, Dublin City University, Glasnevin, Dublin 9, Ireland.

Although a substantial body of atomic, molecular and plasma physics research has been conducted on the single laser produced plasmas, to date, very little work has been done with colliding plasmas despite its genesis in the early 1970s [1]. This often overlooked area of plasma physics has a wide parameter space to be explored and controlled and concomitantly has much to offer by way of potential applications. Our specific interest is to develop this dynamic system as an atomic, molecular and cluster source for materials deposition – a variant on traditional Pulsed Laser Deposition (PLD). We are currently building a new laboratory facility to exploit 'Colliding Plasma PLD' with in-situ optical-spectroscopic and particle diagnostics. The focus of our contribution will be on the design of the system and on the characterisation of plasma diagnostics toolkit for the experiment.

When two plasmas collide there are two extreme scenarios that can play out - the plumes can either interpenetrate or stagnate. The key determinant is the collisionality parameter 'ζ' [2], expressed as the ratio of the experimental scale (D), which is usually taken as the separation between the 'seed' plasmas, to the ion-ion mean free path (λ_{ii}). An experimental setup resulting in a high value for ζ, will favour stagnation layer formation. Since λ_{ii} scales approximately as T_e^2, for a given D, high temperature plasmas will tend to interpenetrate whereas low temperature plasmas tend to stagnate, i.e., the two plumes decelerate rapidly to form a high density, relatively hot layer, the so-called stagnation layer. We aim to 'design' or prepare the initial conditions for each plume individually and develop optimal target configurations which will give us significant scope for engineering exotic chemistry at the stagnation layer. In addition to optical spectroscopy [3], we will add laser interferometry [4] and Thomson scattering [5] to provide reliable methods of determining plasma parameters in the stagnation layer from initiation to expiration. In addition, time of flight mass spectroscopy [6] will enable us to identify and quantify atomic, molecular species in the stagnation layer.

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Mo2-8

LASER-ION SOURCE FOR EXPERIMENTS WITH ROVIBRATIONALLY SELECTED MOLECULAR IONS

N. de Ruette[1], X. Gillon[1], B. Fabre[2], X. Urbain[1]

[1]Département de physique/PAMO, Université catholique de Louvain, chemin du cyclotron 2, B-1348 Louvain-la-Neuve, Belgium
[2]CELIA, Université Bordeaux 1, cours de la Libération 351, F-33405 Talence cedex, France

A laser-ion source has been developed for the production of beams of ro-vibrationally selected molecular ions. The gas is introduced through a thin needle between two electrodes producing an electric field compensating for the strong space-charge repulsion that results from the high ionization degree in the focal volume of a pulsed laser beam. Alternately, a focused electron beam can be produced by a hot filament for DC operation as a conventional electron impact ion source. In both modes, the ions are extracted and formed into a beam of several keV for laser and electron impact experiments.

The selectivity is achieved in H_2 by 3+1 REMPI via the C $^1\Pi_u$ state [1]. The absolute number of ions has been determined by means of a calibrated electron multiplier, and easily exceeds a million per laser shot (3 ns duration, 25 mJ at 300 nm). The rotational lines are barely resolved due to both power broadening and ac-Stark shift of the intermediate levels. The source has been characterized with the help of our dissociative charge exchange apparatus, consisting of a potassium target and a pair of position-sensitive detectors operating in coincidence. The resonant electron capture ensures the vibrational distribution to be preserved in the molecule. When resonant with v=0 and v=1 in the C $^1\Pi_u$ state, the laser pulses produce a large fraction (>95%) of the ions in the same vibrational state. This selection is visible in the kinetic-energy-release spectrum, both as a sharp predissociation peak of the c $^3\Pi_u$ state and the reflection of the vibrational wavefunction of the a $^3\Sigma_g^+$ state by the repulsive b $^3\Sigma_u^+$ potential upon radiative decay.

The vibrational selectivity of the REMPI process appears however to be altered for the upper levels by their large photodissociation probability in the UV range. This effect has been verified by time-of-flight spectroscopy, where protons are seen to dominate over H_2^+ ions when aiming at vibrational states above v=1.

The laser ion source may serve as a beam injector for ion storage rings for vibrationally selected DR and SEC studies [2], and provides a convenient ion source for photodissociation and Coulomb explosion experiments [3].

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Mo2-9

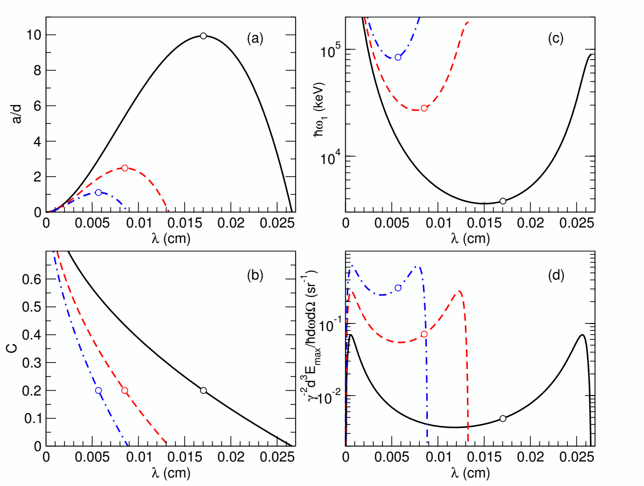
Feasibility of a crystalline undulator for ultra-high-energy electrons

A.V. Korol, M. Tabrizi, A.V. Solov'yov, W. Greiner

Frankfurt Institute for Advanced Studies, Johann Wolfgang Göthe-Universität,
Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

In the present work we prove the feasibility of a crystalline undulator of the novel type based on the effect of a planar channeling of ultra-relativistic electrons ($E \sim 50\,\mathrm{GeV}$) in a periodically bent crystal. It is shown that to overcome the restriction due to the smallness of the dechanneling length, an electron-based crystalline undulator must operate in the regime of higher energies than a positron-based one [1] does. We carried out numerical analysis of Si and C electron-based undulator for $E = 50$ GeV. The figure illustrates the dependences of undulator amplitude a (scaled by interplanar distance d), parameter C [1], the photon energy and the peak intensity on undulator period λ for a 50 GeV electron channeling in a periodically bent Si(111) crystal. In each graph the three curves correspond to different numbers of undulator periods N_d within the dechanneling length: the solid curves stand for $N_d = 5$, the dashed curves - for $N_d = 10$, the chained curves - for $N_d = 15$. For each N_d the open circles indicate the parameters of undulator with $C = 0.2$ (see graph (b)). The results show that such crystalline undulator is feasible.

We acknowledge support from the European Commission (the PECU project [2], Contract No. 4916 (NEST)).



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3. Clusters and Nanoparticles

Mo3-1

SPECTRUM AND DYNAMICS OF A TWO-ELECTRON DOUBLE QUANTUM DOT MOLECULE

R. Nepstad, V. Popsueva and J. P. Hansen

Department of Physics and Technology , University of Bergen.
Allégaten 55, 5007 Bergen, Norway

Coupled quantum dots confined in two dimensional metallic structures and typically containing a few active electrons defines a new scene for “molecular physics on the solid state” [1]. Electron tunnelling from one well to another typically occurs on nanosecond time scales which opens for precise manipulation of electronic states. Two coupled quantum wells containing two active electrons thus define a two-dimensional analogue of the H_2 molecule.

In the present work we have diagonalised the two-electron Hamiltonian of this system based on a one-center basis state expansion [2]. Following the observation that the spectrum of singlet and triplet molecular states group into narrow bands we classify the spectrum. In Figure 1 the one-electron probability density of three electronic states are shown.

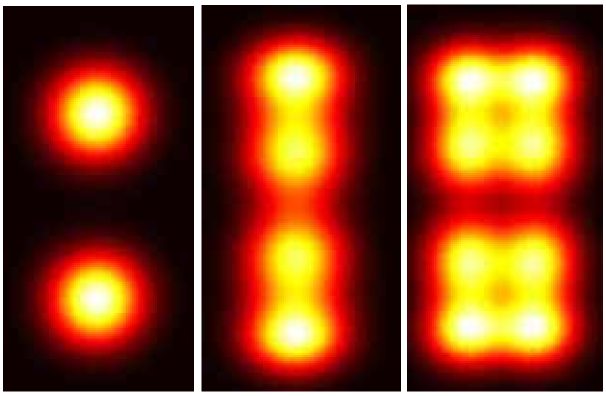

Figure 1: Single electron probability density of the ground state, 10’th and 18’th excited state (from left to right) of a two-electoron double dot with 80nm well separation in the vertical direction.

By solving the time dependent Schrödinger equation we study the response of the system to time dependent electromagnetic fields [3]. The role of the “Overhauser effect”, the singlet-triplet mixing due to interactions with the nuclear spins pertaining to ~10^5 atoms surrounding the quantum dot, is particularly considered.

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Mo3-2

NON-METALLIC BEHAVIOR OF C_{60} ELECTRON SHELL

M. Ya. Amusia[1, 2] and A. S. Baltenkov[3]

[1]Racah Institute of Physics, the Hebrew University, Jerusalem 91904, Israel
[2]Ioffe Physical-Technical Institute, St.-Petersburg 194021, Russia
[3]Arifov Institute of Electronics, Tashkent, 700125, Uzbekistan

The dynamical and static dipole polarizabilities of the C_{60} molecule have been calculated on the basis of the experimental data on the cross section of the fullerene photoabsorption [1]. It has been shown that the fullerene shell in the static electric field behaves most likely as a set of separate carbon atoms, rather than as a conducting sphere [2].

We demonstrate that by studying photoabsorption cross-section of a mesoscopic object one can conclude whether its electron system forms a “conductor” or “dielectric”. Of course, these notions characterize the ability of the object to conduct electricity and are applicable, only to macroscopic bodies. However, for mesoscopic objects that include many atoms, the feature of conductivity can also become meaningful starting from the certain number of constituent atoms. This makes sensible the question whether a mesoscopic system behaves as a conductor, i.e. whether its electrons can move freely under the action of an external electric field.

As a feature that characterizes a conductor we use a quite natural definition that a static external electric field cannot penetrate inside a conducting body. As an object of investigation and as a particular example of the mesoscopic system, in this talk we choose the fullerene C_{60} molecule. We calculate the effective electric field $\mathbf{E}_{eff}(\omega)$ that is at the fullerene center when the external electric field $\mathbf{E}(\omega)$ with frequency ω is applied to C_{60}. The modification of the external field comes from the effect of the dynamic dipole polarizability $\alpha_d(\omega)$ of the fullerene C_{60} that is expressed via its total photoionization cross-section $\sigma(\omega)$. We calculate the frequency dependence of the ratio $\eta(\omega) \equiv \mathbf{E}_{eff}(\omega)/\mathbf{E}(\omega)$ and then investigate whether $\eta(0)$ is equal to zero or not.

The equality of the ratio $\eta(\omega)$ to zero in the static limit $\omega \to 0$ is the critical condition being general for a conducting body with any form. In the case of the fullerene C_{60} this ratio is $\eta(0) \approx 2$, i.e. C_{60} is not a hollow metallic sphere at all.

For the nonzero frequencies of radiation ω the metallic sphere stops to be an ideal screen for the incidental radiation and the alternating electric field penetrates into the conducting sphere. However, as is shown in the talk, the frequency dependence of the ratio of the fields $\eta(\omega)$ at the center of the C_{60} molecule and outside it has nothing to do with $\eta(\omega)$ for the conducting sphere [2], which is additional evidence that the C_{60} shell is strongly non-metallic.

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Mo3-3

Surface Photochemistry from First Principles

Thorsten Klüner

Carl von Ossietzky University Oldenburg, Institute of Pure and Applied Chemistry,
Theoretical Chemistry, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

Photodesorption of small molecules from surfaces is one of the most fundamental processes in surface photochemistry. Despite its apparent simplicity, a microscopic understanding beyond a qualitative picture still poses a true challenge for theory. While the dynamics of nuclear motion can be treated on various levels of sophistication, all approaches suffer from the lack of sufficiently accurate potential energy surfaces, in particular for electronically excited states involved in the desorption scenario.

In the last decade, we have developed a systematic and accurate methodology to reliably calculate accurate ground and excited state potential energy surfaces (PES) for different adsorbate-substrate systems. These potential energy surfaces serve as a prerequisite for subsequent quantum dynamical wave packet calculations, which allow for a direct simulation of experimentally observable quantities such as velocity distributions.

In this contribution, I will focus on recent results obtained for photodesorption of NO and CO from a NiO(100) and a Cr_2O_3(0001) surface, respectively. In contrast to previous studies, we were able to construct highly accurate potential energy surfaces based on correlated quantum chemical calculations (CASPT-2/CCSD(T)). Despite the enormous computational cost, this level of theory turns out to be crucial, since less sophisticated approaches such as density functional theory (DFT) cannot even provide a reliable description of ground state properties, not to mention electronically excited states.

These potential energy surfaces were used in subsequent wave packet studies which reveal new desorption mechanisms. In the NO/NiO(100) case, we observed an *anti-Antoniewicz* scenario in which the wave packet is initially repelled from the surface but eventually reaches a turning point before it is back-scattered from the surface. State resolved desorption velocity distribution have been calculated, and the results are in good agreement with experimental findings [1]. In the CO/NiO(100) system, we observe the formation of a genuine covalent bond upon photoexcitation for the first time. As demonstrated in the current study, this chemical bond formation is the crucial step in the desorption mechanism for this system [2]. Again, our results are in good agreement with recent experiments. Furthermore, recent results on the rotational alignment of desorbing CO molecules from a Cr_2O_3(0001) surface and state resolved lateral and desorption velocity distributions are presented and compared with experiment [3,4].

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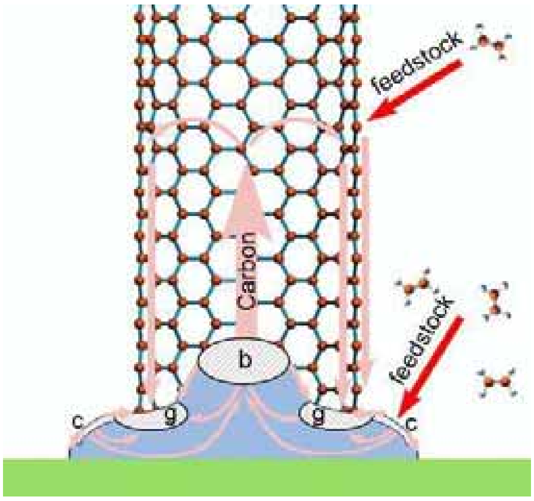
Mo3-4

KINETIC MODEL FOR NANOTUBES GROWTH

O. I. Obolensky, I. A. Solov’yov, A. V. Solov’yov, W. Greiner

A.F. Ioffe Physical Technical Institute, 194021 St. Petersburg, Russia
Frankfurt Institute for Advanced Studies, 60438 Frankfurt am Main, Germany

Size selected nanoclusters of such metals as Ni, Fe, Co are widely used as catalysts in the chemical vapor deposition (CVD) techniques of production of carbon nanotubes [1]. The characteristics of the nanotubes as well as the parameters of their growth are closely related to the size and properties of the catalytic particles [1]. Despite of intensive studies the physical mechanism responsible for the catalytic action of the nanoclusters leading to the nanotubes growth is not yet known.



We have developed a kinetic model describing the process of catalytically assisted growth of carbon nanotubes. The model describes the flow of carbon atoms starting from the catalytic decomposition of the feedstock molecules at the surface of the nanocluster and ending at their embedding into the nanotube. In the figure we show a cross section of the nanocluster and the nanotube with the schematic representation of the carbon flows which are accounted for by the model.

Feedstock molecules are decomposed on the catalytically active part of the nanocluster surface, which is exposed to the environment and not screened by any additional inactive layers (region “c”). The carbon atoms from this region diffuse (either along the surface or through the bulk of the cluster) into the other parts of the cluster. We single out the growth region from which the atoms embed themselves into the nanotube walls (region “g”) and the near-surface region inside the nanotube (region “b”). From the region “b” carbon atoms can reach the growth region by surface or bulk diffusion or they can evaporate. Some of the evaporated atoms are deposited on the nanotube walls and reach the growth region by surface diffusion. We also account for the possibility of decomposition of the feedstock molecules directly by the nanotube walls.

Thus, we present a model comprehensively describing the kinetics of the nanotube growth. The model allows one to predict with a reasonable accuracy the distribution of carbon within the catalytic nanoparticle, the relative importance of various growth mechanisms, the nanotube growth rate, etc. However, the results are rather sensitive to the input parameters (e.g., diffusion coefficients, activation energies for embedding into the nanotube) which are to be obtained from accurate quantum mechanical calculations or experiments.

We acknowledge partial financial support from INTAS (contract 03-51-6170) and from European Commission (project EXCELL).

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AB INITIO POTENTIAL SURFACE AND VIBRATIONAL PREDISSOCIATION DYNAMICS OF HeI_2(B) CLUSTER

R. Prosmiti, A. Valdés, P. Villarreal, G. Delgado-Barrio

Instituto de Matemáticas y Física Fundamental, C.S.I.C.,
Serrano 123, 28006 Madrid, Spain

We report here *ab initio* calculations on the $B(^3\Pi)$ excited state of the HeI_2 complex [1]. The lowest triplet $^3A'$ and $^3A''$ states are calculated at the UCCSD(T) level of theory, employing large-core relativistic peudopotentials for the iodine atoms. Spin-orbit coupling effects are not included and the three-dimensional potential energy surface for HeI_2(B) is represented in terms of the average of the $^3A'$ and $^3A''$ adiabats. The UCCSD(T) surface presents a global minimum at the T-shaped configuration, and a secondary one at linear configurations for elongated r bond distances.

Spin-free bound state calculations for $J=0$ are carried out for the above surface. The binding energy, and vibrationally averaged structure are determined and compared with the experimental measurements by Levy and coworkers [2], as well as recent experiments by Loomis's group [3].

To our knowledge, this is the first *ab initio* study on the B excited state of HeI_2. For HeI_2(B) complex more experimental data are available from vibrational predissociation dynamics experiments [2,3,4] for low and high υ excitations. Therefore, for a global evaluation of the present *ab initio* PES, further theoretical dynamics simulations are carried out [5]. Spectral blueshifts and vibrational predissociation lifetimes are computed and their comparison with the experimental data is discussed.

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Mo3-6

CLUSTER ORIGIN OF TRANSFER OF NANOTUBES

Francisco Torrens and Gloria Castellano

Institut Universitari de Ciència Molecular, Universitat de València, Edifici d'Instituts
de Paterna, P. O. Box 22085, 46071 València, Spain

It is discussed the existence of single-wall carbon nanotubes (SWNTs) in organic solvents in the form of clusters. A theory is developed based on a *bundlet* model, which enables describing the cluster-size distribution function. Comparison of calculated solubilities with experiments would permit obtaining energetic parameters characterizing the interaction of an SWNT with its surrounding. Fullerenes and SWNTs are objects whose behaviour in many physical situations is characterized by peculiarities, which show up in that these systems represent the only soluble forms of carbon, what is related to their molecular structures. The fullerene molecule is a virtually uniform closed spherical–spheroidal surface, and an SWNT is a smooth cylindrical unit. Both structures give rise to weak interactions between the neighbouring units in a crystal and promote their interaction with solvent molecules. Another peculiarity is related to their trend to form clusters consisting of a number of fullerene molecules or SWNTs. The phenomena have a unified explanation in the bundlet model, in which the free energy of an SWNT in a cluster is combined from two components, *viz*. a volume one proportional to the number of molecules n in a cluster, and a surface one, proportional to $n^{1/2}$ (Fig. 1a). The *membranous character* of growth process in clusters allows explaining the dispersion of data. Growth mechanisms of fractal clusters in fullerene solutions are analyzed along with similarity laws determining the thermodynamic characteristics of fullerite crystals (Fig. 1b). We thank Universitat de València–Mediscovery.

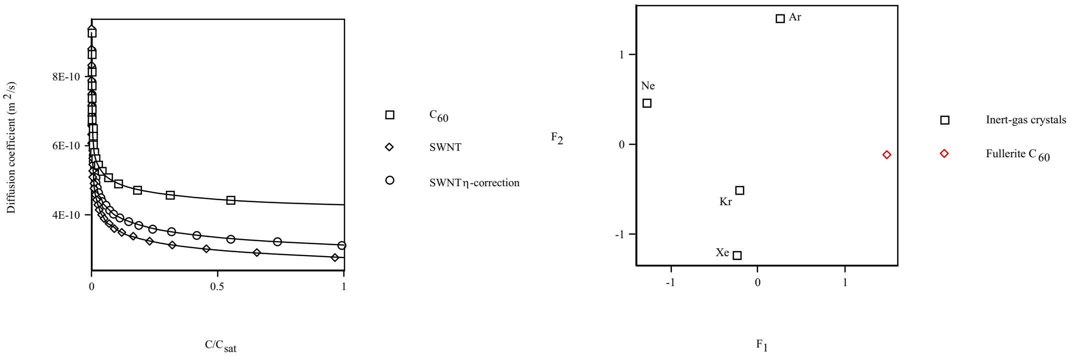

Fig. 1. (a) Concentration dependence of the diffusion coefficient of C_{60}/SWNT at $T = 298.15$K. (b) Hierarchical PCA F_2–F_1 plot for properties of inert-gas/C_{60} crystals.

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MULTIPLY CHARGED NEON CLUSTER IONS: CRITICAL SIZE AND COULOMB EXPLOSION

I. Mähr[1], F. Zappa[1], S. Denifl[1], D. Kubala[2], O. Echt[3], T. D. Märk[1,2] and P. Scheier[1]

1. *Institut für Ionenphysik und Angewandte Physik, Leopold Franzens Universität Innsbruck, Technikerstr. 25, A-6020 Innsbruck, Austria.*
2. *Department of Experimental Physics, Comenius University, SK-84248 Bratislava, Slovak Republic*
3. *Department of Physics, Univers. of New Hampshire, Durham, NH 03824, USA*

Multiply charged neon cluster ions are formed upon electron impact ionization of large neutral clusters and analyzed utilizing a two sector field mass spectrometer applying techniques developed recently [1,2,3].
The critical size for doubly charged neon cluster ions is determined experimentally with isotopically pure ^{20}Ne to be 287. In spectra of natural neon, the presence of doubly charged clusters can be observed as an increase of the ion yield at the same cluster size confirming the above result. This method allows in addition an approximate determination of the critical sizes for triply charged cluster ions. Utilizing a beam deflection method [4] it is possible to observe (for the first time) directly the asymmetric fission of multiply charged neon clusters right after the ionization event. The most abundant low mass fragment ion from this reaction process is the dimer ion. The yield of larger fragment ions decreases exponentially with the fragment size. The kinetic energy of the emitted low mass fragment ions is of the order of 200 meV which is surprisingly low when comparing the results with a simple point charge model taking into account the critical cluster sizes presently determined.

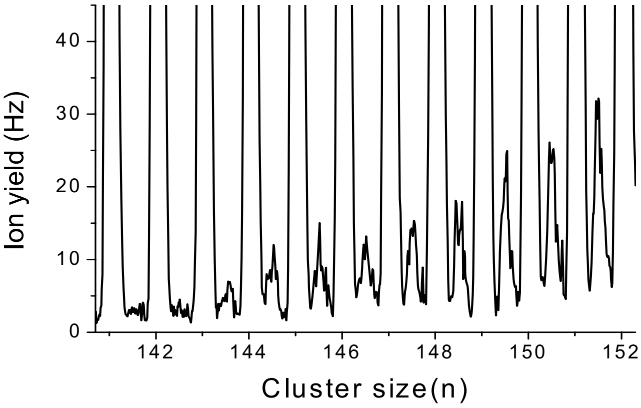

Fig. 1 Part of a mass spectrum for a Ne_n cluster beam consisting of isotopically pure ^{20}Ne.

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Mo3-8

ELECTRON SPIN RELAXATION IN ALKALI SAMPLES ON THE SURFACE OF HELIUM NANODROPLETS

Johann Nagl, Gerald Auböck, Carlo Callegari, and Wolfgang E. Ernst

Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria
Email: wolfgang.ernst@tugraz.at

Helium nanodroplets formed in a supersonic expansion of high pressure gas from a low temperature source (10 to 20K) represent finite size superfluid samples with 0.4 K internal temperature. Using a helium backing pressure around 100 bar, nanodroplets of average size $N=10^4$ atoms are generated. In a molecular beam apparatus, the droplets pass through a pick-up cell containing a gas at low pressure, where each droplet is doped with a statistical number of atoms or molecules. Most degrees of freedom of these dopants are immediately cooled to 0.4 K, and the released energy leads to evaporation of a corresponding number of helium atoms from the droplet. The cold environment can be used to cool individual molecules for a spectroscopic study of their lowest energy configuration, to produce weakly bound molecular complexes, or study cold collisions between different dopant species residing in the same droplet. In the analysis of condensed matter samples, electron spin resonance is a common experimental technique. ESR spectroscopy could become a versatile tool to investigate oligomers formed on He droplets after an examination of spin lifetimes and the development of a detection method for spin states. This paper reports the first magnetic study of any species in or on helium droplets as well as approximate relaxation times for electron spin states of potassium atoms and molecules on helium droplets.

Alkali atoms were one of the first chromophores ever attached to a helium droplet, and are unique in that they do not become solvated inside the droplet, but instead remain in a dimple on its surface. Further, because of the smaller binding energy released into the droplet, it is the high spin complexes (triplet dimers, quartet trimers) which preferentially survive the formation process [1]. We now investigated their electronic spin in the low-symmetry environment offered by the surface of a droplet. In a first step, we have measured magnetic dichroism spectra of potassium atoms residing on the surface of He nanodroplets 1) to estimate the spin-relaxation time; 2) to demonstrate that a spin-polarized sample can be easily created and that optical detection is a viable technique for ESR in He droplets. Laser induced fluorescence was used to probe the K 4p←4s atomic transition and the $1^3\Pi_g \leftarrow 1^3\Sigma_u$ band of K_2. A magnetic field of 2.9 kG was applied and the laser beam polarization continuously varied with a Pockels cell from σ^- through π to σ^+. By measuring the circular dichroism, the populations of Zeeman sublevels were probed. No dichroism was observed for the atomic potassium sample on helium droplets, indicating that the sublevels have not thermalized and putting a lower limit to the spin relaxation time of 1.9 ms [2], based on the geometrical conditions in the molecular beam apparatus.

Dichroism spectra of K_2 molecules on helium droplets showed a different behavior. Their analysis yields a population of Zeeman sublevels close to thermal equilibrium with the helium droplet. Geometric considerations put an upper limit of ~40 μs to the spin relaxation time in this case [2].

Further to the exploration of spin lifetimes whose different values will have to be explained on the basis of the interaction of the alkali atoms and molecules with the helium environment, the optical saturation of the spectra was measured and will be used for the preparation of spin polarized samples on cold droplets.

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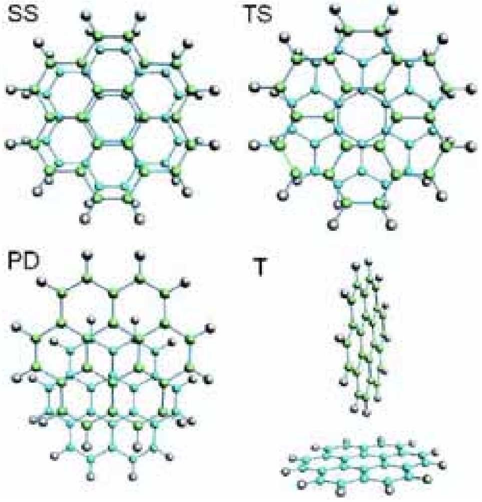
Mo3-9

STRUCTURE OF CORONENE CLUSTERS

O. I. Obolensky, A. V. Solov'yov, W. Greiner

A.F. Ioffe Physical Technical Institute, 194021 St. Petersburg, Russia
Frankfurt Institute for Advanced Studies, 60438 Frankfurt am Main, Germany

Clusters of polycyclic aromatic hydrocarbons (PAH) and their ions are believed to be one of the most probable species in the interstellar space responsible for converting the UV radiation of the stars into the intensive IR radiation, known as unidentified infrared bands [1,2]. The current knowledge of structure and properties of PAH clusters is very limited. Laboratory studies have just started to appear while reliability of the theoretical results is limited due to the subtle interplay between the van der Waals polarization forces and the electrostatic interaction [3].



We have recently performed density functional theory (DFT) calculations of energies for four plausible configurations of dimer of coronene ($C_{24}H_{12}$) [3] (shown on the left). The stack configurations (superimposed stack (SS), twisted stack (TS) and parallel-displaced (PD) stack) are favoured by the van der Waals forces while the T-shaped configuration is favoured by the electrostatic interaction. In order to get a better description of the van der Waals interaction, the DFT results were corrected by a phenomenological London-type $1/r^6$ term. Depending on the magnitude of this term, both the T-shaped and the PD stack configurations can be the global minimum configuration of the system. It is quite surprising that the T-shaped configuration is energetically competitive for such a large system for which a graphite-like stacked structure had been *a priori* expected. On the basis of the DFT calculations we developed a model in which each coronene molecule is represented by a set of four charged rings [3]. Adjusting the parameters of these rings both the T-shaped and the stack configurations can be made energetically preferable configurations.

We found the global energy minimum structures of the coronene clusters in the situation when the electrostatic interaction dominates and in the situation when the van der Waals forces prevail (also studied previously [4]). Rotational constants and the normal modes in the obtained sets of structures are distinctively different making possible to distinguish experimentally between the two situations.

We acknowledge partial financial support from INTAS (contract 03-51-6170) and from European Commission (project EXCELL).

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Mo3-10

Radiative Cooling of Al_4^-

Y. Toker, O. Aviv, M. Eritt, M.L. Rappaport, O. Heber, D. Schwalm, D. Zajfman
Weizmann Institute of Science
PO Box 26
Rehovot 76100
Israel

The radiative cooling of small metal clusters, Al_4^-, has been measured using delayed electron emission as a temperature probe. Delayed electron emission is a process in which cluster after being irradiated by a laser, emit an electron not in coincidence with the laser but hundreds of microseconds later. By measuring the rate at which the electrons are emitted the temperature of the clusters prior to irradiation can be deduced, and studied as it varies with time. It is found that Al_4^- radiative cooling rate is very similar to the rate of black body radiation, and is proportional to the temperature to the power of 3.5+/- 0.2.

Contact Information :
Email : jtoker@weizmann.ac.il
Telphone : 972-8-9343373
Address :
Yoni Toker
Department of Particle Physics
Weizmann Institute of Science
PO Box 26
Rehovot 76100
Israel

Mo3-11

INTERPLAY OF ELECTRONIC AND GEOMETRY SHELL CLOSURES FOR NEUTRAL AND CHARGED Sr CLUSTERS

Andrey Lyalin, Ilia Solov’yov , Andrey Solov’yov, and Walter Greiner

Frankfurt Institute for Advanced Studies,
Max von Laue Str. 1, D-60438 Frankfurt am Main, Germany

The optimized structure and electronic properties of neutral, singly and doubly charged strontium clusters have been investigated using *ab initio* theoretical methods based on density-functional theory. We have systematically calculated the optimized geometries of those clusters consisting of up to 14 atoms, their average bonding distances, electronic shell closures, binding energies per atom, dissociation energies and the gap between the highest occupied and the lowest unoccupied molecular orbitals [1]. It is demonstrated that the size-evolution of structural and electronic properties of strontium clusters is governed by an interplay of the electronic and geometry shell closures. It is shown that the excessive charge affects the optimized geometry of strontium clusters. Ionization of small strontium clusters results in the alteration of the magic numbers. Stability of positively charged strontium clusters towards fission is analysed [1,2]. The obtained results are compared with the available experimental and theoretical data.

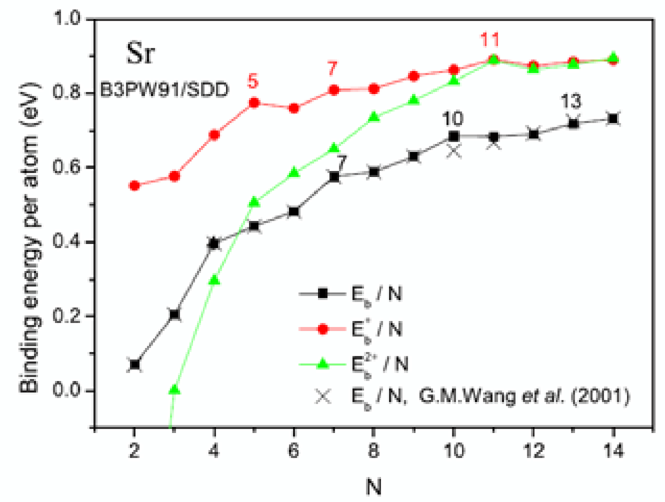

Figure 1: Binding energy per atom for the most stable neutral (filled squares), singly charged (filled circles) and doubly charged (filled triangles) Sr clusters.

This work is partially supported by the European Commission within the Network of Excellence project EXCELL, and by INTAS under the Grant No. 03-51-6170.

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Mo3-12

MAGNETIC PROPERTIES OF La CLUSTERS

Andrey Lyalin, Andrey Solov'yov, and Walter Greiner

Frankfurt Institute for Advanced Studies,
Max von Laue Str. 1, D-60438 Frankfurt am Main, Germany

We have performed a systematic theoretical investigation of optimized ionic structure, electronic and magnetic properties of La clusters within the size range N < 14 [1]. We found a giant enhancement of magnetism in La_4, La_6, and La_{13} clusters. We also found that the ground states of La_2, La_3, La_5, La_7, La_9-La_{11}, and La_{14} clusters possess nonzero magnetic moments, that ranged from 0.1 μ_B to1.0 μ_B per atom. This clearly indicates that small La clusters display magnetic behavior, even though bulk La has no magnetic ordering. We show that magnetism in La clusters is governed by unpaired valence electrons, in contrast to the local-moment magnetism in clusters of heavy rare-earth elements. In addition to the ground state isomers of La clusters we found an ensemble of energetically low-lying spin isomers. We predict an increase of the average magnetic moments for ensembles of La_2, La_3, La_5, La_8, La_9, La_{11}, La_{12}, and La_{14} clusters with temperature due to the thermal population of the spin isomers. For ensembles of La_4, La_7, and La_{13} clusters, the average magnetic moment decreases with temperature. Such an anomalous behavior of the magnetic moment with temperature can be detected in Stern-Gerlach deflection experiments.

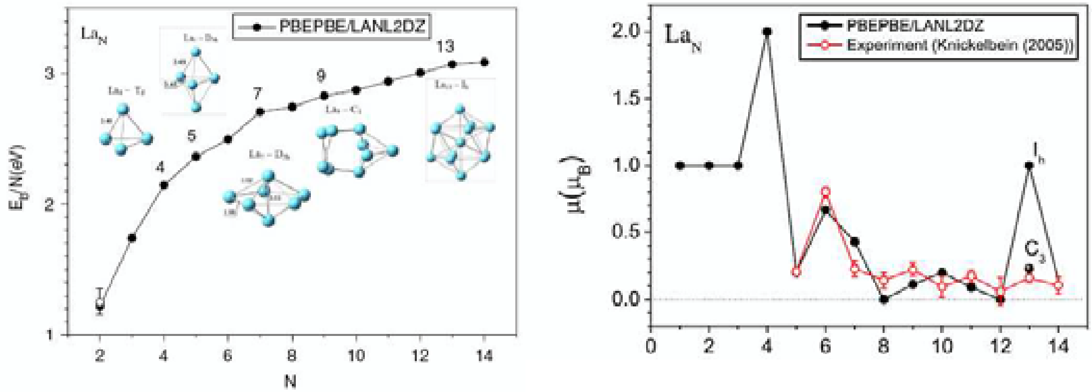

Figure 1. Binding energy per atom for the most stable La clusters (left); magnetic moments per atom for La clusters as a function of cluster size. Open circles present the results of experiment by Knickelbein [2] (right).

This work is partially supported by the European Commission within the Network of Excellence project EXCELL, and by INTAS under the Grant No. 03-51-6170.

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Mo3-13

ATOM DECAY WITHIN CLUSTERS OF DIELECTRIC AND METALLIC NANOPARTICLES

V. Yannopapas[1,2] and N. V. Vitanov[2,3]

[1]Department of Materials Science, University of Patras, Rio, 26504, Greece
[2]Department of Physics, Sofia University, James Bourchier 5 blvd., 1164 Sofia, Bulgaria
[3]Institute of Solid State Physics, Bulgarian Academy of Sciences,
Tsarigradsko chaussée 72, 1784 Sofia, Bulgaria

A Green's tensor formalism of the electromagnetic field for a single scatterer as well for a cluster of finite number of scatterers is presented. The formalism, based on the multiple-scattering theory for classical waves, provides a means to calculate the number of states, the density of states, as well as the local density of states (LDOS) of the electromagnetic field. The last quantity determines the spontaneous emission (SE) rate of atoms embedded within a cluster of spherical bodies. We present calculations of the LDOS for a finite planar photonic-crystal slab of titania spheres in air. We focus on calculations of the SE rate for a two-level atom placed near a metallic Drude-type nanosphere as well as within clusters of nanospheres. We examine the convergence of the above quantities in terms of the angular expansion of the electromagnetic field. The frequency and spatial dependence of the local density of states and of the corresponding spontaneous emission rate is also studied by depicting the relevant spectra for different cluster sizes and configurations. We have found, in particular, that, within the frequency region of the surface-plasmon resonances, the spontaneous emission rate is influenced by the near field of the spheres which are closer to the atom rendering the contribution of farthest spheres almost negligible. Depending on the distance from the surface of the sphere(s) the spontaneous emission rate in the cluster assumes values which can be several orders of magnitude larger than the corresponding rate in vacuum. Finally, we examine the differences which arise when an experimentally available dielectric function is employed, instead of the Drude type.

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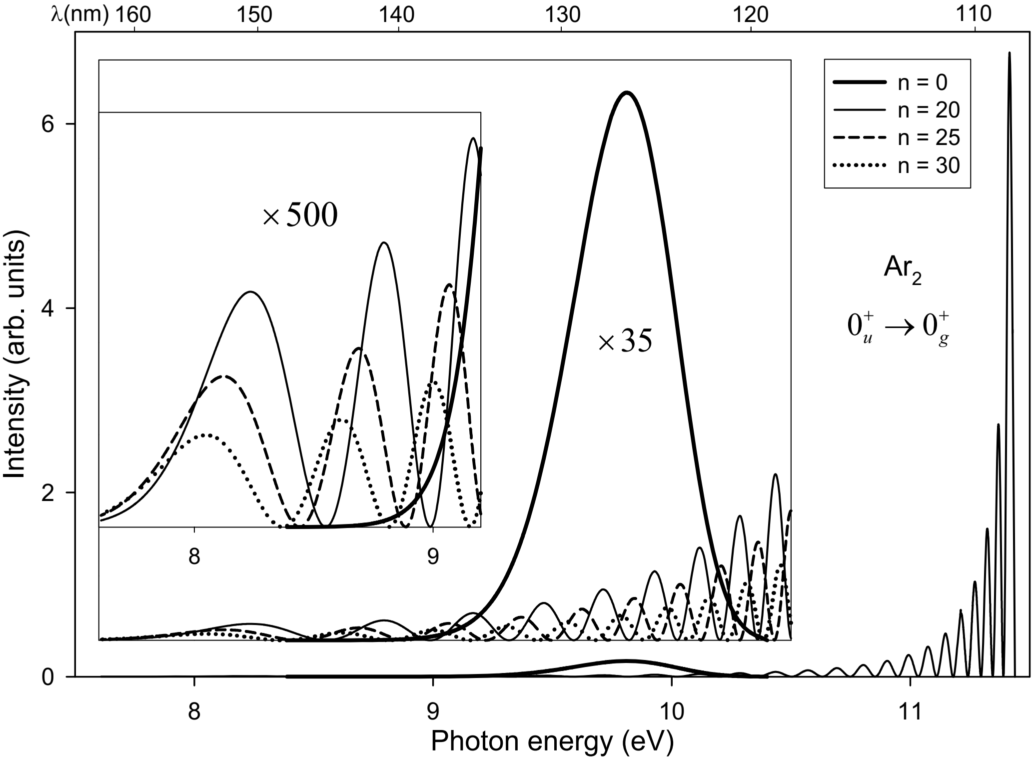
Mo3-14

THEORETICAL STUDIES OF RARE GAS EXCIMERS

Matti Selg

Institute of Physics of the University of Tartu, Riia 142, 51014 Tartu, Estonia

Diatomic rare gas (RG) molecules are unstable in their ground electronic state, but one can create strongly bound excited molecules (excimers) in these media. Radiative decay of the excimers results in two intense continua, which may be considered the most important spectroscopic features of RGs. As is generally accepted, the so-called first continuum stems from higher vibrational levels, while the second continuum corresponds to vibrationally relaxed excimers. A uniform theoretical treatment of RG emission continua has been recently given [1, 2], and successfully applied to Xe_2^*. In this report the same approach is used for Ar_2^*.



The figure shows Franck-Condon factors for the selected vibrational levels. Using the above model [1], one can ascertain statistical weights of the levels, and then calculate the overall time-dependent emission spectrum. The results are in good agreement with experimental data, including the weak oscillatory spectrum from the excimers' left turning point (LTP) region (see the inset). However, the peak-like feature with sharp maximum at 155 nm, observed in Ar under particle beam excitation, cannot be associated with the LTP region of Ar_2^*. Instead, another interpretation is proposed, which assigns this feature to $^1\Sigma_u^+ \to {}^1\Sigma_g^+$ transition in double ionized excimer Ar_2^{++}.

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Mo3-15

Resonances in Transition Metal Complexes by TDDFT calculations

P. Decleva, G. Fronzoni and M. Stener

Universita' di Trieste
Dipartimento di Scienze Chimiche,Via Giorgieri, 1
I-34127 Trieste, Italy

Time Dependent Density Functional Theory (TDDFT) has been shown to be a powerful and accurate description of photoionization processes, including interchannel coupling, in small systems [1,2]. A new direct algorithm for the solution of the equations in complex molecules has been presented [3], which eliminates convergence problems which hinder application of the classical SCF approach to large systems, and a parallel implementation is being developed. Applications to the description of resonances, both shape and autoionization, in organometallic systems [4] will be presented, together with a discussion of chemical effects on the position and strength of the resonances.

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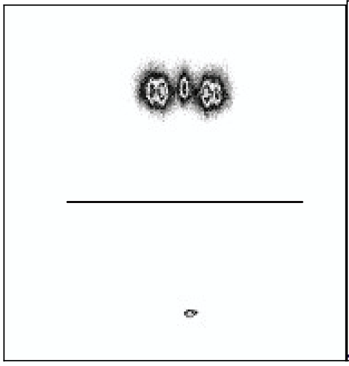
Mo3-16

Diffraction of keV atoms and molecules on surfaces

Roncin P, Khemliche H, Rousseau P and Borisov AG.

Laboratoire des Collisions Atomiques et Moléculaires,
LCAM UMR 8625, CNRS Université Paris-Sud, 91405, Orsay France

Diffraction of cold and ultra cold atoms on surface is known for long [1,2] but it is only this year that diffraction of keV atoms has been simultaneously reported [3,4] on surfaces. A simple way to interpret this grazing diffraction is to consider that the projectile movement can be separated into a fast component parallel to the surface and a slow one, normal to the surface. The fast oscillations of the projectile surface potential in the projectile frame tend to have zero net integral contribution [4,5] so that only the potential averaged (along the direction of the fast movement) affects the trajectory. The surface then appears as made of parallel furrows. The long wavelength $\lambda_\perp$ (on the Å scale) associated to the slow motion normal to the surface diffracts on these furrows. Following this model, the "Hard Wall" model, which showed successful to interpret thermal helium scattering, may be used to calculate the diffracted intensities. For He colliding on LiF(100) and NaCl(100) a simple sine potential is enough to well represent the diffraction pattern. Taking $Z(y)=h.\sin(2\pi y/d)$ with y perpendicular to the furrows, d the spacing between furrows and h the corrugation. The intensities of the various diffraction orders is simply given by the square of the associated Bessel function. $I_n=J_n(4\pi h/\lambda_\perp)^2$. The figure 1a display the 2D diffraction pattern while the figure 1b shown the fit with a common line shape and a corrugation parameter h=0.393. The accuracy both on the lattice parameter and the corrugation is estimated in the 10^{-3} range. Note that the normal energy is closed to one eV, much larger than that used in thermal helium scattering. This allows getting much closer to the surface. New results on semi conductors will be presented.



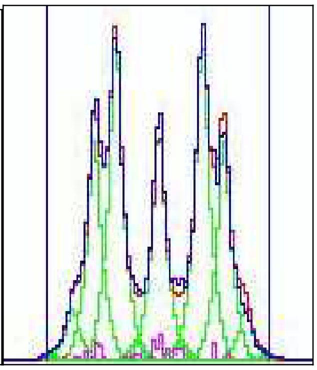


Figure 1a (left): Image of the 2D scattering profile of 2 keV He atoms colliding at 1 deg. on a LiF single crystal oriented along a (100) channelling direction. The horizontal line is a projection of the surface plane

Figure 1b. (right) A horizontal slice of the 2D intensity is fitted by a Bessel function (see text)

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GUIDED TRANSMISSION OF LOW ENERGY ELECTRONS BY HIGHLY ORDERED Al_2O_3 NANOCAPILLARIES

A. R. Milosavljević[1], Gy. Vikor[1], Z. D. Pešić[1a], S. Mátéfi-Tempfli[2],
M. Mátéfi-Tempfli[2], L. Piraux[2], P. Kolarž[1], D. Šević[1], and B. P. Marinković[1]

[1] Institute of Physics, Pregrevica 118, 11080 Belgrade, Serbia
[2] Unité de Physico-Chimie et de Physique des Matériaux, Université Catholique de Louvain, Place Croix du Sud, 1, B-1348 Louvain-la-Neuve, Belgium

Since the first reported results by Stolterfoht *et al.* [1], the guided transmission of charged particles through insulating nanocapillaries has attracted considerable attention. The capillary guiding has potential for investigation of interaction of charged particles with the insulators, characterizing of the inner walls of nanocapillaries and for possible applications (e.g. manipulation of the charged particles on the nanoscale) [2]. Therefore, a number of both experimental and theoretical results have been published on this topic in the last two-three years, mostly focused to highly charged ions (HCIs) as projectiles [3-5] (and references therein). Still, a full understanding of complex processes involved in guiding effect has not been achieved. In particular, the characteristics of *electron guiding* are considered to be unknown at the present.

We present an experimental investigation of guiding of low-energy electrons (200-350 eV) by insulating nanocapillaries [6]. The nanochannels array was prepared using self-ordering phenomena during a two-step anodization process of a high purity aluminium foil. The experimental results clearly show the existence of the guiding effect, as found for HCIs. The guiding of the electron beam was observed for the tilt angles up to 12°. As seen for HCIs, the guiding efficiency increases with decreasing the incident electron energy. The transmission efficiency appeared to be significantly lower than observed for HCIs and, moreover, the intensity of transmitted electrons significantly decreases with decreasing the incident energy.

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[a] Present address: Physics Department, Western Michigan University, Kalamazoo, MI, 49008, USA and Advanced Light Source, LBNL, Berkeley, CA, 94720, USA

Mo3-18

ELECTRONIC STRUCTURE AND STABILITY OF C_{70}^{q+} (q=0-14)

H. Zettergren, G. Sánchez, S. Díaz-Tendero, M. Alcamí and F. Martín

Dep. de Química, C-9, Universidad Autónoma de Madrid, 28049-Madrid, Spain

We have evaluated the ionization potentials and dissociation energies of multiply charged C_{70} fullerenes at the B3LYP/3-21G* and B3LYP/6-31G* level of theory, complementing a recent study of multiply charged C_{60} [1,2]. As there are more possibilities to extract a C_2-unit from a C_{70} than from a C_{60} fullerene [3], fifteen C_{68} isomers have been included in the present study. Eleven corresponded to all the classical fullerene structures (only pentagonal and hexagonal faces) with a minimum number of adjacent pentagons (2 pairs). The remaining four corresponded to non classical structures (with one heptagonal face) originating from the four distinct possibilities to extract a C_2 from the most stable C_{70} isomer (with D_{5h} symmetry). The relative stabilities between the C_{68} isomers were found to change dramatically as functions of charge state. This behaviour could be explained by a simple rule based on how the pyrenes (a bond surrounded by four hexagonal faces) are distributed.

Fig. 1 shows the dissociation energies corresponding to the $C_{70}^{q+} \rightarrow C_{68}^{q+} + C_2$, $C_{70}^{q+} \rightarrow C_{68}^{(q-1)+} + C_2^{+}$, $C_{70}^{q+} \rightarrow C_{68}^{(q-2)+} + C^{+} + C^{+}$, $C_{70}^{q+} \rightarrow C_{68}^{(q-3)+} + C^{2+} + C^{+}$, and $C_{70}^{q+} \rightarrow C_{68}^{(q-4)+} + C^{2+} + C^{2+}$ decay channels. The competition between the different pathways were found to be similar to the C_{60}^{q+} case [2] but the absolute energies (and the slopes) for a given decay channel were different. These differences give information on the relative stabilities between C_{70}^{q+} and C_{60}^{q+}.

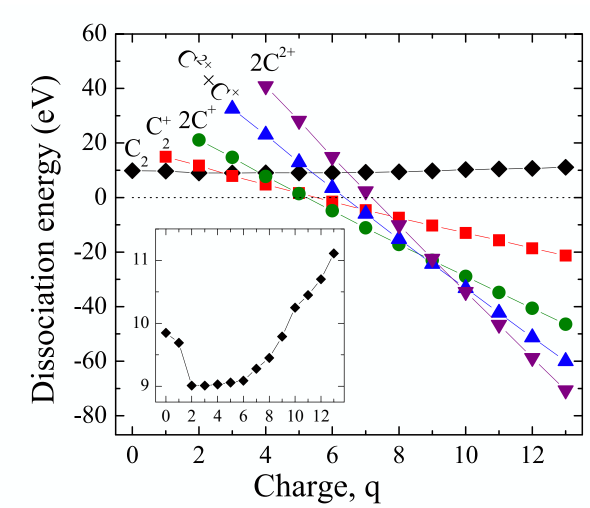

Figure 1: The dissociation energies corresponding to different decay pathways for C_{70}^{q+} ($C_{70}^{q+} \rightarrow C_{68}^{(q-1)} + C_2$ also shown as inset).

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Mo3-19

Femtosecond laser induced fusion of gas phase fullerenes

K.Hansen[1*], M.Kjellberg[1], A.V.Bulgakov[2], E.E.B.Campbell[1]

1. Dept. of Physics, Göteborg University, SE-41296 Göteborg, Sweden
2. Institute of Thermophysics, SB-RAS, 1 Lavrentyev Ave. 630090 Novosibirsk, Russia
* email: klavs@physics.gu.se

van der Waals bound clusters of fullerenes have been observed to undergo intra-cluster fusion when exposed to femtosecond laser light [1,2,3,4]. The fusion is followed by fragmentation with loss of C_2 units, demonstrating both the fullerene nature of the products and the large thermal energy of the fusion product. Fusion is absent when the clusters are exposed to a nanosecond laser pulse, where the decay channel is instead loss of intact fullerene molecules.

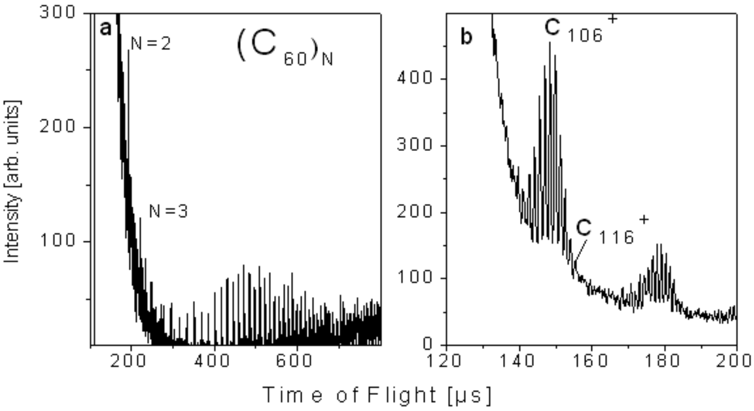

Fig.1 (a) Time-of-flight mass spectrum obtained by single-photon ionisation of $(C_{60})_N$ clusters from a gas aggregation source. (b) Part of ion time-of-flight mass spectrum from an identical cluster distribution ionized with 200 fs laser pulses providing evidence for intra-cluster molecular fusion.

Fusion-fragmentation products of precursors up to $(C_{60})_5$ and $(C_{70})_5$ have been observed but only as singly charged species. These facts suggest that the fusion process involve timescales similar to the ones found for the quasi-thermal electron emission from fs-heated fullerenes, of several hundred femtoseconds. This has been confirmed with pump-probe experiments where the total fragment yield was measured [2].

The degree of post-fusion fragmentation is fairly invariant to source conditions and laser fluence. The number of C_2 units lost from the fusion products grows linearly with the precursor size and reaches 30 for $(C_{60})_5$. The shape of the dimer fusion product distribution can be understood in terms of the fusion barrier which provides the high mass (low energy) cutoff and, for the low mass (high energy) cutoff, as the tendency for more highly charged and hotter van der Waals bound clusters to *fission*[3,4].

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Mo3-20

EFFECT OF DIFFUSION ON NANOCLUSTER NUCLEATION

D.N. Korolev, M.V. Sorokin, A.E. Volkov*

Russian Research Centre 'Kurchatov Institute', Kurchatov Sq.1, Moscow, 123182,
Russia, (*) volkov@dni.polyn.kiae.su

Decomposition of a solid solution supersaturated with impurity atoms results in creation of nanoclusters. Descriptions of such decomposition are based on the adiabatic principle which declares that diffusion currents of monomers in the vicinity of clusters adjust themselves to the actual cluster sizes. In this case the probabilities of absorption/desorption of atoms on the cluster interfaces depend only on these sizes and clustering is a Markovian stochastic process completely described by these probabilities [1], [2].

The thermodynamical approach assumes that forming clusters do not disturb the supersaturated solution [3] and the absorption probability depends on the average monomer concentration in the system. We will consider a more general case, when the absorption/desorption probabilities depend on the kinetics of impurity atoms in the vicinity of the cluster interface including their interaction with this interface, and the difference between the absorption and desorption rates of monomers coincides with the value of the diffusion current at the cluster interface.

This current results from the spatially non-uniform impurity concentration induced by a forming cluster. Having in mind the adiabatic principle the current can be determined from the solution of the steady-state diffusion problem in the vicinity of the selected cluster. The average concentration of monomers in the system and their absorption by other clusters form the boundary conditions for this problem. Thus, the absorption/desorption mechanisms couple the kinetics of impurity atoms at the cluster interface with impurity diffusion which depends on monomer annihilation at other clusters.

We demonstrate that such coupling can result in deviation of the forms of parameters governing clusterization from those predicted by the thermodynamic approach [2]. For illustration of this effect we choose the steady-state nucleation mode [4]-[6] when the nucleation barrier determines the steady-state nucleation rate of clusters.

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Mo3-21

Probing finite-size properties of small carbon clusters with delayed detachment process.

F. Pagliarulo[1], B. Baguenard[1], F. Calvo[1], P. Parneix[2], B. Concina[1], F. Lépine[1] and C. Bordas[1]

[1]Université Lyon 1 ; CNRS ; LASIM UMR 5579, 43 boulevard du 11 novembre 1918, F-69622 Villeurbanne Cedex, France

[2]LPPM Batiment 210 et 350 Université Paris SUD 91405 Orsay Cedex

When an atomic cluster is excited with a nanosecond laser pulse, the absorbed energy can be redistributed over the nuclear skeleton. This heating process can lead to the delayed ionization of the system. This electron emission can be regarded as a statistical process and be very well described using Weisskopf's model.
In this model the kinetic energy spectrum of the emitted electrons depends on the electron attachment cross section and on the density of states. It can be approximated by:

$$P(\varepsilon) \propto \varepsilon^{\gamma} \exp\left(\frac{-\varepsilon}{k_B T_d}\right)$$

Under the assumption of a spherical daughter cluster interacting with the emitted electron via a Langevin potential the exponent γ is set to 0.5.

We have measured the electron emission from size selected small carbon cluster anions C_n^- ($10 \leq n \leq 22$) excited by nanosecond laser (Xe:Cl, 308 nm, or Xe:Cl pumped dye laser). Time-resolved velocity-map imaging [1] allows us to measure Kinetic energy spectra of emitted electrons and to discriminate direct and delayed emission [2]. Determination of the kinetic energy spectrum can be considered as a thermometric measurement as it provides a direct access to the cluster temperature T_d.

In a first approximation, measured daughter temperatures T_d are in good agreement with the statistical predictions when $\gamma = ½$ is assumed. However, a detailed analysis shows significant differences with the model. A γ-free model has been used to characterize this disagreement. It shows a variation of γ and T_d with the cluster size (from $\gamma = 0.2$ to 0.6). Combining DFT and PST calculations [3] a more refined understanding of delayed processes is obtained and reveals that the shape of the electron spectrum is a signature of cluster's finite-size properties. In this contribution we will discuss how this electron spectrum is altered when the geometry of the system evolves from linear (carbon chains) to spherical or planar (carbon rings) geometry. Thermionic emission could be a useful probe of the geometry of clusters and complex molecules.

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Mo3-22

SCREENING OF A CONFINED ATOM BY A FULLERENE OF FINITE THICKNESS

S. Lo[1], A.V. Korol[1,2] and A.V. Solov'yov[1]

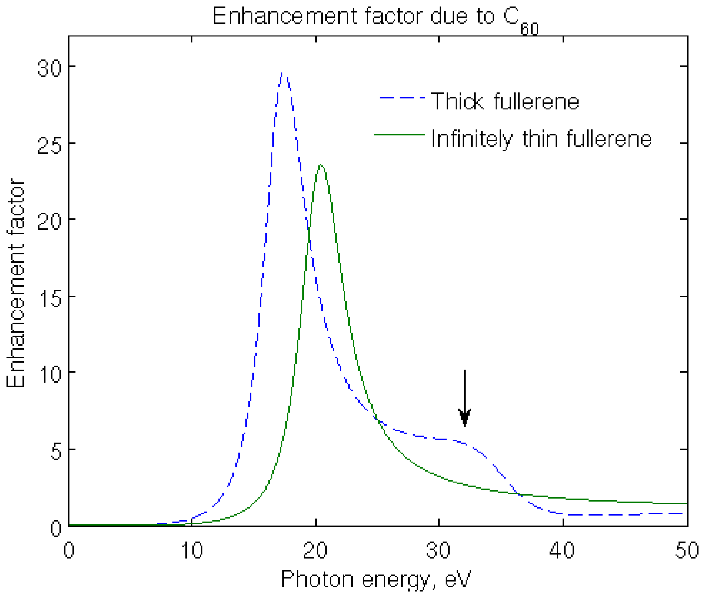
[1] Frankfurt Institute for Advanced Studies, Johann Wolfgang Goethe-Universität,
Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

[2] Department of Physics, St. Petersburg State Maritime Technical University,
Leninskii prospect 101, St. Petersburg 198262, Russia

Email: lo@fias.uni-frankfurt.de

An atom confined within a fullerene is dynamically screened from the external electromagnetic field - it experiences a field that is amplified - leading to an enhancement of the photoabsorption of the confined atom. The amplification occurs in a certain frequency range determined by the plasmon excitation in the confining fullerene. This enhancement factor was discussed by Connerade and Solov'yov in [1] for the case of the infinitely thin fullerene.

The dynamical enhancement factor due to a fullerene of finite thickness is presented here. The existence of a second surface of this fullerene is significant as this allows for the presence of two surface plasmon modes [2], in contrast to the single plasmon considered in [1]. The figure is a plot of the enhancement factor for the infinitely thin fullerene and the fullerene of finite thickness. The profile of the enhancement factor for the thick fullerene has an additional feature, which is due to the manifestation of the second plasmon mode, as indicated by the arrow in the figure.



This work was supported in part by INTAS (project number 03-51-6170) and by EU through the EXCELL project.

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SPECIFIC FEATURES OF POLARIZATION BREMSSTRAHLUNG ON ELECTRON SCATTERING BY XENON CLUSTERS

E.V. Gnatchenko, A.N. Nechay, A.A. Tkachenko

Verkin Institute for Low Temperature Physics and Engineering, National
Academy of Sciences of Ukraine, 47 Lenin Ave, 61103, Kharkov, Ukraine,
E-mail: egnatchenko@ilt.kharkov.ua

Until recent time the polarization bremsstrahlung (PBS) which arises due to dynamic polarization of the target particle by the field of the incoming electron on collisions of electron and free atom [1,2], and solid [3,4] is studied well enough. In these investigations, the wide resonance structures in the region of photon energies where the dynamic polarizability of the target particle is large were found. However, there are no experimental data on PBS manifestations on electron scattering by clusters, whereas the theoretical works [5,6] predict the effect of cluster size on the energy position, shape and intensity of PBS resonance.

In this report we present the results of the first experimental study of bremsstrahlung spectra including ordinary bremsstrahlung and PBS on electron scattering by free clusters of xenon. The experiments were carried on a setup consisting of an X-tube with xenon supersonic jet as an anode and an X-ray spectrometer [1]. Clusters were formed in the process of isoentropic expansion of an ultrasonic jet of xenon flowing into vacuum. Cluster size was varied from 50 to 10^3 at/cl. The cluster jet was crossed by an electron beam with the energy 0.6 keV. The range of photon energies studied was 70-220 eV.

The effect of the cluster size on spectrum form as well the dependence of bremsstrahlung intensity on the cluster size is studied. The comparison of experimental results and theoretical calculations is carried out.

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Mo3-24

The photon-assisted transport and Maxwell potential in mesoscopic devices

ARAFA. H. ALY[1,2], SANG W. RYU[1]
[1]Department of Physics, Chonnam National University, Gwangju, Korea
[2]Physics department, Faculty of Sciences, Beni-Suef University, Egypt.
arafa16@yahoo.com

We analyzed theoretically the phenomenon of **photon-assisted** quantum transport in Superconductor-Semiconductor mesoscopic by suggesting a Maxwell potential at the interface. Sub-gap structure in the I-V characteristics could be explained by multiple Andreev reflections. The electrical properties are strongly determined by the interface between superconductor and semiconductor. The I-V characteristics were found to be very sensitive to the photon frequency. Good agreement between the calculated and the measured curves leads us to the conclusion that photon-assisted transport is observed in superconducting-semiconductor junctions with an enhanced current density. Our formula obtained could give a general sight into the quantum characteristics of the S-N junction. The effect of the photon-assisted quantum transport can be utilized to develop a very high frequency detector in the range of THz.

Mo3-25

IS CADMIUM DIMER A TRULY VAN DER WAALS MOLECULE: ROTATIONS AT THE $^{1}0_{u}^{+}(5^{1}P_{1})\leftarrow X^{1}0_{g}^{+}$ AND $^{1}1_{u}(5^{1}P_{1})\leftarrow X^{1}0_{g}^{+}$ TRANSITIONS

M. Strojecki, M. Ruszczak, M. Łukomski and J. Koperski

Smoluchowski Institute of Physics, Jagiellonian University,
ul. Reymonta 4, 30-059 Kraków, Poland

Rotational profiles of the ^{228}Cd$_2$ isotopomer recorded in the $(\upsilon',\upsilon'') = (26,0)$, (27,0), (45,0), (46,0) and (48,0) vibrational bands of the $^{1}0_{u}^{+}(5^{1}P_{1})\leftarrow X^{1}0_{g}^{+}$ transition were investigated (see Fig. 1). As a result, the $B'_{\upsilon=26}=0.0309(5)$ cm^{-1}, $B'_{\upsilon=27}=0.0308(5)$ cm^{-1}, $B'_{\upsilon=45}=0.0277(5)$ cm^{-1}, $B'_{\upsilon=46}=0.0274(5)$ cm^{-1} and $B'_{\upsilon=48}=0.0271(5)$ cm^{-1} excited- as well as the $B''_{\upsilon=0}=0.0206(5)$ cm^{-1} ground-state rotational constants were determined. A multi-band and multi-branch analysis allowed direct determination of absolute values of the $R'_e=2.94(3)$ Å and $R''_e=3.77(4)$ Å excited- and ground-state bond lengths, respectively. Analysis of a rotational profile recorded in the $(\upsilon',\upsilon'') = (38,0)$ band of the same isotopomer recorded at the $^{1}1_{u}(5^{1}P_{1})\leftarrow X^{1}0_{g}^{+}$ transition allowed estimation the $B'_{\upsilon=38}=0.0317(5)$ cm^{-1} rotational constant in the $^{1}1_{u}$ state. The result provides a contribution to the discussion on purity of the ground-state van der Waals bonding and presence of a covalent admixture to the bonding.

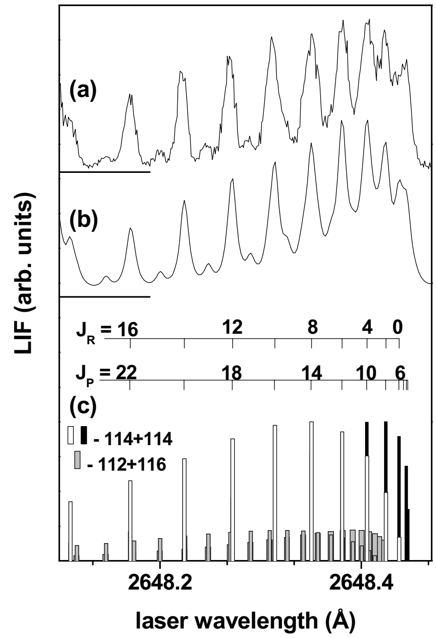

Fig. 1. Rotational profile of the ^{228}Cd$_2$ isotopomer recorded in the $(\upsilon',\upsilon'') = (26,0)$ vibrational band of the $^{1}0_{u}^{+}\leftarrow X^{1}0_{g}^{+}$ transition. (a) Experimental trace, (b) computer simulation obtained as a result of convolution of every rotational transition with a Voigt function corresponding to the 0.08 cm^{-1} bandwidth of the laser beam and 0.12 cm^{-1} Doppler broadening as well as 6 K rotational temperature, (c) *P*-branch (full bars) and *R*-branch (open bars) of the ^{114}Cd^{114}Cd isotopomer, *P*- and *R*-branches of the ^{112}Cd^{116}Cd isotopomer (grey bars).

Mo3-26

FERROMAGNETIC COUPLING IN FINITE Mn LINEAR CHAINS

Andrey Lyalin, Andrey Solov’yov, and Walter Greiner

Frankfurt Institute for Advanced Studies,
Max von Laue Str. 1, D-60438 Frankfurt am Main, Germany

The study of evolution of magnetic properties from atoms to the bulk is important for the development of magnetic nanomaterials with specific properties and for understanding the fundamental principles of spin coupling in finite and low dimensional systems. In this work we report the results of a systematic theoretical investigation of optimized structure, electronic and magnetic properties of linear chains of Mn atoms and organometallic sandwich clusters $Mn_N(C_6H_6)_{N+1}$ within the size range $N \leq 6$ [1]. The choice of Mn is stipulated by the fact that the Mn atom possesses a large magnetic moment due to the half-filled 3d electron shell, and thus, manganese is a good candidate for strong nanomagnets. Our calculations are based on *ab initio* theoretical methods invoking density-functional theory with the gradient-corrected exchange-correlation functional of Perdew, Burke and Ernzerhof (PBEPBE). The standard LANL2MB basis set of primitive Gaussians have been used to expand the electronic orbitals formed by the $3s^2 3p^6 3d^5 4s^2$ outer electrons of Mn (15 electrons per atom). We show that the finite linear chains of Mn atoms exhibit novel magnetic properties that differ from those of the corresponding Mn bulk and one-dimensional infinite chains. Thus, we demonstrate that finite one-dimensional monoatomic chains of Mn atoms possess ferromagnetic order in spite of the fact that the most stable crystal structure of Mn exhibits antiferromagnetic behaviour. We demonstrate that magnetic ordering in finite linear chains depends on its length and therefore can be controlled by the fixing chain’s geometry. We also predict enhancement of magnetism in organometallic sandwich clusters $Mn_N(C_6H_6)_{N+1}$.

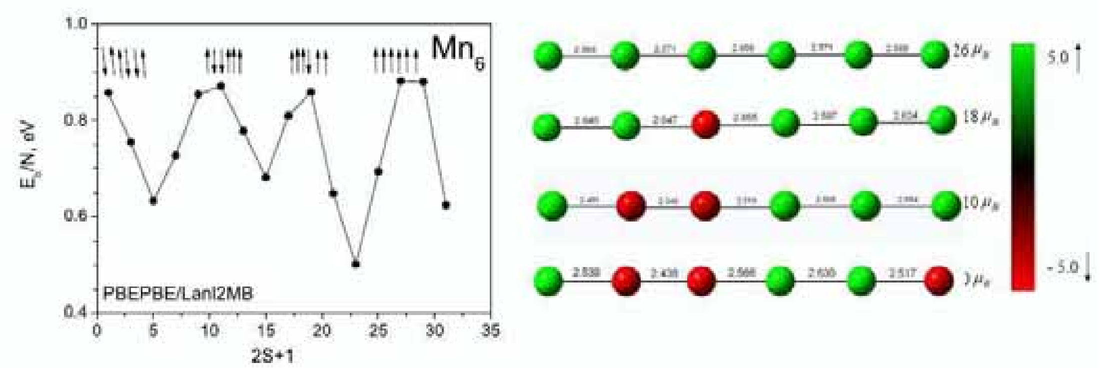

Figure 1: Binding energy per atom for Mn_6 linear chain as a function of multiplicity 2S+1 (right). Mulliken atomic spin densities for different spin isomers of Mn_6 chain (left). Interatomic distances are given in angstroms.

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Mo3-27

Vaporization of Rubidium and Potassium Clusters by a Low Power CW Atomic Resonant Laser Radiation

Alexander Plekhanov[1], Sergey Atutov[2], Roberto Calabrese[2], Lucca Tomassetti[2], Vincenzo.Guidi[2], Anatoly Shalagin[1]

[1]Institute Automation and Electrometry, Russian Academy of Science, Novosibirsk, Russia, fractal@iae.nsk.su
[2]Istitito Nazionale di Fisica Nucleare, Sezione di Ferrara, Ferrara, Italy.

Is it possible to vaporise some small pieces of metal immersed in a atmospheric pressure buffer gas by a relatively weak CW laser radiation? Someone could say it is definitely not possible, because a metallic surface reflects practically all light incidents upon the surface and thus a vaporisation needs at least a few tens Watts power of laser radiation. Anyway the answer on this question is ”yes”, if these pieces of metal are, as we found, so called metallic microclusters[1].

Here we demonstrate that relatively weak (less than ~ 0,3 Вт/см^2) CW red or infrared laser radiation can vaporise metallic clusters of K or Rb. This intriguing and unexpected effect occurs in a commonly used in many optical and spectroscopic experiments heat - pipe - oven (HPO) cell. It was found surprising that the effect exists only when the frequency of the laser is sharply detuned to the exact maximum of resonant optical absorption line of atoms from which the clusters consist of. The observed vaporisation is fast enough to overcome diffusion of the atoms out of the laser beam and create compact, dense and bright atomic “clouds”. The fluorescence spectrum of the K or Rb clouds corresponds to K or Rb plasma recombination. It shows practically all atomic emission lines of these atoms including the lines which correspond to the the ionisation levels of the atoms. Electrical conductivity of these clouds is found to be very high. The clouds are periodically generated and then move along of the cell opposite to the direction of propagation of the laser beam inside of the cell. The clouds exhibit “solitonlike” behaviour, i.e. there no change in shape, size and brightness during propagation over distance that can be much longer with respect to the cloud size[2].

This phenomenon was observed for K, Rb, and also for Na[3] clusters, so this effect should be also observable with other kind of clusters. We have, for example, evidence of the fast vaporization iodine clusters in iodine molecules vapor excited directly by Ar$^+$-laser radiation. Thus, the phenomenon, we observed, is not strictly confined to the physical or chemical properties of the clusters but it is a more general effect. We believe that the present work reveals the existence of new physical phenomena in clusters physics as a interaction of clusters with radiation in presence of resonantly exited atoms or molecules

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Mo3-28

Two-dimensional distributions of slow Ne^{7+} transmitted through SiO_2-nano-capillaries

P. Skog, HQ. Zhang, and R. Schuch

Atomic Physics, Fysikum, AlbaNova Physics Centre, S-106 91 Stockholm, Sweden

The transmission of highly charged ions (HCI) through insulating nano-capillaries has attracted considerable attention during recent years [1-3]. In the case of HCI impingent on insulating capillaries at angles larger than the angle given by the aspect ratio, substantial transmission of ions in the initial charge state and at the initial kinetic energy was found[1-3].. The ion-guiding of insulating capillaries has been studied by our group using capillary membranes in different materials, such as SiO_2, Al_2O_3 [2-3]. The guiding of HCI through insulating capillaries has been attributed to the formation of near-entrance charge patches, preventing incident ions from coming in close contact with the walls [1,4]. The further propagation of ions, after the first deflection near the entrance, through the capillaries is attributed to guiding by an electric field from all charges deposited on the capillary walls. The angular distributions are then broadened by the inhomogeneous electric field at the capillary exit due to end effects.

The guiding effect is time dependent; ions hitting the capillary walls deposit positive charge, which will deflect ions incident at a later instant. Full transmission is achieved when equilibrium between deposition and diffusion of charge is reached.

Our group has manufactured highly ordered, parallel, capillaries in 100 nm thick SiO_2 on Si, 25 μm in length and 100 nm in diameter and with wall thicknesses of 100 nm [5]. We have studied the two-dimensional distribution of 7 keV Ne^{7+}-ions guided through these SiO_2-capillaries, using ions from the 14 GHz ECR ion source located at the Manne Siegbahn Laboratory, Stockholm. Figure 1 shows the distributions of Ne-ions guided by the SiO_2-nano-capillaries for different tilt angles of the capillary membrane, ranging from -3° to +3°.

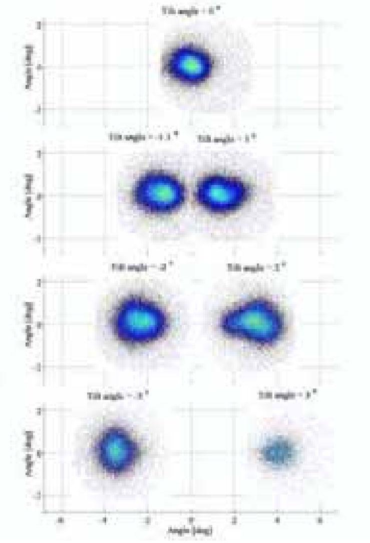

Fig. 1 Two-dimensional distributions of Ne-ions guided by SiO_2-nano-capillaries for capillary tilt angles of -3° - +3°.

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Mo3-29

POLAR MOLECULES IN HELIUM CLUSTERS: BOSONIC VERSUS FERMIONIC ENVIRONMENTS

M. P. de Lara-Castells, R. Prosmiti, G. Delgado-Barrio,
D. López-Durán, and P. Villarreal*

Instituto de Matemáticas y Física Fundamental (CSIC)
Serrano 123, E-28006-Madrid, SPAIN

Accurate CCSD(T) *ab initio* calculations on He-ICl(X) and further on He_2-ICl(X) [1] show that this surface can be described as the sum of two triatomic potentials plus the He-He interaction. Extension of this model to He_N-ICl(X) clusters allows to simulate, by using Hartree/Hartree-Fock approachs [2], their infra-red (IR) spectra depending on the statistics of the surrounding helium atoms. For ^{4}He boson species, the simulated IR absorption spectra exhibits well defined P and R branches with lack of Q branches, which only appear in fermionic environments of ^{3}He. Moreover, in the later scenario, there is a quasi-degeneration of spin multiplets contributing to the congestion of the spectrum. This is in perfect agreement with the experimental findings on a similar molecule, linear OCS, in helium nano-droplets [3] , where the well structured spectra observed in ^{4}He, in contrast with the broad profiles observed in ^{3}He, were interpreted as a manifestation of superfluidity of bosonic helium at a microscopic scale.

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* e-mail: p.villarreal@imaff.cfmac.csic.es

Mo3-30

SWEEPING-OUT-ELECTRONS EFFECT UNDER IMPACT OF LARGE MOLECULES AND CLUSTERS

Edward S. Parilis

California Institute of Technology, 200-36, Pasadena, CA, 91125, U.S.A.

Abstract

This paper presents the most intriguing of the effects of non-additivity under impacts of polyatomic molecules and clusters, observed up to now only in a variety of electronic energy loss phenomena: electron emission, light emission, and projectile charge state formation. The sublinear effect consists in a reduction of the yields per atom, caused by the mechanism of sweeping-out-electrons that is discussed and clarified.

The non-linear effects that have been studied in cluster-solid interactions usually consist in an enhancement, in some cases very drastic, of the yield per atom, with increasing number of atoms in the cluster. All of them are connected to the nuclear stopping and could be regarded as a natural result of the synergetic action of the cluster constituents.

What was puzzling and intriguing and yet not completely explained was the existence of some non-additivity effects, in which the total yield is sublinear, i.e., it is less than proportional to the number of atoms in the cluster. The extent of reduction increased with the increasing number of cluster constituents. It looked like the atoms were mutually blocking or screening each other, diminishing the resulting effect.

All the sublinear effects were observed only in the electronic stopping related phenomena.. It was supposed that the sublinear reduction is due to a sweeping-out-electrons effect, consisting in removing some electrons from the cluster trek by the front running cluster atoms, leaving fewer available for the rear ones .

The purpose of this review is to describe different manifestations of the mechanism and the corresponding formalism, to clarify its general character and to discuss other possible effects of sweeping out electrons under cluster impacts.

Mo3-31

FRAGMENTATION AND FORMATION AS PHASE TRANSITION IN FULLERENES

Adilah Hussien, Ilia Solov'yov, Andrey V. Solov'yov and Walter Greiner

Frankfurt Institute for Advanced Studies
Johann Wolfgang Goethe University
Max-von-Laue-Str. 1
60438 Frankfurt am Main, Germany
E-mail: hussein@fias.uni-frankfurt.de

We investigate the various fragmentation and formation channels of fullerenes using a statistical description first applied to polypeptide folding [1]. In this formalism, the growth and fragmentation of fullerenes are treated as phase transitions, and we present a scheme of constructing a parameter-free partition function describing such a process. Thus, we develop a theory describing all essential thermodynamical properties such as heat capacity, free energy and the phase transition temperature. The predictions of our theory are compared with available experimental measurements on the melting of fullerenes [2] and with results from molecular dynamics simulations [3].

Two examples of possible fragmentation channels of C_{60} are shown in Figure 1. Channel (a) corresponds to the transition of C_{60} in the gas phase of 30 C_2 molecules, while channel (b) corresponds to the polymerization of the fullerene.

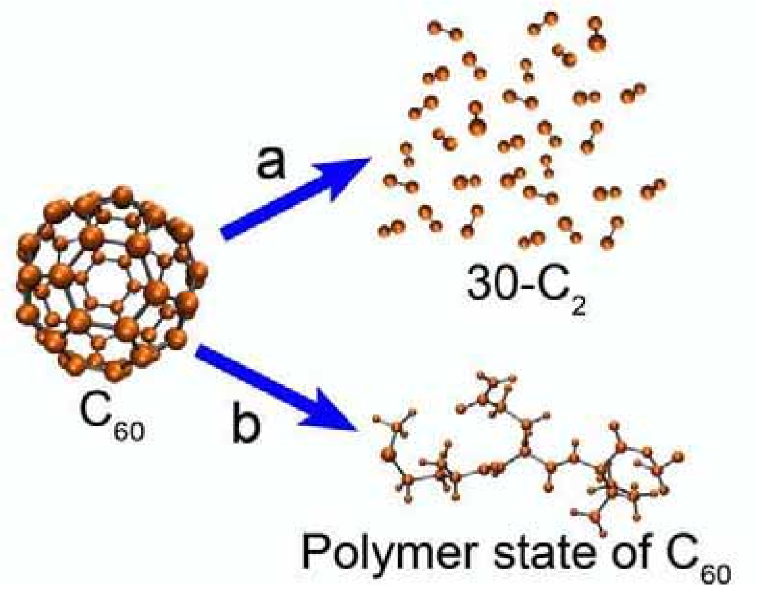

Figure 1: Possible fragmentation channels of C_{60} into a gas or polymer phase.

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Mo3-32

DFT CALCULATIONS OF GOLD CLUSTERS WITH S, Se and Te COMPOUNDS

Pablo López-Tarifa, Fernando Martín and Manuel Alcamí

Departamento de Química, C-9, Universidad Autónoma de Madrid, Cantoblanco,
28049 Madrid, Spain

We present a systematic study at DFT level of the interaction of gold atom and clusters (Au_n n=1-5) with different compounds containing S, Se or Te as the main reactive centre. In particular the series of compounds H_2X, $(CH_3)HX$, $(CH_3)_2X$, $(CH_3CH_2)HX$, HClX and $H(NH_2)X$ with X=S, Se and Te have been considered.

These results allow us to study the evolution of the binding energies as a function of the nature of the basic centre and the size of the cluster. Binding energies increase in the order S < Se < Te, being in some cases the interaction of a single gold atom with Te derivatives 40% stronger than with the corresponding S compound. The interaction energy increases when the size of the cluster increases, in particular the binding energies duplicate when going from Au to Au_2, but the differences in the interaction energies among S, Se and Te become smaller when Au clusters are considered, i.e. the effect of increasing the size of the cluster has a larger effect in the enhancement of the interaction energies in S than in Te compounds. We have also analyzed the effect of the different substituents. In general, methyl and electronegative substituents reinforce the interaction with gold.

For the larger clusters (Au_4 and Au_5) the interaction with two molecules has also been studied and in some specific cases we have evaluated the singlet-triplet energy gap. The structure of all the species has been fully optimized and the changes in the structure upon formation of the complex with gold have been analyzed. Finally the nature of the interactions and the electronic effects has been analyzed by using the electronic density (AIM method) and the natural bond orbitals (NBO method).

Mo3-33

Quantum Monte Carlo Simulation of Small Boson-Helium Clusters with Fermion-Helium Impurities

Dr. Cono Di Paola[1,2], Prof. Gabriele Morosi[1,3], Dr. Dario Bressanini[1,4]

Insubria University, Via Lucini, 22100 Como (Italy)[1]
cono.dipaola@uninsubria.it[2] gabriele.morosi@uninsubria.it[3]
dario.bressanini@uninsubria.it[4]

In recent years weakly bound helium clusters and droplets have attracted the attention of a growing number of experimentalists and theoreticians. The combination of the extremely weak interaction between helium atoms and the small atomic masses makes helium clusters very weakly bound and by far the most intriguing van der Waals clusters with highly quantum features.

Initial investigations were devoted to pure ^{4}He clusters and droplets. More recently a growing number of studies have focused on pure ^{3}He clusters and droplets. While all ^{4}He clusters, starting from dimer, are bound, it is not yet known what is the minimum number of ^{3}He atoms necessary to form a stable cluster. In an early investigation, Pandharipande et al [1] found that eight ^{3}He atoms would form a bound state if they were bosons, despite the lighter mass, and eight ^{4}He atoms would be bound even if they were fermions, but eight ^{3}He fermions do not form a bound state.

The information on the mixed ^{3}He/^{4}He systems is even poor. The stability of the clusters ^{3}He^{4}He$_N$ for N>1 was predicted by Bressanini et al. [2] and later shown experimentally. In the same paper, it is examined the stability of a cluster containing the ^{3}He. They showed that the system ^{3}He$_2$^{4}He is unstable, while the trimer ^{3}He^{4}He$_2$ is very weakly bound with a total energy an order of magnitude smaller than the pure trimer ^{4}He$_3$. Nevertheless, it is possible to add a second ^{3}He atom and form the stable species ^{3}He$_2$^{4}He$_2$ with the odd feature of having five out of six unbound pairs.

The stability of pure ^{3}He$_M$ and mixed ^{3}He$_M$^{4}He$_N$ clusters is a delicate balance between the fermionic nature of the ^{3}He that introduces nodes in the ground state wave function, the weakly attractive He-He potential, and the kinetic energy effects due to the lighter mass of the fermionic isotope. A first attempt to study mixed clusters with more than three ^{3}He atoms has been recently published [3].

The exploration of the stability diagram of ^{3}He$_M$^{4}He$_N$ is just at the beginning and very complicated, due to the fact that for each cluster it is not even known what are the preferred spin multiplicity and angular momentum. The simulation of the ground state was obtained using the Quantum Diffusion Monte Carlo Method [4].

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Mo3-34

QUANTUM STRUCTURING AND MICROENERGETICS OF IONIC DOPANTS IN ^{4}HE DROPLETS FROM STOCHASTIC CALCULATIONS

E. Coccia, E. Bodo, F.A. Gianturco

Dept. of Chemistry and CNISM, University of Rome "La Sapienza", Italy
coccia@caspur.it

Helium nanodroplets provide a very interesting medium that acts as a "quantum matrix" where one can probe ro-vibrational and electronic spectroscopy of atoms and molecules "solvated" in it and where the nonclassical effects caused by the surrounding He atoms [1-2] can be observed.

The discovery [3] that also ions can be captured inside helium nanodroplets opens the way to a new class of experiments and theoretical approaches which are useful to understand the quantum behaviour and the structure of these systems. A charged impurity is expected to strongly modify the local environment of the liquid He: a positive alkali ion polarizes the surrounding helium atoms and a region of increased density, characterized by some kind of solid order, is present (the *snowball* model [4]).

We have carried out Variational Monte Carlo (VMC) and Diffusion Monte Carlo (DMC) calculations [5] to study the clusters of $Li^+(He)_n$, $Na^+(He)_n$ and $K^+(He)_n$ with n up to 15 [6]. We focus our attention on the energetics (total energy and evaporation energy) and on several geometric observables, such as M^+- He and He-He distances, three-body angles and angular probability distributions from a four-body correlation function. We are also interested in showing the possible coexistence of different "resonance" quantum structures from our stochastic simulation: the generation of 3-D representations of the atomic density shows the localization of the helium atoms around the impurity.

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Mo3-35

Spatial arrangements and stability shells for bosonic He clusters around ionic impurities: a genetic algorithm study.

F. Marinetti[1], E. Bodo[1], F.A. Gianturco[1], E. Yurtserver[2], M. Yurtserver[3], E. Yildrim[3]

[1]Department of Chemistry and CNISM, University of Rome La Sapienza, Rome, Italy
[2]Department of Chemistry, Koç University, Rumelifeneri Yolu, Istanbul, Turkey
[3]Department of Chemistry, Istanbul Technical University, Istanbul, Turkey

marinett@caspur.it

The spectroscopy performed with a superfluid He matrix allows to study molecular species which are difficult to observe in the usual gas phase spectroscopy. Such species are ions, weakly bound molecules like triplet diatoms and highly reactive species like radicals. These experiments provide highly resolved spectra because of the increased dopant lifetime and the small coupling with the environment. For cationic species, it is possible to observe a solid-like behaviour in the region of the droplet which is close to the impurity. Therefore, the inner solvation shells are highly structured (snowball effect) and present an increased helium density with respect to the bulk phase (electrostriction effect). The high localization enable us to treat these shells as they would be behaving as classical objects[1].
In our work therefore we use a classical optimization procedure, based on a genetic algorithm[2], in order to find absolute minima of the potential energy for the systems $X^+(He)_n$. We have focused our attention on the shell structure by analysing the evaporation energies and the geometries and we have compared our results with accurate quantum Monte Carlo calculations[4].
The potential energy has been built up with a sum of pairwise potentials which are calculated with an high quality ab initio approach[3]. Several calculations has been carried out for cationic system like: alkali metals[4], their ionic dimers, OH^+[5], and He_n^+.

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Mo3-36

STRUCTURE OF THE PCBM FULLERENE DERIVATIVE AND ITS DIMERS

Yang Wang, Manuel Alcamí, Fernando Martín

Departamento de Química, C-9, Universidad Autónoma de Madrid, Cantoblanco,
28049 Madrid, Spain

Among the promising applications of fullerenes, {1-(3-methoxycarbonylpropyl)-1-phenyl[6,6]methanofullerene} (PCBM)[1,2] is one of the best examples. This methanofullerene derivative has been proposed as an efficient electron acceptor component in bulk heterojunction organic solar cells.[3] It has been shown that the blends of PCBM with conjugated polymers can lead to enhanced power conversion efficiencies.[3,4] Despite the frequent use of PCBM, there have been relatively few computational studies on this fullerene derivative so far. Therefore, we present here a computational study of PCBM based on density functional theory (DFT). The B3LYP/6-31G* optimized geometries of PCBM monomer in gas phase are comparable with values from crystal structures.[2] In order to investigate how PCBM molecules interact with each other, several possible PCBM dimers were proposed and characterized computationally. Among these possible dimers, the two most stable ones have disassociation energies of 6.85 and 4.15 kcal/mol at the level of B3LYP/6-31G*, and 2.15 and 2.19 kcal/mol after considering the basis set superposition effect (BSSE). Weak C-H---O hydrogen bonds[5,6] are found in these two dimers, which contribute to the main part of the interaction between the two PCBM molecules. Our results for the dimers may give some hints on understanding the interaction in bulk structures of PCBM.

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Mo3-37

Photo – atomic induced processes in dryfilm coatings and nanoporous silica

A. Burchianti, A. Bogi, A. Cappello, C. de Mauro, S. Di Renzone,
A. Khanbekyan, C. Marinelli, C. Maibohm, E. Mariotti, L. Moi

Università di Siena, Dipartimento di Fisica, via Roma 56 Siena, I-53100, Italy
email:mariotti@unisi.it

During the last years numerous investigations have been devoted to the study of atom-dielectric surface interaction in the presence of light. This interest is due to the possibility to obtain a more in-depth understanding of the complex system, atom-surface-light, and to develop applications in atomic spectroscopy and in nanotechnologies. Nano-porous silica and silane compounds offer a wide class of different properties to study in this direction.

The possibility of build up atomic sources controlled only by light for spectroscopic experiments, was in the last years one of the main reason in studying the features of light induced atomic desorption (LIAD) effect from organic coatings: when a coated cell is shined even with non-resonant incoherent light a huge increase of the vapor density could be observed [1]. We decided to test dry-film coatings and in particular OTS that has been studied in the past [2] and it is currently used in many experiments where a weak adsorption energy surface and UHV conditions, as in a magneto optical trapping (MOT) experiment, are needed. We observed the first experimental evidence of non-thermal light induced atomic desorption from a dry-film coating, with an efficiency which is about one order of magnitude greater of those measured with other organic coatings such as PDMS or OCT [3]. Furthermore, our experimental data confirm that the theoretical model elaborated for PDMS and OCT is correct and that it is also valid for OTS. This result expands the list of materials showing such an effect and increases the possibilities to get suitable light controlled atomic sources for spectroscopy and applications, in particular for a fast and efficient loading of a MOT [4].

LIAD has been also observed from nano-porous silica, even if the same macroscopic behaviour originates from different microscopic process with respect to organic coatings. In addiction to LIAD, we investigate the optical response of atoms and nano-particles embedded in nano-porous silica samples. Green-blue desorption light induces cluster formation taking advantage of the enormous number of desorbed atoms, which diffuse in the nano-cavities. Red-infrared desorption light excites the surface plasmon oscillations of nano-particles embedded inside the glass matrix, causing atomic evaporation from metallic clusters [5]. Both processes are completely reversible and are even visible to the naked eye.

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Mo3-38

EXCITATION AND IONIZATION OF CLUSTERS OF CHIRAL FLUORINATED MOLECULES BY R2PI SPECTROSCOPY

A. Giardini [1,2], F. Rondino [3], A. Paladini [2], M. Speranza [3], S. Piccirillo [4], M. Satta [5]

[1] Dipt. di Chimica, Università di Roma "La Sapienza", 00185 Roma, Italy
[2] CNR-Istituto Metodologie Inorganiche e Plasmi, 85050 Tito Scalo (Pz), Italy
[3] Facoltà di Farmacia, Dip. di Studi di Chimica e Tecnologia delle Sostanze Biolog. Attive, Università di Roma "La Sapienza", 00185 Roma, Italy
[4] Dipt. di Scienze e Tecn. Chimiche, Università di "Tor Vergata", Roma, Italy
[5] CNR-Istituto Sistemi Complessi, via dei Taurini 19, 00185 Roma, Italy

contact details: anna.giardini@uniroma1.it, tel. +39 06 49913358, fax +39 06 490324

There has been considerable recent interest in the properties of unsymmetric molecules which play a crucial role in selectivity and function of biological molecules. Over recent years, considerable progress has been made in detailed characterization of their structure, reactivity and bonding using techniques as laser spectroscopy and supersonic beam production. The influence of weak interaction as van der Waals hydrogen bond, dispersion and repulsion forces on the shape and conformation of these compounds and of their complexes with chiral and achiral molecules is here discussed at the light of experimental results on laser absorption and ionization studies and theoretical investigation.

Our group has been involved in the study of gas phase chiral supramolecular recognition systems since many years. Chiral discrimination has been performed in many gas phase chiral complexes between a chromophore and alcohols, amines, neurotransmitters, lactates, ethers, etc. by Resonant Two Photon Ionization laser (R2PI) spectroscopy in supersonic beam.

Recently we have chosen organofluorine chromophores in order to investigate the effect of fluorine atom in complex formation. It is already established that substitution of fluorine into a molecule generally introduces minimal steric alterations, so facilitating interaction with receptor recognition sites and mechanistic studies [1]. The effect of fluorine as a substituent in bioactive compounds is based on its strong electron withdrawing effect and also on an electron pair donating mesomeric effect in conjugated systems [1].

As an example, we will report on the R2PI spectroscopy and mass spectrometry of complexes of (R)-1-phenyl-2,2,2-trifluoroethanol with various chiral and achiral partners.

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Photoabsorption cross sections for the fullerene ions C_{60}^{+} and C_{60}^{++}.

A.K. Belyaev[1], V.K. Ivanov[2], R.G. Polozkov[2], A.S. Tiukanov[1],
A.V. Solov'yov[3] and W. Greiner[3]

[1] Herzen University, Moika 48, 191186 St.Petersburg Russia
[2] St. Petersburg State Polytechnic University, Politechnicheskaya 29,
195251 St.Petersburg Russia
[3] Frankfurt Institute for Advanced Studies, Johann Wolfgang Goethe University,
Robert-Mayer Str. 10, D-60054 Frankfurt am Main, Germany

The photoionization cross sections of the fullerene positive ions C_{60}^{+} and C_{60}^{++} are calculated within the photon energy range from the ionization thresholds up to 80 eV and compared with the recent experimental data [1] and other calculations for C_{60}^{+} [1, 2]. The main features of the theoretical framework used in the present work has been developed earlier by us [3] and applied for the description of photoionzation of C_{60} and C_{60}^{+} [2, 3]. In the present work the theoretical approach is improved by means of using the Perdew-Wang parametrization for the exchange-correllation energy functional.

The total photoionization cross section is calculated as a sum of partial cross sections for each orbital. The ionization amplitude of each orbital is calculated both within the single-electron approximation and also by taking into account many-electron correlations. At the first stage, the frozen core model and the local density approximation (LDA) are used assuming that there is a single electron transition during the process. Then, the correlations between the transitions from different states are taken into account within the random phase approximation. Single-electronic states of a fullerene ion are calculated within the spherical jellium model with the self-consistent potential [3] determined within LDA. The basic Kohn-Sham equations are used for determining of the single-electronic wave functions.

The calculated photoionization C_{60}^{+} and C_{60}^{++} cross sections indicate the giant plasmon resonances with positions of $\approx$ 20 eV for both ions. This is in a good agreement with the classical Mie theory and the experimental data [1]. The analys shows that the dominant contribution in the giant resonance for the total cross sections is due to the ionization from the $6g$ and the $5f$ shells with some contribution from the $4d$ and $2s$ shells. The photoionization cross sections calculated in the present work fulfill the sum rule for both fullerene ions C_{60}^{+} and C_{60}^{++}, so in contrast to the previous calculations [2, 3] they are not scalled by any factor.

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Mo3-40

STABILITY OF MULTIPLY CHARGED FULLERENE DIMERS

H. Zettergren, S. Díaz-Tendero, M. Alcamí and F. Martín

Dep. de Química, C-9, Universidad Autónoma de Madrid, 28049-Madrid, Spain

We have calculated vertical ionization energies and the dissociation energies of multiply charged fullerene dimers ($[C_{60}]_2$) by means of Density Functional Theory. Several functionals (B3LYP, BLYP, MPW1B95, and B971) have been used to test the applicability of DFT methods to describe the van der Waals type neutral system, but all failed to catch an essential part of the dispersion interaction. In order to circumvent this problem, we have used an empirical dispersion correction to the BLYP functional as proposed by Grimme [1]. This approach gave a binding energy of 336 meV for the neutral system in accord with the experimental value of 275 ± 80 meV [2], which justifies the use of the empirical correction for this system. Once the dimer system is charged, the introduction of the long range Coulomb interaction means that an accurate description of the dispersion interactions are of minor importance. The sequence of vertical ionization energies for dimer charge states q=0-6 were deduced from single point calculations carried out at the binding distance of the neutral dimer system (center-center distance is R=10 A) .

In this communication, the ionization energies are compared with recent theoretical results concerning multiply charged *monomer* C_{60} [3] and discussed in view of recent experimental results on multiple ionization of fullerene dimers [4]. In addition, the calculated kinetic energy releases associated with the prompt decay of the multiply charged dimers (q>1) are compared with the corresponding experimental values [4].

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Mo3-41

AB INITIO INTERMOLECULAR POTENTIALS AND DYNAMICS OF Rg_2-DIHALOGEN CLUSTERS

R. Prosmiti, A. Valdés, C. Diez-Pardos, P. Villarreal, G. Delgado-Barrio

Instituto de Matemáticas y Física Fundamental, C.S.I.C.,
Serrano 123, 28006 Madrid, Spain

The intermolecular forces between atoms and molecules are of great importance in studies of solids, liquids and clusters. Over the last decade, enormous advances have been made in understanding of interaction potentials of small molecules. In particular, up to now accurate potentials have been obtained for triatomic vdW systems either by fitting the potential parameters to experimental data obtained from high resolution spectroscopic methods or by performing state-of-the-art electronic structure calculations. Studies of larger species are more complex and the construction of *ab initio* potential energy surfaces for such polyatomic molecular systems (including heavy atoms in our case) is a computationally prohibitive task. Thus, given the high quality *ab initio* PESs calculated for triatomic species, attempts are made using pairwise 3-body interaction potentials to represent PESs of larger Rg_nXY complexes.

In the present study the pairwise additivity of the 3-body interactions, derived from the He_2 and He-dihalogen CCSD(T) potentials, investigated by means of a*b initio* electronic structure and quantum-mechanical calculations [1]. The intermolecular interactions and structural properties of these clusters, which consist of homopolar and heteropolar halogens, are analyzed and the importance of additional effects, such like introducing electric dipole moment and larger reduced mass of the complex, is evaluated. Calculations of vibrational energies, including all 5 degrees of freedom, are performed and compared with experimental data from high resolution spectroscopy. Different structural models, such as 'police-nightstick' and 'linear', together with the traditional tetrahedral ones are predicted. For first time results on energetics and vibrationally averaged structures of such species are presented and their comparison with recent experimental predictions attributes to evaluate the quality of the surface [2]. Such PESs continue to be in demand since molecules are probes of superfluidity in He nanodroplets. In this sense, our current studies might serve to bridge the gap between the small cluster and the large cluster limits [3].

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Mo3-42

ATOM-SURFACE VAN DER WAALS INTERACTION IN THE NANOMETRIC RANGE

A. Laliotis, I. Maurin, P. Todorov, I. Hamdi, G. Dutier, S. Saltiel,
M.-P. Gorza, M. Fichet, D. Bloch and M. Ducloy

Laboratoire de Physique des Lasers, UMR7538 du CNRS et de l'Université Paris13,
93430 Villetaneuse, France email: bloch@lpl.univ-paris13.fr

The atom-surface interaction is one of the simplest prototype of the universal dipole-dipole interaction between neutral bodies and a key phenomenon in the ultimate cohesion of the matter. The electrostatic van der Waals (vW) regime, scaling in $C_3 z^{-3}$ (z: the atom-surface distance) should cover a considerable distance range ~1-1000 nm, *i.e.*. about 10 orders of magnitude in energy. However, little has been done to test the predicted dependence, and various subtle corrections are now currently predicted. Here, we report on a spectroscopic investigation of the vW interaction exerted onto the excited atoms of a vapour nanocell, whose nanometric thickness varies locally. This allows to reach distances as short as in the most recent comparable measurements [1], with record energy shift owing to the use of excited atomic levels.

Our method relies on a spectral analysis and on a fitting of the simultaneously recorded transmission and reflection spectra, with theoretical lineshapes. These two signals, originating in linearly independent spatial combinations of the atomic response, are processed independently. They yield however consistent results. A full series of measurements was completed for the high-lying state Cs ($6D_{5/2}$), for a thickness range 40-130 nm (NB : for a 40 nm thickness, 20 nm is the maximal atom-surface distance). A single set of parameters is enough to predict the transmission and the refection lineshapes for various thicknesses, showing [2] that the C_3 coefficient appears to be constant for all thickness within our experimental accuracy, yielding a check of the z^{-3} scaling law. Reproducibility of the spectra for various regions of the nanocell, and an estimate of the possible residual Stark shift, demonstrate that the observed spectral shift and distortions can be traced back to the Cs interaction with the YAG surface itself. The estimated value C_3 value (~ 14 ± 3 kHz.μm^3) is found to be in very good agreement with the theoretical prediction (~15 kHz.μm^3). This is a remarkable agreement, because various subtleties could affect the accuracy of the prediction, including corrections related to the nonzero-temperature of the vacuum, and short distances (non retarded) contributions of the electronic core.

The surface-induced vW energy-shift, exceeding several GHz (*i.e* 0.25 K) is much larger than obtained in all previous investigations. This corresponds to a considerable acceleration (~ 8.10^7 g for a Cs(6D) atom 20 nm away from one of the wall), that exceeds by orders of magnitude the one obtained in laser cooling techniques. This may open a realm of exotic possibilities, such as a gradient of density for an atomic gas in the extreme vicinity with the surface. Complementary experiments are now conducted on the D_1 resonance line. In spite of more delicate experimental issues, a reproducible investigation of cell thicknesses down to 25-30 nm appears now to be feasible. A preliminary analysis seems however to indicate a C_3 value exceeding theoretical predictions.

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Mo3-43

THE LATTICE PHONON STUDIES OF CCVD GROWN CNTs

R. Malekfar[1] and H. Asadi[2],
[1]Physics Department, Faculty of Basic Sciences, Tarbiat Modarres University,
P.O. Box 14115-175, Tehran, I.R. Iran, Malekfar@Modares.ac.ir
[2]Physics Department, Faculty of Sciences, Islamic Azad University,
North Tehran Branch, Tehran, I.R. Iran.

Abstract: Carbon nanotubes (CNTs) have been synthesized by Catalytic Chemical Vapour Deposition, CCVD at temperatures by 900 ˚C. A prepared catalytic source with a specific grain size was used [1, 2]. The powders of trivalent oxides with different grain nano sizes were prepared by using nitrate co-precipitation and solid state reaction techniques. Acetylene gas was used as carbon source material, hydrogen and argon gases were also used as the carrier gases.

We will report a complete analysis here on the effects of some different kinds of catalysts containing the oxides of transition metal particles and also their alloy combinations on the process of the length, shape, phonon lattice modes and the structural properties of the produced CNTs.

The sizes of the catalysts on silicon oxide or quartz substrates varied in a rather controlled manner by adjusting the conditions of the precursor powders with repeated mechanical mixing and extensive heat treatments at different temperatures. In order to monitor the effects of catalysts sizes on the nanotube growth parameters, we used different sizes of catalysts in micro and nano dimensions during CVD process.

For CNTs structural characterization and diameter measurement purposes, we used a Scanning Electron Microscopy system, SEM, model XL-30 manufactured by Philips. The synthesized CNTs qualities were also determined by Raman Scattering Spectroscopy, Thermo Nicolet Almega Dispersive Micro-Raman Spectrometer, which used a laser excitation line at 532 nm line in a backscattering configuration. The slit width was set to 20 μm and a Raman spectrum resolution of about 4 cm^{-1}. The detection system was a low temperature CCD detector operating at -50 ˚C. A typical Raman spectrum is shown in figure 1.

We believe the present results provide useful information for achieving diameter-controlled growth and the behaviour of catalyst particles on CNTs growth.

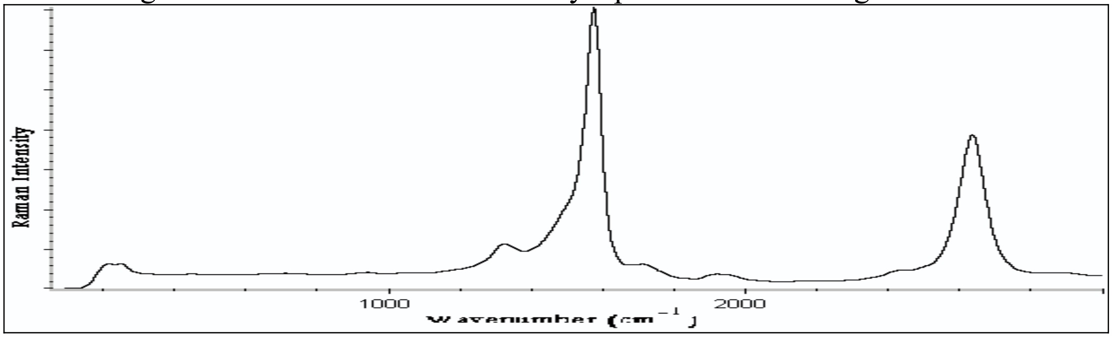

Fig. 1: A typical Raman Spectrum of CNTs in RBM, D and G region, obtained by excitation of 532 nm laser line.

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Mo3-44

ENERGETICS AND STABILITY OF CARBON NANOTUBES OF DIFFERENT CHIRALITIES

Maneesh Mathew, Ilia A. Solov’yov, Andrey V. Solov’yov and Walter Greiner

Frankfurt Institute for Advanced Studies
Johann Wolfgang Goethe University
Max-von-Laue-Str. 1
60438, Frankfurt am Main, Germany
E-mail: mathew@fias.uni-frankfurt.de

We systematically study carbon nanotubes of various chiralities and their stabilities to understand how the chirality influences the binding energy of nanotubes. Both *ab initio* and molecular mechanics methods are used for the investigation. The *ab initio* density functional theory (DFT) calculations are performed with the use of Gaussian 03 software package [1] and the molecular mechanics calculations are performed with the use of NAMD software package [2]. The results obtained through these studies are used for a better understanding of the growth mechanism of carbon nanotubes [3, 4]. The mechanism which controls the growth of a nanotube of desired chirality is poorly understood. Our studies can be used for the theoretical investigation of the dependence of growth of carbon nanotube on its chirality. The following figure explains the concept of the chirality of a nanotube by depicting how a nanotube of certain chirality, characterized by two integer numbers n and m, can be constructed from a graphite sheet. The figure below shows the structure of a chiral nanotube, corresponding to n=7 and m=4, being a typical conductive nanotube.

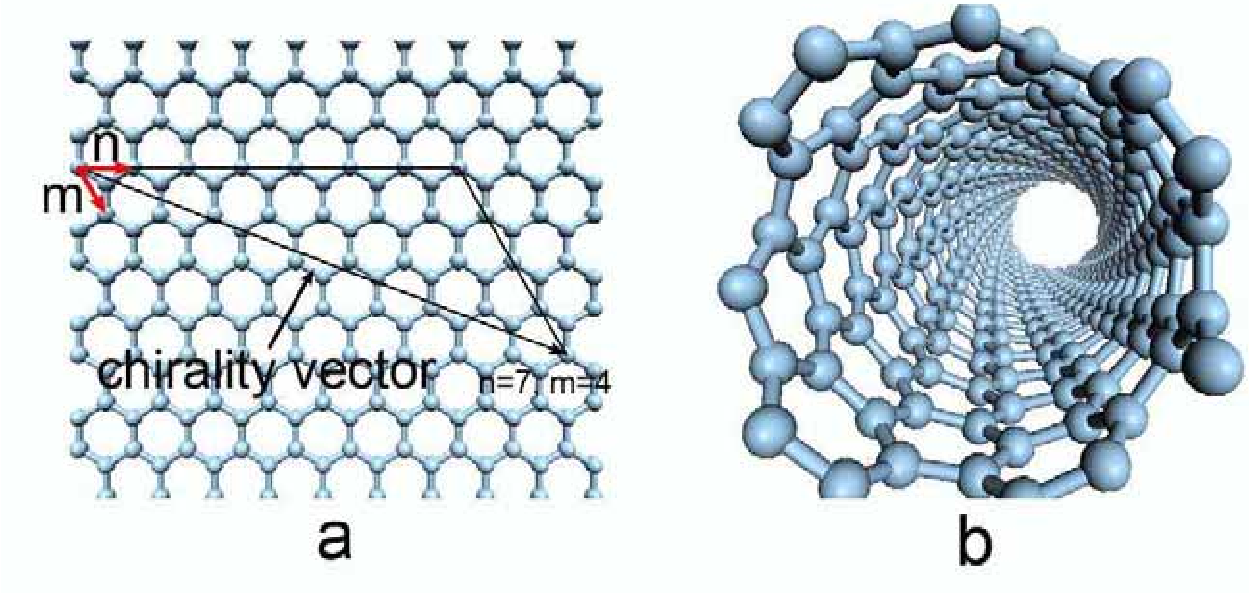

Figure 1: (a) Chirality vector shown in a graphite sheet; (b) The nanotube formed after folding the graphite sheet in figure-(a) along the chirality vector.

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Mo3-45

PRODUCTION, ANALYSIS AND MANIPULATION OF SILICON NANOPARTICLE FILMS

S. Jaksch[1], F. Zappa[1], P. Scheier[1]
[1]Institut für Ionenphysik und Angewandte Physik, Leopold-Franzens-Universität Innsbruck,
Technikerstrasse 25, A-6020 Innsbruck, Österreich
e-mail: stefan.jaksch@uibk.ac.at

Abstract

Films of silicon nanoparticles are formed by a magnetron sputtering and deposition onto freshly cleaved highly oriented pyrolitic graphite (HOPG). The effect of different parameters such as the distance between magnetron and graphite surface, pressure, discharge current and deposition time is analyzed with a variable temperature scanning tunneling microscope (STM). Well defined manipulation in the nanometer regime of the films with the STM tip is demonstrated and electronic properties of the films are probed by local scanning tunneling spectroscopy (STS).

Experimental

Silicon nanoparticles are formed by magnetron sputtering of a pure silicon target and deposited onto HOPG. The sample preparation chamber is directly connected to the STM which enables a fast transfer into the ultra high vacuum of the analyzing part of the instrument The structure of the deposited silicon nanoparticles is studied with high resolution STM images and the electronic properties of the films and individual particles is probed with local STS. The presently utilized STM enables to investigate the silicon nanoparticles in a temperature range from 25K to approximately 1300K.

Results and discussion

The growth of very homogeneous films of silicon nanoparticles is observed and studied. In the present work the effect of the distance between magnetron and HOPG substrate, the argon pressure, the current, and also the deposition time is carefully investigated. The distance turns out to be the most sensitive parameter: only for a distance between magnetron and HOPG of approximately 8cm stable films of nanoparticles are formed. The pressure of the Ar used for sputtering affected the deposition rate and the sticking coefficient of the silicon nanoparticles.

Modifications like vaporization, fusion and removal of nanoparticles with the STM tip on the nanometer scale are demonstrated. These techniques enable a novel kind of nanolithography where real grey scale patterns can be formed. Fig. 1 shows a grey scale pattern formed by increased tunneling currents. The right diagram shows a sectional scan at the position of the white line in the STM image.

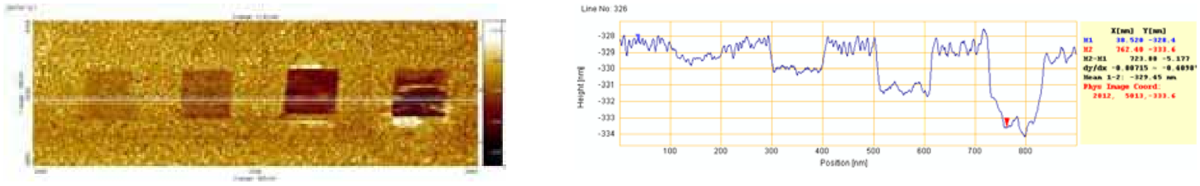

Fig 1: Greyscale series by different tunneling currents

Increased bias-voltage, applied between the tip and the silicon nanoparticle film, fuses silicon nanoparticles into larger objects with substantially increased electronic density of states. Finally it is possible to wipe all nanoparticles with the STM tip away by scanning an area with low (0.1 V) bias voltage. Surprisingly, most of the times this procedure does not affect the resolution of the STM tip.

It is planned to determine the conditions for a film that has optimum properties for subsequent nanolithography as described above. A high resolution grey scale image will be imprinted on such a film. The stability of the films and the nanolithography is going to be studied at elevated temperature.

This work is supported in part by the FWF, Wien, the European Commission through the I3 ITS-LEIF and the West Austian Initiative for Nano Networking (WINN).

Mo3-46

NONADIABATIC PHOTODISSOCIATION DYNAMICS IN $(HI)_2$ INDUCED BY INTRACLUSTER COLLISIONS

S. López-López, R. Prosmiti and A. García-Vela

Instituto de Matemáticas y Física Fundamental, C.S.I.C.,
Serrano 123, 28006 Madrid, Spain

The sequential photodissociation process has been investigated experimentally in small $(HI)_n$ clusters, with n=2 being the dominant cluster size [1]. Upon photodissociation of the HI monomer with 266 nm radiation, the measured H fragment translational energy spectrum displays two peaks at 12830 and 5287 cm^{-1}, which correspond to the $I(^2P_{3/2})$ and $I(^2P_{1/2})$ (hereafter referred to as I and I*, respectively) co-fragments. When $(HI)_n$ clusters with n=2 being the dominant size are photolyzed with 266 nm radiation, an additional peak with very small but detectable intensity is observed, corresponding to H atoms with around 20285 cm^{-1} of translational energy. This additional peak is separated from the higher energy monomer peak of 12830 cm^{-1} by 7455 cm^{-1}, which is nearly the energy difference between the I and I* states due to spin-orbit splitting. Such a peak was attributed to intracluster H/I* collisions produced upon photodissociation of a second HI moiety within the I*-$(HI)_{n-1}$ complex left behind after photodissociation of the first HI bond in $(HI)_n$ [1]. Some of the H/I* collisional events can induce a nonadiabatic electronic transition producing deactivation of I* to the lower I state, with the H fragment acquiring nearly all the excitation energy of I*.

The above process has been investigated [2] by means of a nonadiabatic wave packet simulation, assuming that $(HI)_2$ is the parent cluster photodissociated. In the model applied it is assumed that photodissociation of the first HI moiety in $(HI)_2$ has already occurred, and the simulation starts from the photodissociation of HI within the I*-HI complex left behind. The photodissociation dynamics occurs in two electronic surfaces, those associated with the $^3\Pi_{0+}$ and $^1\Pi_1$ states of HI [3] (which correlate with I* and I, respectively), that are coupled by spin-rotation coupling. The dependence of the spin-rotation coupling on the H-I* (or H-I) separation has been computed through high level *ab initio* calculations [2]. The dynamical simulation shows that indeed a nonadiabatic transition takes place from the $^3\Pi_{0+}$ electronic state to the $^1\Pi_1$ one as a consequence of intracluster collisions between H and I*, leading to deactivation of I* and very hot fragments. The H translational energy spectrum for 266 nm radiation is calculated and compared to the experimental one, showing good agreement. The fragment state distributions of the nonadiabatic photodissociation process are also investigated and discussed.

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POSTERS

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4. Coherent Control

Mo4-1

CONTROLLING DISSOCIATION PATHWAYS IN THE DEUTERIUM MOLECULAR ION WITH INTENSE ULTRASHORT LASER PULSES

I D Williams[*], C R Calvert[*], J McKenna[*], D S Murphy[*], W A Bryan[†],
E M L English[†], J Wood[†], I C E Turcu[δ], W R Newell[†] and J F McCann[*].

[*] School of Mathematics and Physics, Queen's University Belfast, Belfast, UK
[†] Department of Physics and Astronomy, University College London, London, UK
[δ] Central Laser Facility, CCLRC Rutherford Appleton Laboratory, Chilton, UK

Advances in laser technology, including the control of intensity, coherence, spectral range and duration of pulses, are of great interest and widespread application. The ultrashort infrared pulses currently available have durations which are shorter than the vibrational periods of even the fastest molecular ions (e.g. $H_2^+ \sim 15$ fs, $D_2^+ \sim 24$ fs). This has presented the opportunity of using these femtosecond pulses to create and image coherent dynamic vibrational wavepackets in these ultrafast systems [1,2].

At this meeting we will present a scheme [3] for controlling the quantum nature of the photodissociation process in diatomic molecules i.e. whether dissociation occurs via a one-photon or two-photon process. The scheme is dependent on the production of a coherent vibrational wavepacket and we demonstrate its application in the deuterium molecular ion, D_2^+. Using a theoretical model, a novel method for controlling the ratio of single- to two-photon dissociation is proposed and the experimental realization of such a control scheme is demonstrated by means of a pump-probe technique.

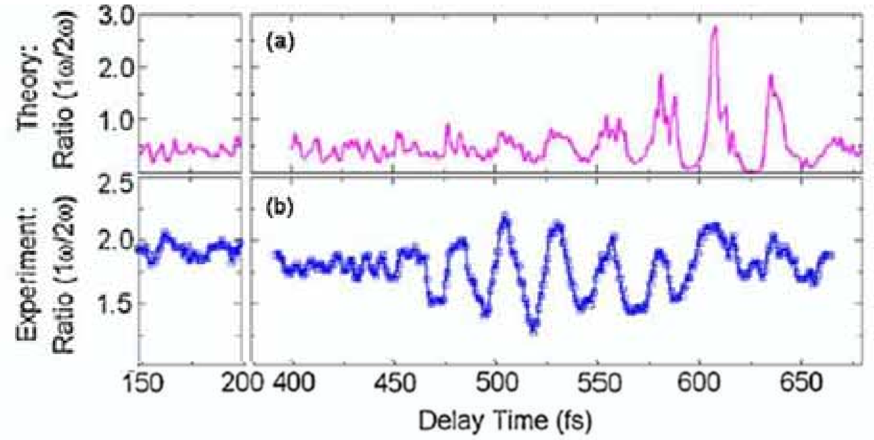

Figure 1: Demonstration of control over D_2^+ wavepacket photodissociation. The ratio of single-photon (1ω) to two-photon (2ω) dissociation is shown to be dependent on the delay time (after the initiation of D_2^+ wavepacket) at which the molecule is probed. Plot (a) displays the theoretical prediction for the 1ω/2ω ratio. The experimental data in plot (b) confirms the application of this technique.

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Mo4-2

PUMP-PROBE SPECTROSCOPY IN DEGENERATE TWO-LEVEL ATOMS WITH ARBITRARILY STRONG FIELDS

T. Zigdon, A. D. Wilson-Gordon, and H. Friedmann
Department of Chemistry, Bar-Ilan University, Ramat Gan 52900, Israel

In our previous work [1] on pump-probe spectroscopy in realistic degenerate two-level systems (TLS) and model systems, we discussed the role of transfer of coherence (TOC) and transfer of population (TOP) between the ground and excited hyperfine states in producing electromagnetically-induced transparency (EIA) peaks in the probe spectrum, when an $F_g \rightarrow F_e = F_g + 1$ transition in an alkali-metal atom interacts with a strong pump and ***weak*** probe that have perpendicular or parallel polarizations. These spectra were calculated using a computer program that both constructs and solves the relevant optical Bloch equations.

In our recent work, we consider the effect of a ***strong*** probe on the pump absorption and refraction spectra when the pump and probe polarizations are perpendicular. The problem is tractable for all pump and probe polarizations, apart from σ polarization. A number of interesting differences from the weak-probe case are found. For example, when the probe is sufficiently strong, the pump and probe spectra show complementary behavior (see Fig. 1). The four-level *N* system can be used to model the degenerate TLS interacting with a σ^+ polarized pump and a π polarized probe. Insight into the origin of the complementary behavior can be gained from a comparison of the contributions to the total pump and probe absorption spectra from the individual Zeeman transitions in the realistic degenerate TLS, and in the model *N* system.

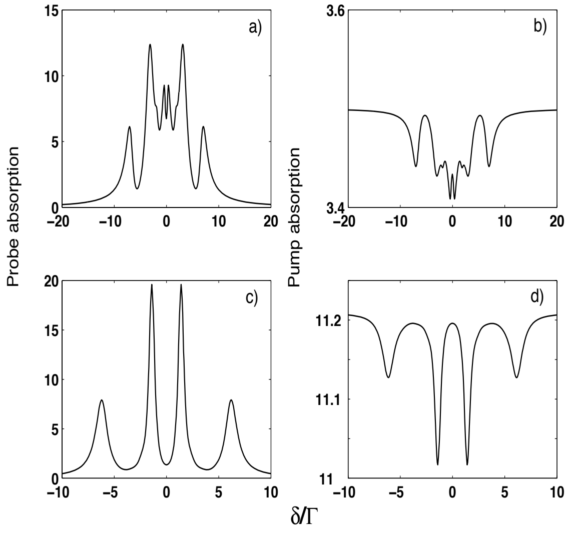

Fig. 1 Complementary behavior of probe and pump absorption spectra for (a,b) artificially closed $F_g = 1 \rightarrow F_e = 2$ and (c,d) cycling $F_g = 2 \rightarrow F_e = 3$ transition in ^{87}Rb.

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Mo4-3

Manipulation of dark states with white light

M.Auzinsh [1], N.N.Bezuglov [2], K.Miculis [1]

[1]University of Latvia, Dept. of Physics, Zellu Street 8, LV-1002 Riga, Latvia
[2]V.A.Fock Institute of Physics, St. Petersburg State University, 198904, Russia

Atoms and molecules prepared in well-defined quantum states are widely used in modern atomic physics. The conventional way to manipulate quantum states exploits atomic interactions with two coherent laser fields [1] and requires highly monochromatic light: frequency fluctuations spoil coherent effects easily. We demonstrate, nevertheless, that the control of atomic states can be attained by exciting an atom having $J = 1$ ground (g) and $J = 0$ excited (e) states (Fig.1) with broad-band (white) light. The radiation is elliptically polarized, so that the cyclic components $E^{\pm 1}$ couple simultaneously g-sublevels $m = \pm 1$ with e-state $m = 0$. The upper state decays spontaneously (total decay rate Γ_0) onto g-sublevels with partial rates $\Gamma_{0i} = \Gamma_0 / 3$. The evolution of the atomic system under the interaction with white radiation is described via the equation of motion for the density matrix $\rho_{i,j}^{(g,e)}(t)$ [2,3]. It allows a simple stationary solution

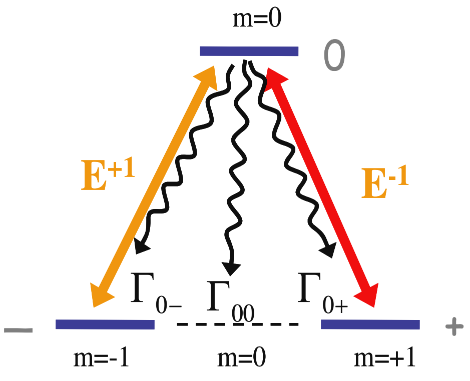

Fig.1 Energy levels diagram

$$\rho_{ii}^{(g)} = \tilde{\Omega}_i \tilde{\Omega}_i / \left(\tilde{\Omega}_+^2 + \tilde{\Omega}_-^2 \right); \qquad \rho_{ij}^{(g)} = -\tilde{\Omega}_i \tilde{\Omega}_j / \left(\tilde{\Omega}_+^2 + \tilde{\Omega}_-^2 \right) \ (i,j=+,-); \ \ \rho_{00}^{(e)} = 0, \qquad (1)$$

which contains effective “Rabi frequencies” (ERF) $\tilde{\Omega}_\pm \ \ \| d \| E_\pm / \hbar$. Solution (1) has two distinguishing futures: (i) the absence of an e-state population, which results in zero spontaneous emission; (ii) evident structure of pure superposition of g-sublevels $m = \pm 1$. In another words, Eq. (1) describes a dark state formed with white light. This fact opens new perspectives for atom control based on dark states. As an example, we present the efficiency of the STIRAP-type population transfer [1] from the $m = -1$ sublevel (initially populated) to the $m = +1$ sublevel (initially empty). It is demonstrated, in particular, that two pulses of identical amplitudes $\tilde{\Omega}_\pm = \tilde{\Omega}_0 \times \exp(-(t - \Delta_\pm)^2 / 2\sigma^2)$ with duration $\sigma = 2$ ns and offset in time by $\Delta = \Delta_+ - \Delta_-$=2 - 4 ns, may provide the desired transfer with practically 100% efficiency.

This work was supported by Russian FBR, Grant 05-02-16216, EU TOK project LAMOL, NATO Grant EAP.RIG.981378, and the European Social Fund.

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Mo4-4

COHERENTLY CONTROLLED ADIABATIC PASSAGE TO MULTI-CHANNEL CONTINUUM STRUCTURE

Ioannis Thanopulos* and Moshe Shapiro

Department of Chemistry, University of British Columbia, Vancouver B.C., Canada

*E-mail: ioannis@chem.ubc.ca

We present the merging of Coherent Control (CC) and Adiabatic Passage (AP) and the type of problems that can be solved using the recently developed ``Coherently Controlled Adiabatic Passage'' (CCAP) method [1].

We start by discussing the essence of CC as the guiding of a quantum system to arrive at a given final state via a number of different quantum pathways.

The guiding is done by ``tailor-made" external laser fields. We show that selectivity in a host of physical and chemical processes can be achieved by controlling the interference between such quantum pathways. We then discuss the AP process, in which a system is navigated adiabatically along a single quantum pathway, resulting in a complete population transfer between two energy eigenstates. The merging of the two techniques (CCAP) is shown to achieve both selectivity and completeness, demonstrated in a series of applications involving bound-states.

We lastly present a solution to the ``Multi-Channel Quantum Control'' problem, where the CCAP is successfully applied for first time to a system including continuum structures. Selective and complete population transfer from an initial bound state to M energetically degenerate continuum channels is achieved under loss-free conditions. The control is affected in an adiabatic fashion proceeding via N bound intermediate states. In a realistic situation, where presence of real loss is inevitable, we further demonstrate that the control efficiency remains significant. We illustrate the viability of the method by computationally controlling the multi-channel photodissociation of methyl-iodide [2,3].

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Mo4-5

QUANTUM DYNAMICS OF A KICKED HARMONIC OSCILLATOR

Calvin Stubbins
Department of Physics, Franklin & Marshall College,
Lancaster, Pennsylvania, USA
E-mail: calvin.stubbins@fandm.edu

A classical system of two masses connected by a spring and subjected to a time-dependent pulse is used to model a kicked quantum harmonic oscillator in free space. This model is of interest because it is related to the Mössbauer effect where the kick is due to the emission of a gamma ray. Furthermore, the model results in coherent states and can be solved analytically.

If x_1 and x_2 are the positions of the masses, m_1 and m_2, the potential energy of the system is written as the sum of energy due to the potential of the spring and the energy bestowed by the force, $F(t)$, acting on m_2

$$V = \frac{1}{2}\mu\omega^2(x_2 - x_1)^2 - F(t)x_2. \tag{1}$$

In center of mass coordinates, this potential is used to motivate the form of the Schrödinger equation for the quantum system. The wave function is found using two extended Galilean transformations [1] and the separation of variables technique [2].

The force applied to the system is specified as a Gaussian pulse, and the expectation value for the energy of a system initially in the ground state is calculated. Before the pulse is applied, the system has energy equal to that of an unperturbed harmonic oscillator plus that of the entire system as a free particle. The energy increases as the force acts on the system and is constant once the pulse has died off.

The probability that the system is in an unperturbed harmonic oscillator state is calculated to have the form

$$|C_m|^2 \propto e^{-|z|^2}\frac{z^{2m}}{m!}, \tag{2}$$

indicating that our model produces coherent states [3]. We further show that any force acting on the system in a stationary state will produce coherent states once the force has gone to zero, except in the case where the force is turned off at the moment when the oscillator is at its equilibrium position with zero velocity. In this case, the wave function is the original stationary state.

Finally, we examine the case of a delta-function pulse acting on a particle in a general potential, $V(x)$. We find a form for the wave function and investigate the system's behavior if it was initially in a stationary state.

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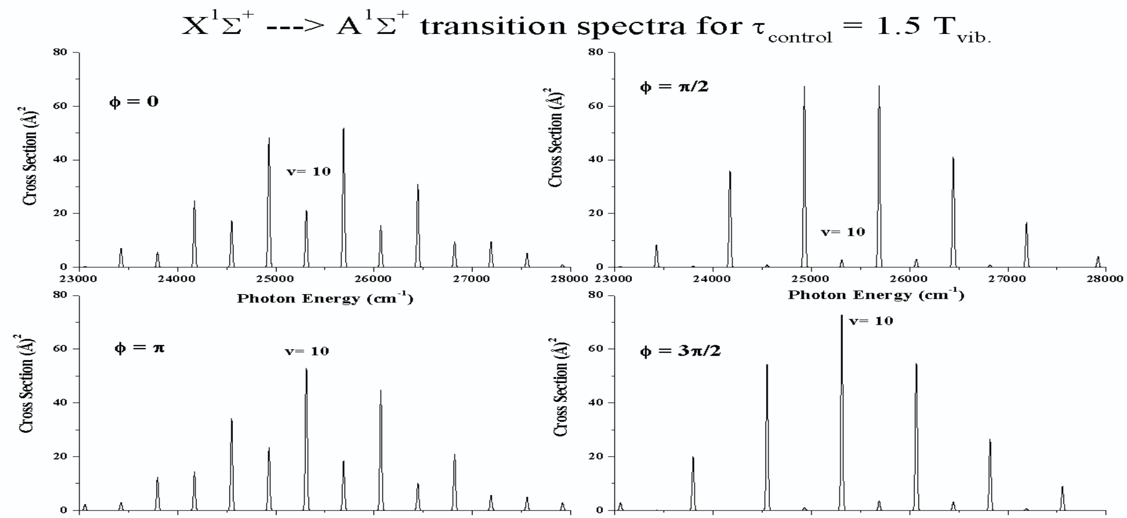
Mo4-6

Control of wavepacket interference and vibrational distribution by control of phase between ultrashort pulses

Anindita Bhattacharjee[i] and Krishna Rai Dastidar[ii]

Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032

By ab-initio calculation we have shown that quantum interference [1] between two vibrational wave packets in NaH molecule can be controlled by using two phaselocked ultrashort pulses. In NaH molecule, two consecutive 4 fs (FWHM) Gaussian pulses (pump and control pulses) generate two wave packets on the $A^1\sum^+$ state around the vibrational level v'=10. The second pulse (control) is delayed by $\tau_{control}$ from the first pulse (pump). Interference between two wavepackets is dependent on the delay $\tau_{control}$ and the phase difference φ between two pulses. For a particular delay time, we have found that the phase difference φ controls the vibrational distribution of population on the $A^1\Sigma^+$ state. For delay $\tau_{control}$ ~1.5 T_{vib}. where, $T_{vib.}$ is the average vibrational period of the levels v'= 6-14 of the $A^1\Sigma^+$ state and for different relative phases, φ= 0, $\pi/2$, π and $3\pi/2$ between the pulses, the group of even and odd vibrational levels are populated differently from each other. In Fig. 1, spectra for excitation of the molecule from v=0 level of ground state to different vibrational levels of $A^1\sum^+$ state by the pump and control pulses are shown. When φ= $\pi/2$, cross section for excitation of odd vibrational levels is high whereas that for even vibrational levels is nearly zero. This feature is reversed when φ= $3\pi/2$, i.e. even vibrational levels have large population. This is the result of quantum interference between two wavepackets on the $A^1\sum^+$ state that produces beats in the excitation spectrum depending upon the relative phase difference between the wavepackets.



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[i] E-mail : anny_b_2000@yahoo.com

[ii] E-mail : spkrd@iacs.res.in

Mo4-7

A GENERAL SCHEME FOR CONSTRUCTION OF COHERENT STATES OF ANHARMONIC OSCILLATORS

Marcin Molski

Adam Mickiewicz University of Poznań, PL 60-780 Poznań, ul. Grunwaldzka 6
e-mail: marcin@rovib.amu.edu.pl

Coherent states are very useful tool for investigation of the phase-space properties of quantum systems and interactions of molecules with high-frequency electromagnetic fields. Studies of the latter require construction of coherent states for general anharmonic potentials describing vibrational displacements of nuclei in molecules. Such potentials take into account both the harmonic limit in the vicinity of the potential minimum and the dissociation limit for highly extended bonds. The notion *coherent* reflects the fact that such states remain localized on the corresponding classical trajectory and do not change their functional form with time. Coherent states of anharmonic oscillators are defined in the following manner:

i. they are eigenstates of the annihilation operator $\hat{A}|\alpha\rangle = \alpha|\alpha\rangle$,
ii. they minimize the generalized uncertainty relation $(\Delta q)^2(\Delta p)^2 \geq \langle g\rangle^2/4$ in which q and p denote the vibrational coordinate and conjugated momentum respectively, whereas g is defined by the commutation relation $[q,p] = ig$;
iii. in the harmonic limit they are states that arise from the operation of the unitary displacement operator $\exp(\alpha\hat{A}^{+} - \alpha^*\hat{A})|0\rangle = |\alpha\rangle$; here $\alpha^*$and $\langle\alpha^*|$ denote the eigenvalue and eigenstate of the creation operator $\langle\alpha^*|\alpha^* = \langle\alpha^*|\hat{A}^{+}$.

The coherent states of anharmonic oscillators have been constructed using several alternative approaches. In the method proposed by Nieto and Simmons [1] the position and momentum operators are chosen in such a way that, in these variables, the resultant Hamiltonian resembles that for an harmonic oscillator whose coherent states are well known. In the approach developed by Perelomov [2] the construction of generalized coherent states is connected with irreducible representations of a Lie group. Appling this formalism Kais and Levine [3] have constructed coherent states of anharmonic Morse oscillator employing the energy dependent SU(1,1) representation.

Mo4-8

SELECTION OF UNRESOLVED HYPERFINE STATES OF MOLECULES USING THE AUTLER-TOWNES EFFECT

T. Kirova[1], A. Ekers[1], M. Auzinsh[1], N. Bezuglov[2], K. Blushs[1]

[1] Institute of Atomic Physics and Spectroscopy, University of Latvia, Riga, Latvia
[2] Fock Institute of Physics, St. Petersburg State University, St. Petersburg, Russia

The Autler-Townes (AT) effect [1] is the high-frequency analogue of the splitting of two degenerate levels by a dc Stark field. It has potential for development of new applications to molecular spectroscopy, like obtaining the transition dipole moment matrix element [2, 3] and as well as lifetime and branching ratios of highly excited molecular states using cw laser fields [3]. The possibility to achieve quantum state control using the AT effect has been studied by using the Nonresonant Dynamic Stark Effect (NRDSE) [4] and the Selective Population of Dressed States (SPODS) [5] techniques. An all-optical method for aligning non-polar molecules for chemical reactions was demonstrated [2b] based on AT effect and its dependence on the molecular magnetic quantum number (M_J). The latter enables resolution of individual M_J peaks, leading to additional state selectivity and better control of the molecular properties.

In our present work we extend the quantum control schemes to more complex energy level systems. In particular, the effect of coupling between nuclear and electronic angular momentum, which leads to occurrence of hyperfine structure, is studied in molecular level systems. Each molecular hyperfine level is 2F+1-fold degenerate over the projection of F (i.e., M_F). Since the coupling of hyperfine components by the laser field depends on the hyperfine and magnetic quantum numbers F and M_F, this will lead to a different AT splitting for each involved hyperfine level. Simulations based on solving the density matrix equations of motion show that application of a strong coupling field leads to lifting of the M_F degeneracy, thus giving the opportunity to selectively address hyperfine components of excited molecular states. Future calculations will be performed to predict possible experimental applications of the control mechanisms.

The work is expected to yield novel approaches allowing one to gain control over the actual molecular eigenstates under the conditions when hyperfine splitting cannot be resolved using the usual spectroscopic means.

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Mo4-9

ELECTROMAGNETICALLY INDUCED TRANSPARENCIES IN CIRCULARLY POLARIZED LIGHT IN CROSS MAGNETIC FIELDS

J. Dimitrijević, A. J. Krmpot, M. M. Mijailović, Z. D. Grujić, D. Arsenović, and B. M. Jelenković

Institute of Physics, University of Belgrade, 11080, Belgrade, Serbia

We have investigated theoretically and experimentally transmission of circularly polarized light through Rb vapour, when light is resonant to the closed $F_g \rightarrow F_e = F_g + 1$ transitions in ^{85,87}Rb and atoms are subject to cross magnetic fields. Typically, we scan magnetic field parallel to the laser wave-vector, and apply additional transverse magnetic fields. Theoretically, the light absorption is obtained from calculated populations of magnetic sublevels of the excited state. Experimentally, laser absorption was measured by detecting the signal from the photo-diode and recorded by the digital oscilloscope operated in the average mode.

It is known that linearly polarized light for $F_g \rightarrow F_e = F_g + 1$ transitions leads to electromagnetically induced absorption (EIA) [1]. Elliptically polarized light, in a Doppler broadened media, can enhance EIA nearly ten fold [2]. When circular polarization, on the other hand, is interacting with a two level system, subject to magnetic field parallel to the laser wave vector, optical trapping leads to the population accumulation in "edge" magnetic sublevels. In this case there are not coherence effects that will lead to change of the light absorption when magnetic field varies around zero value. Additional magnetic field, transverse in respect to axial magnetic field, dramatically changes this picture via new quantization axis and light polarization which can induce transmission gain through coherence effects. Another coherence effect that leads to transmission gain, electromagnetically induced transmission (EIT) is observed in atomic systems for which $F_g \rightarrow F_e \leq F_g$. We can call the transmission gain, obtained with input circular light, a circular electromagnetically induced transmission (CEIT). Through more quantitative study this work extends the previous work on Hanle effects with circular light [3]. We have calculated amplitudes and widths of CEIT as a function of two orthogonal magnetic fields, at different laser intensities, without and with Doppler effect. We have shown that both amplitudes and widths of CEIT (at zero value of scanning magnetic field) fast increase when transverse magnetic fields increases from ~1 mG to ~200 mG. Experimental transmission curves for laser intensities between 0.1 to 100 mW/cm^2 were compared with theoretical curves and observed similarities and differences were discussed.

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Mo4-10

ANALYTICAL SOLUTION OF THE DEGENERATE LANDAU-ZENER MODEL

G. S. Vasilev[1], S. S. Ivanov[1] and N. V. Vitanov[1,2]

Department of Physics, Sofia University, James Bourchier 5 Boulevard, 1164 Sofia, Bulgaria[1]

Institute of Solid State Physics, Bulgarian Academy of Sciences, Tsarigradsko Chaussée 72, 1784 Sofia, Bulgaria[2]

The exact analytical solution of the degenerate Landau-Zener model [1], wherein two bands of degenerate energies cross in time, is presented [2]. This model can be viewed as the unsolved limiting case of the multiple-crossings grid models for vanishing level spacing. The model also represents the unsolved limiting case of the bow-tie models when all energies that cross at the same time coalesce into only two different slopes. It also generalizes the solution by Kyoseva and Vitanov [3], which assumes one degenerate and one nondegenerate level. The solution is derived by using the Morris-Shore transformation [4], which reduces the fully coupled system to a set of independent nondegenerate two-state systems and a set of decoupled states. Each of the independent two-state systems represents a standard, nondegenerate LZ problem, whereas the decoupled states do not evolve. The solution of the degenerate LZ problem is constructed by this set of two-state LZ solutions, which interfere and produce interesting features in the probabilities in the original basis. In particular, it turns out that not all transition probabilities are defined, as far as an infinite interaction duration is concerned, due to the divergence of the phase of the off-diagonal element of the propagator in the original Landau-Zener model. In general, apart from some special cases, only the transition probabilities between states within the same degenerate set exist, but not between states of different sets.

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Mo4-11

ENHANCED FOUR-WAVE MIXING IN MERCURY ISOTOPES, PREPARED BY STARK-CHIRPED RAPID ADIABATIC PASSAGE

Martin Oberst*, Jens Klein, and Thomas Halfmann**

Department of Physics, University of Kaiserslautern, 67653 Kaiserslautern, Germany

We demonstrate significant enhancement of four-wave mixing (FWM) in coherently driven mercury isotopes to generate vacuum ultraviolet radiation at 125nm [1]. The enhancement is accomplished by preparation of the mercury atoms in a state of maximum coherence, i.e. maximum nonlinear-optical polarization, driven by Stark-chirped rapid adiabatic passage (SCRAP) [2,3]. In this technique a pump laser at 313 nm excites the two-photon transition between the ground state $6s^2\ {}^1S_0$ and the target state $7s\ {}^1S_0$ in mercury. A strong, off-resonant radiation field at 1064 nm generates dynamic Stark shifts. These Stark shifts serve to induce a rapid adiabatic passage process on the two-photon transition. The maximum coherence permits efficient four-wave mixing of a pump laser and an additional probe laser at 626 nm. The efficiency is further enhanced, as the SCRAP process allows to stimulate the complete ensemble of different mercury isotopes to participate in the frequency conversion process. This enlarges the effective atomic density of the medium. Thus, we observe the generation of vacuum-ultraviolet radiation at 125 nm enhanced by more than one order of magnitude [1] with respect to conventional frequency conversion (see fig. 1). Parallel to frequency conversion, we also monitored the evolution of the population in the medium by laser-induced fluorescence. These data demonstrate efficient coherent population transfer by SCRAP.

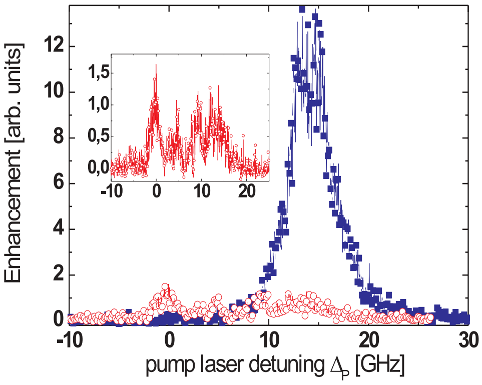

Fig. 1: Relative intensity of the vacuum-ultraviolet radiation, when the pump laser frequency is varied in the vicinity of the two-photon resonance (hollow circles, red line). The ordinate is normalized to the peak value of the signal, when the Stark laser is switched off. The zero of the abscissa is calibrated to the two-photon resonance for the mercury isotope ^{202}Hg. When the Stark laser is switched on, i.e. the system is driven to maximum coherence by SCRAP, the efficiency of the FWM-process increases significantly (solid squares, blue line). The enhancement with respect to conventional frequency conversion is more than one order of magnitude. The inset shows the spectrum when the Stark laser is switched off.

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** oberst@physik.uni-kl.de*　　*** http://www.quantumcontrol.de*

Mo4-12

Controlling statistical properties of stored light

Sylwia Zielińska-Kaniasty[1], Andrzej Raczyński[2], Karolina Słowik[2]
and Jarosław Zaremba[2]

[1] Instytut Matematyki i Fizyki, Uniwersytet Technologiczno-Przyrodniczy,
Bydgoszcz, Poland

[2] Instytut Fizyki, Uniwersytet Mikołaja Kopernika, Toruń, Poland

A medium of atoms in the tripod configuration, irradiated by two control fields, has recently been shown theoretically to act as a flexible and effective beam splitter [1]. Two time-separated incoming light pulses can be stored in two orthogonal combinations of atomic coherences, which can in turn be later transformed back into two time-separated outgoing pulses. Statistical properties of the latter are determined by the amplitudes and phases of the releasing control pulses.

Combinations of both classical and nonclassical pulses will be examined. The probability distributions and/or statistical moments of the number of outgoing photons will be shown as functions of the parameters of the control pulses. The external manipulations of the atomic system at the storage stage are taken into account and their influence on statistical properties of stored light will be discussed. Also the case of two stored pulses which overlap partially will be considered .

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Mo4-13

COHERENT CONTROL OF LIGHT-SHIFTS AND APPLICATION TO SLOW-LIGHT AND PULSE AMPLIFICATION.

M.A.Bouchene , J-C.Delagnes, F.A. Hashmi

Laboratoire CAR, Université Paul Sabatier, 118 Route de Narbonne 31062 Toulouse cedex, France
E-mail : aziz@irsamc.ups-tlse.fr

The interaction of strong laser fields with matter causes light-shifts that play an important role in many fields as quantum optics, molecular physics and chemistry. These effects induce dramatic changes in both the structure and the dynamics of the driven systems [1] and are strongly enhanced when laser pulses are used. Rapid adiabatic passage, stimulated Raman adiabatic passage (STIRAP) and Stark-chirped adiabatic passage (SCRAP) are non-exhaustive examples of effects where light-shifts also play a crucial role. Although light-shifts prevail in so many phenomena, only little possibilities are offered to control their influence. This is generally done by controlling the laser intensity or the detuning when the interaction is not resonant. Here, we describe an experiment where we achieve coherent control of light-shift [2]. We consider a duplicated two-level system (fig. a) where a strong femtosecond pulse drives each of the two-level system and a weak resonant femtosecond pulse connects cross transitions. In the adiabatic representation, the dressed states are connected by the weak pulse with a coupling strength that differs whether the states are identically or oppositely light-shifted, and that also depends on the relative phase of the optical waves. The control comes from adjusting this phase, which we achieve experimentally by varying the time delay between the pulses (fig. b). Depending on the relative phase, the weak pulse can be amplified, or transmitted without any modification. Likewise in coherent control experiments, here the control results from the interference between two excitation quantum paths, corresponding to the absorption and to the emission by the dressed atomic system of one photon from/on the weak field mode respectively. This effect paves the way to many applications and we will describe a new method to slow the light in an atomic medium.

(a)Excitation scheme of rubidium in cross polarisation. A strong π polarised pulse connects each of the two-level system whereas a weak σ polarised pulse connects cross transitions.

(b) Output energy of the σ pulse. Oscillations occur although the weak and the strong pulse are orthogonally polarized. The measured period is half the optical period.

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Mo4-14

Stimulated Raman Adiabatic Passage (STIRAP) in a Pr:YSO crystal

Jens Klein, Fabian Beil, and Thomas Halfmann

Fachbereich Physik, University of Kaiserslautern, Germany

STIRAP [1] is an efficient and robust technique to manipulate population distributions in atoms and molecules. Therefore, STIRAP is an interesting tool for optical data storage and quantum information processing. Experimental studies of STIRAP have been mainly constricted to media *in the gas phase*. However, it is solid media which are (due to their high density and scalability) of special interest for applications, but usually ultra-fast decoherence processes in solids prevent the implementation of coherent excitations. Rare earth ion doped inorganic crystals combine the advantages of solids and the coherent properties of atoms. Therefore, a growing number of studies on coherent excitations are performed in these media at present. Recently, first evidence for STIRAP in a doped crystal has been reported [2].

We implemented STIRAP in a Pr^{3+}:Y_2SiO_5 crystal (Pr:YSO) [3]. The experiment yielded striking data on adiabatic population transfer in a solid. The experiment follows our successful implementation of rapid adiabatic passage in Pr:YSO [4]. Population is transferred between two hyperfine levels of the $^3H_4$ ground state of an selected ensemble of Pr^{3+} ions (see fig. 1). The population of the target state is observed by absorption of a delayed probe pulse. The variation of the transfer efficiency vs. the delay of the Stokes laser pulse with respect to the pump laser pulse is shown in fig. 1. Efficient, adiabatic transfer is observed for negative delay (STIRAP) as well as for positive delay. The latter is due to an alternative adiabatic passage process via dressed states. In both adiabatic processes, the transfer efficiency clearly exceeds the value for excitation by coincident pulses.

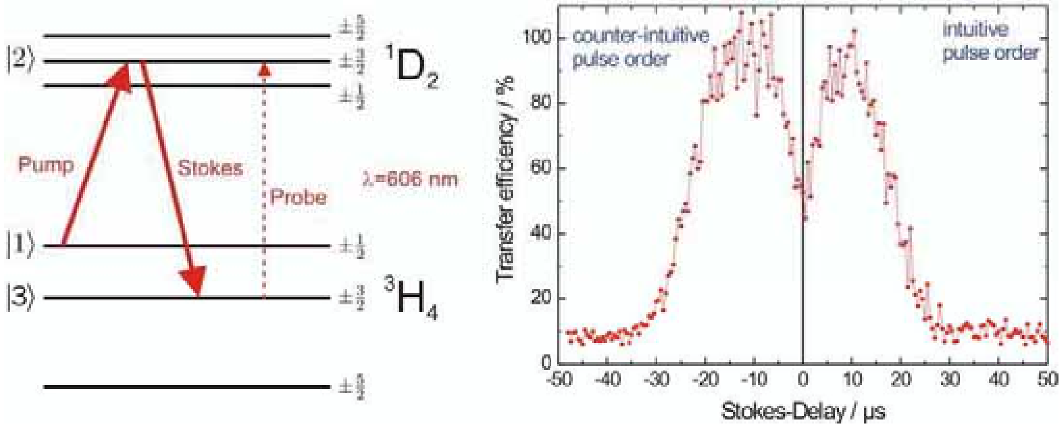

Figure 1 Coupling scheme for STIRAP in Pr :YSO. The scheme shows the transitions for STIRAP and the probe process. Variation of the transfer efficiency vs. the delay between Stokes and pump pulse.

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Mo4-15

Picosecond to Nanosecond Pulse Shaping via a Chirp-Transform Scaling Technique

N. Forget, A. Cotel*, T. Oksenhendler, C. Le Blanc*, D. Kaplan and P. Tournois

Fastlite, Bat 403, Ecole Polytechnique, 91128 Palaiseau, France
**LULI, Ecole Polytechnique, 91128 Palaiseau, France*

Numerous applications require a careful control of the phase and amplitude of pulses with GHz to THz spectral widths: coherent control of atomic systems with GHz linewidths, amplitude pulse shaping for nanosecond high-intensity laser systems… In this talk, we present an original technique based on a broadband acousto-optic programmable dispersive filter (AOPDF) to fill the technological gap between time-domain (bandwidth < 10GHz) and spectral-domain (resolution > 100 GHz) pulse shaping devices.

An input broadband and ultrashort laser pulse of center frequency ν_1 is sent into a dispersive device, stretching the pulse to a length τ_2. This stretched pulse is then seeded in an optical parametric amplifier (OPA) which is pumped by a long single-frequency laser pulse of frequency $\nu_0 > \nu_1$. The amplified signal pulse is then shaped in phase and amplitude by a wideband ultrafast pulse shaper and then mixed in a nonlinear crystal with the idler output of the OPA (of center frequency $\nu_0 - \nu_1$). The laser pulse generated by sum frequency generation (SFG) is a narrowband pulse of frequency ν_0 shaped in phase and amplitude. This technique allows to magnify the pulse-shaping resolution of the broadband programmable dispersive filter by a factor close to the chirp ratio of the stretched short pulses [1]. With chirp ratios of $\sim 10^3$ (a 100fs pulse stretched to 100 ps for example), the spectral resolution in increased by $\sim 10^3$ and one can control the shape of the output narrowband pulses with a picosecond time resolution.

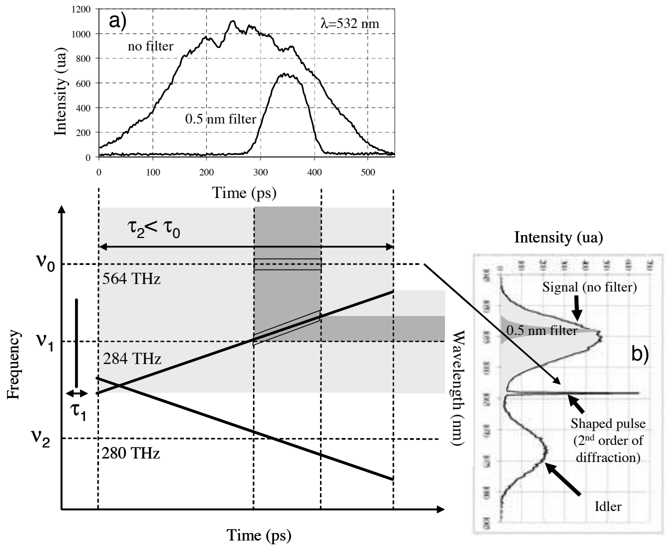

Fig. 1: a)Two different shaped pulses : gaussian pulse of 450ps FWHM (no filter) and top-hat pulses of 85 ps (0.5 nm filter). b) spectra at the output of the SFG crystal : signal pulse (1055 nm, broadband), idler pulse (1073 nm, broadband) and reconstructed narrowband pulse at 532 nm.

We applied this technique to 7ns pulses at 532nm originating from a commercial seeded, Q-switched, frequency-doubled Nd:YAG laser. The spectral width of linearly chirped broadband pulses pulses is of 4.5nm with a stretch factor of ~100 ps/nm and a central wavelength of 1055nm. Fig 1b shows the spectral composition of the three beams at the output of the SFG crystal : as expected, the reconstructed pump pulse is narrowband with a central wavelength of 532nm. The temporal profile of the reconstructed pulses were then measured with a streak camera.When a broadband filter (10nm) was implemented by the AOPDF, a gaussian pulse of 300ps pulse was measured.With passband filters of 3nm and 0.5nm, top-hat pulses of 300ps and 85 ps were recorded (Fig 1a). These durations are in good agreement with the stretch factor of the signal pulse (100ps/nm) given the resolution of the streak camera. The 10%-90% rise-time of the top-hat pulse is about 50ps, which is also in agreement with the spectral resolution of the AOPDF.

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Mo4-16

NEW WAY TO INDUCE AND CONTROL ELEMENTARY CHEMICAL TRANSFORMATIONS ON A GAS-SOLID INTERPHASE BY MEANS OF RESONANT LASER RADIATION

V. V. Petrunin

Physics and Chemistry Department, University of Southern Denmark
5230 Odense M, Denmark

We will briefly review different approaches used in laser chemistry. By considering them under a specific angle and using basic theoretical arguments, we will point out that one particular possibility to conduct laser-induced chemical transformations is left unexplored.

It will be shown how this theoretical prediction can be realized experimentally. In contrast to the majority of photochemical studies dealing with molecular fragmentations, our recent experiment [1] reports a highly endothermic associative chemical reaction, in which only a small fraction of the excitation energy being lost to heat, whereas the rest is used to establish new chemical bonds. We will present several experimental observations justifying the interpretation of the phenomenon and show how microscopic amount of the outcome of the reaction can be produced.

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Mo4-17

LASER-CONTROLLED PORPHYRIN-BASED MOLECULAR CURRENT ROUTER

Ioannis Thanopulos* and Emmanuel Paspalakis

Department of Chemistry, University of British Columbia, Vancouver B.C., Canada
Materials Science Department, University of Patras, Patras, Greece
*E-mail: ioannis@chem.ubc.ca

The fast expanding field of molecular electronics [1,2] investigates the electrical behavior of a molecular system, where the molecule acts as a barrier for incoming electrons, as in the original idea of “conduction as scattering” by Landauer [3]. A central question in this research area is the features of electric charge transfer through molecular junctions [4]. Furthermore, molecular junctions with several stable configurations receive particular attention in recent years [5].

In this work we introduce a novel molecular junction based on a thiol-functionalized porphyrin derivative. This junction possesses two energetically almost degenerate equilibrium molecular structures, which define two orthogonal directions of maximal electric charge transfer, respectively. We further demonstrate computationally how to switch between the two equilibrium molecular structures of the compound by optical means in two steps acting in tandem, which further enables the control of maximal current flow direction along the junction. The mechanism of optical switching is presented in the relevant configuration sub-space of the compound after obtaining the corresponding potential and electric dipole surfaces by ab initio methods. We propose using such a porphyrin-based molecular junction as a laser-controlled molecular current router [6].

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Mo4-18

THE IMPORTANCE OF CARRIER BEAMS IN THE LOSSLESS PROPAGATION OF NONADIABATIC PULSES

A. Eilam, A. D. Wilson-Gordon, and H. Friedmann
Department of Chemistry, Bar-Ilan University, Ramat Gan 52900, Israel

Adiabatons are well-known in the coherently-prepared double Λ system of Fig. 1(a) [1]. The lower Λ system interacts with strong *cw* pumps which establish a coherence between the two lower levels. Complementary adiabatic time-dependent modulations, superimposed on *cw* carrier fields, interact with the upper Λ system. On propagation, the modulations are transferred, via four-wave mixing, onto the pump fields so that pulse matching between all four fields is established. The adiabatons then propagate without further losses, but with reduced group velocity, for long propagation distances.

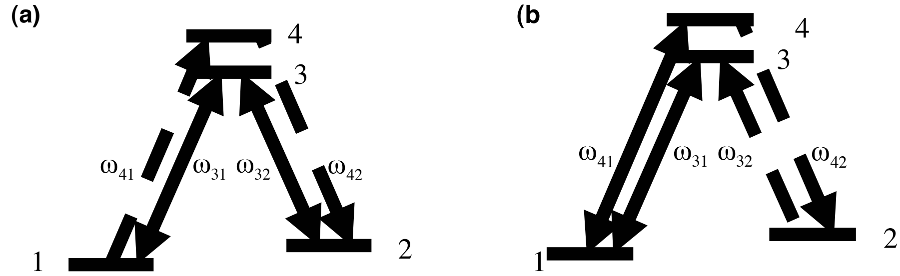

Fig. 1 Double Λ system (a) in coherently-prepared configuration, (b) in double EIT configuration. Pump fields are indicated by full lines and probes by dashed lines.

We have shown that adiabatons can also be demonstrated in the double EIT (electromagnetically induced transparency) system of Fig. 1(b). Moreover, *nonadiabatic* amplitude modulations superimposed on carrier fields (diabatons) can also propagate losslessly once pulse matching is established in both the configurations of Fig. 1. In the absence of the carrier fields, the matched nonadiabatic amplitude modulations experience continuous absorption in the double EIT system, but not in the coherently-prepared configuration [2].

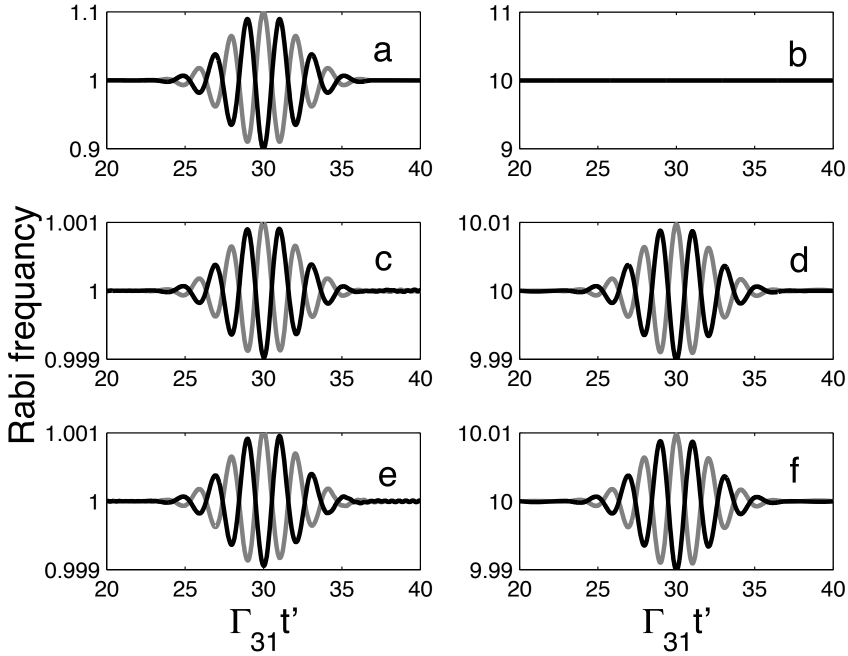

Fig. 2 Diabatons propagating in double EIT system. (a) Initial complementary probe fields, (b) initial pump fields, (c) and (d) complementary probes and pumps at propagation distance $\alpha_0 z = 110$, (e) and (f) at $\alpha_0 z = 150$.

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Mo4-19

COMPLETE POPULATION INVERSION BY A PHASE JUMP: AN EXACTLY SOLUBLE MODEL

B. T. Torosov[1] and N. V. Vitanov[1,2]

Department of Physics, Sofia University, James Bourchier 5 Boulevard, 1164 Sofia, Bulgaria[1]

Institute of Solid State Physics, Bulgarian Academy of Sciences, Tsarigradsko Chaussée 72, 1784 Sofia, Bulgaria[2]

An exact analytic solution to the time-dependent Schrödinger equation is presented for a two-state quantum system coherently driven by a nonresonant pulsed external field. The pulse has a hyperbolic-secant shape, with a phase jump of ϕ at its maximum and the detuning is $\Delta(t)=\Delta_0+B\tanh(t/T)$. In the absence of a phase jump ($\phi=0$) this coincides with the Demkov-Kunike model [1]. Special attention is paid to the cases $\Delta_0=0$ and $B=0$, which reduce to the Allen-Eberly and Rozen-Zener models for $\phi=0$. In the first case ($\Delta_0=0$) the effect of the phase jump is only in a factor of $\cos^2(\phi/2)$ that scales the population in the original Allen-Eberly model. In the second case ($B=0$) it is shown that for detunings larger than the pulse bandwidth and the phase equal to $\pm\pi$, the transition probability approaches unity as the field intensity increases. The population inversion is robust against small-to-moderate variations in the detuning and the intensity, a feature reminiscent of adiabatic passage. The population inversion, however, is not of adiabatic nature; it is induced by a δ-function-shaped nonadiabatic coupling with an area of nearly π [2]. An estimate of the required experimental resources shows that implementation with shaped femtosecond pulses is feasible.

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Mo4-20

ANALYSIS OF THE TRANSIENT EFFECTS OF TWO-LEVEL ATOM IN LASER LIGHT

Saud AL-Awfi, Smail Bougouffa*

Department of Physics, Faculty of Science, Taibah University,
P.O.Box 344, Madina, Saudi Arabia.
*sbougouffa@hotmail.com

For an atom at rest or slowly moving, the mean radiative force is usually split into two parts [1]. The first part is related to the phase gradient of the laser wave (and to the quadrature part of the atomic dipole) and is called dissipative force. The second one, related to the intensity gradient of the laser (and to the in-phase atomic dipole), is called reactive force. The dissipative force is well understood, and its various features [2], such as velocity dependence and momentum discussion, have been analyzed in detail in terms of cycles involving absorption of laser photons and spontaneous emission of fluorescence photons.

On the other hand, the reactive force heats the atoms for a negative detuning and cools them for a positive one. In the majority of theories of atom-light interaction, the steady state approximation or other approximations were used to avoid the complexity of the solutions of the time evolution equations on the Bloch vector or on the internal density matrix [3]. Recently [4] we have presented a separation approach based on a Riccati nonlinear differential equation appropriate for two-level atoms interacting with electric field. In this work we generalize the separation approach of the coupled system. We derived a set of conditions that permit the separation of the optical Bloch equations in the case of a pure radiative decay. The conditions that permit exact solutions of three coupled system are extracted in a natural manner. The case of an atom moving along the axis of a monochromatic wave is treated in some detail including a discussion on the radiation pressure forces exerted by laser light in the transient regime. The resulting equations are solved exactly analytically and relevant quantities such as the dissipative and reactive forces are determined. The present approach persists here with the new conditions of separation and without assuming the exact resonance, strong collisions or intense external field conditions [3]. We emphasize here the fact that with the natural conditions, it is possible to obtain exact analytic solutions which reproduce the most important features of the mechanical effect of light on the moving atom. The cases of sodium atom and Eu^{3+}ion moving along the axis of a monochromatic wave are treated in some detail including a discussion on the radiation pressure forces exerted by light in the transient regime.

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Mo4-21

Manipulation of spatial distribution of excited molecules in a beam via dressed-state interference.

N. N. Bezuglov[1], A. Ekers[2], R. Garcia-Fernandez[3], K. Miculis[2], I. Sydoryk[2],
L. P. Yatsenko[4] and K. Bergmann[3]

[1] V. A. Fock Institute of Physics, St. Petersburg State University,
198904 St. Petersburg, Russia
[2] Dept. of Physics, University of Latvia, LV-1586 Riga, Latvia
[3] Dept. of Physics, University of Kaiserslautern, Kaiserslautern, Germany
[4] Institute of Physics, National Academy of Sciences, 03650 Kiev-39, Ukraine

Manipulation of spatial distribution of state-selected excited molecules using a combination of the Autler-Townes effect [1] under conditions of optical pumping and interference caused by presence of light-induced crossings of the molecular states is studied. In the experiment, a supersonic molecular beam is crossed by two cw laser beams coupled in an open three-level ladder scheme. Lasers are focused in such a way that *strong and short* laser field pulse couples the two lower levels, and *weak and long* laser field pulse couples the two upper levels. Hence, the excitation spectrum of the upper level is strongly affected by the dynamics of optical pumping on the lower transition. Detailed numerical calculations based on the dressed-state picture [2] show that such an arrangement of both laser fields can be used to vary the spatial distribution of highly excited molecules, which can be precisely controlled by varying laser frequencies and intensities. When the frequencies of both laser fields are fixed, the excitation of the upper level can take place at two distinct spatial locations (Landau-Zener transition regions), where the second laser field is resonant with one of the dressed states associated with interaction with the laser field in the first excitation step. This leads to two alternative excitation pathways, whereby the probability amplitude of the upper level at the second Landau-Zener transition region is determined by their constructive or destructive interference. Calculations and experimental results for the case of excitation high lying states of Na_2 are presented. Simulations show (see Fig. 1) that interference fringes in the excitation spectrum of the upper level can be resolved when counter-propagating laser beams are used, which allows elimination of the residual Doppler width.

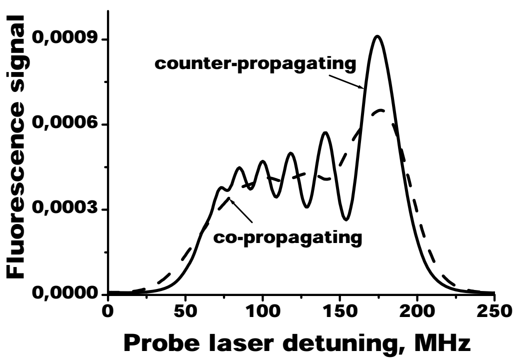

Fig. 1. Calculated fluorescence signal from the upper level of a three-level ladder system, excited by two co- and counter-propagating lasers fields.

This work was supported by the EU TOK Project LAMOL, EU-FP5-RTN QUACS Network, NATO Grant EAP.RIG.981378, European Social Fund, Latvian Science Council, and RFBR Grant 05-02-16216.

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Mo4-22

DEPHASING-DECOHERENCE IN TWO-STATES TRANSITION

X. Lacour[1],† S. Guérin[1], L. P. Yatsenko[2], N. V. Vitanov[3,4] and H. R. Jauslin[1].

[1] Institut Carnot de Bourgogne, UMR 5209 CNRS, BP 47870, 21078 Dijon cedex.
[2] Institute of Physics, Ukrainian Academy of Sciences, prospect Nauki 46,
Kiev-22, 252650, Ukraine.
[3] Department of Physics, Sofia University, James Bourchier 5 Blvd,
1164 Sofia, Bulgaria.
[4] Institute of Solid State Physics, Bulgarian Academy of Sciences,
Tsarigradsko chaussée 72, 1784 Sofia, Bulgaria.

Adiabatic passage is now a widely used tool to control population transfer by external fields [1, 2]. This control is at the heart of many applications such as selective photochemistry [3, 4], and quantum gates [5–8]. The extension of adiabatic passage to open quantum systems, i.e. to quantum systems coupled to an external environment, is of interest since generally adiabatic processes require relatively long times, where decoherence processes may take place.

We describe the effect of pure dephasing upon the time-dependent dynamics of two-state quantum systems in the framework of a Lindblad equation for the time evolution of the density matrix. We derive a uniform approximate formula, which modifies the corresponding lossless transition probability by an exponential factor containing the dephasing rate and the interaction parameters. This formula is asymptotically exact in both the diabatic and adiabatic limits; comparison with numerical results shows that it is highly accurate also in the intermediate range. We consider several two-state models in more detail, including the Landau-Zener, Rosen-Zener, Allen-Eberly, and Demkov-Kunike models, along with several other models, such as a Gaussian model and a Landau-Zener model with a pulsed coupling.

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[†] Electronique address: `xavier.lacour@u-bourgogne.fr`

Mo4-23

INTENSITY DEPENDENT LINE-WIDTHS OF HANLE ELECTROMAGNETICALLY INDUCED ABSORPTION TO TRANSVERSE MAGNETIC FIELDS

A. J. Krmpot, J. Dimitrijević, M. M. Mijailović, Z. Grujić, D. Arsenović, and B. M. Jelenković

Institute of Physics, University of Belgrade, 11080, Belgrade, Serbia

Electromagnetically induced absorption (EIA) [1] is an increase of laser absorption in a gas medium because of coherence and/or population transfer to levels most coupled by a laser light. We investigate, experimentally and theoretically, dependence of EIA contrast and amplitude on the laser intensity and magnetic fields transverse to the scanning axial magnetic field (parallel to the laser propagation). We have done these by monitoring absorption of linearly polarized light locked to the closed $F_g \rightarrow F_e = F_g + 1$ transition in Rb, while additional transverse magnetic fields have different values and orientation in respect to the laser polarization (Hanle configuration).

We made measurements with both 87 and 85 Rb isotopes using Rb cells with different lengths. Theory predics [2] that EIA for cold atoms disappears at very high laser intensities. Experimental EIA, in a Hanle configuration and for Doppler broadened gas medium, is still present even at extremely high laser intensities. With transverse magnetic field zero, experimental EIA width shows line narrowing with increasing laser intensity, which is different from observed behavior of line-widths of electromagnetically induced transparency (EIT) [3]. Such result can be understood from our numerical calculations of the sublevel populations and coherence as a function of the laser intensity at different laser detunings.

Effects of transverse magnetic fields on EIA amplitude and line-widths are similar to those reported for EIT [4]: a) additional magnetic field perpendicular to the laser polarization is destroying conditions for enhanced absorption, decreasing the EIA at zero scanning magnetic field, the more so the larger transverse field is; b) magnetic field parallel to the laser polarization increases both contrast and width of the EIA, by increasing the rate that population is pumped in magnetic sublevels dominantly coupled by the laser.

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Mo4-24

Control of probe response and dispersion in a three level closed Λ system : Interplay between Spontaneously Generated Coherence and Dynamically Induced Coherence

Sulagna Dutta and Krishna Rai Dastidar

Department of Spectroscopy
Indian Association for the Cultivation of Science
Kolkata 700032, India

The dispersion and the absorption properties of a closed three-level Λ system with incoherent pumping have been studied when both dynamically induced coherence (DIC) and the spontaneously generated coherence (SGC) [1, 2] play a significant role. We analyze the interplay between the dynamically induced coherence (DIC) and the spontaneously generated coherence (SGC) on the absorption spectrum to induce different nonlinear processes like amplification without population inversion (AWI), electromagnetically induced transparency (EIT) and electromagnetically induced absorption (EIA) [2]. It has been demonstrated that when the contributions from both the coherences (DIC and SGC) are prominent, the response of a closed three level Λ system with incoherent pumping will change dramatically from the responses obtained either from SGC or from DIC separately. This is because of the fact that these two coherences interfere constructively or destructively depending on their relative magnitude and sign. This control over the response of the system can be achieved by controlling the system parameters like relative values of spontaneous decay widths, Rabi frequencies and the alignment of the dipole transition moments. It has been shown by continuously changing the probe field Rabi frequency, the response of the system can switch over from one nonlinear process to other and hence the probe field Rabi frequency can be used as a knob for switching different nonlinear responses. By changing the relative phase of two fields the response of the system switches over from EIA to EIT or EIT to AWI which can be used as optical switch. Choosing appropriate value of the relative phase and the probe field Rabi frequency, the dispersion and hence the propagation of the probe pulse can be controlled efficiently. Therefore these parameters can be used as a knob to manipulate light propagation from subluminal to superluminal. Exact analytical expressions for the coherences and populations in the steady state limit have been derived (keeping all orders of system parameters) to generalize the analysis and any restriction over the system parameters (e.g. spontaneous decay widths on probe and coherent transitions are equal) have been avoided to make it applicable to various atomic and molecular systems. However the approximate expressions can be derived from these exact values. Numerical values obtained by solving the density matrix equations agreed well with these exact analytical values at large time limit.

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Email: krishna_raidastidar@yahoo.co.in

Mo4-25

Effect of a Two Colour Laser Field and Coherent Phase Control on Electron Impact Excitation of a Hydrogenic Ion

C. Sinha

Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India

The study of multiphoton phenomena in different laser induced /assisted atomic and molecular processes using a two colour (bichromatic) laser field has recently become a subject of particular interest both experimentally [1] and theoretically [2]. The interest mainly seems to stem from the effect of the phase control (commonly known as coherent phase control) i.e. the dependence of the reaction rate on the difference of phase(ϕ) between the two laser fields. By virtue of the modern laser technology it is now possible to produce higher harmonics of a laser field of sufficiently high power and to control (coherent) the phase ϕ between the fundamental field and its harmonics and this new parameter can considerably modify (enhance/reduce) different multiphoton processes (e.g. excitation, ionization etc) .

The present study addresses the electron impact excitation of a hydrogen like ion to n=2 level in presence of a bichromatic laser field consisting of a fundamental frequency ω and its second/third harmonics (e.g. 2ω, 3ω etc.). For the description of the laser field we choose the classical field representation in which the vector potential is given by

$$\vec{A}(t) = A_1\,\bar{\in}_1\ \cos w_1 t\ + A_2\,\bar{\in}_2\ \cos(w_2 t + \phi)\,;\ w_2 = s\ w_1\,,\ s = 2\,,\,3\ \ldots.$$

The collision process is considered in the framework of Coulomb Born approximation . The projectile laser interactions are considered to all orders, while the dressed wave functions of the hydrogenic ion are constructed using a parabolic coordinate representation in the framework of first order time dependent perturbation theory. The parabolic Stark manifolds should be the correct prescription for calculating the excitation probability of a laser assisted hydrogenic ion since in this case the orbital angular momentum is no longer a good quantum number.

A significant suppression is noted in the field assisted differential cross sections (DCS), the suppression being enhanced for the two colour fields as compared to the monochromatic one [3]. Some preliminary result are given in the Table 1 for single photon absorption case with frequencies ω and 2ω. Detailed results and discussions will be presented at the Conference.

Table 1. Phase dependence in the DCS at $\theta = 0^0$ for the laser assisted (two colour) electron impact excitation of the He$^+$ ion (to n = 2 level) for single photon exchange with $\in_0 = 0.01$ a.u. $\omega = 0.043$ a.u.

Energy (eV)	Field free DCS	Monochromatic field DCS	Bichromatic field	
			Phase (ϕ)	DCS
50	0.15816	0.00226	0	0.00021
			90	0.00767

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tpcs@iacs.res.in, chand_sin@hotmail.com

Mo4-26

Rapid Adiabatic Passage in a Pr^{3+}:Y$_2$SiO$_5$ crystal

Fabian Beil, Jens Klein, and Thomas Halfmann

Fachbereich Physik, University of Kaiserslautern, Germany

Recently, rare earth ion doped solids were proposed as potential quantum computer hardware [1]. These media have the advantages of solids, i.e. high density and scalability, while still exhibiting the coherent properties of atoms. Quantum computing requires robust transfer processes [2] for manipulation of population distributions and to control the mutual interaction of qubits. As an example of such processes we examine Rapid Adiabatic Passage in a Pr^{3+}:Y$_2$SiO$_5$ crystal (Pr:YSO) [3]. In our experiments we excite Pr^{3+} ions, initially in their ground state $^3H_4$, to the state $^1D_2$. As both states split up into three hyperfine levels and the optical transition is inhomogeneously broadened, Pr:YSO occurs as a complex spectroscopic system. However, using an appropriate preparation pulse sequence the medium can be prepared by optical pumping and spectral hole burning. This preparation step provides a spectrally isolated two-level-system, which is convenient to study RAP.

When a linearly chirped pump pulse of gaussian temporal shape is applied, complete population transfer to the excited state occurs. We confirm this transfer by absorption spectroscopy, fluorescence detection and observation of amplified spontaneous emission (ASE). Time-resolved measurements serve to monitor the adiabatic population dynamics during the excitation process.

Figure 1 shows results from absorption spectroscopy using a delayed weak probe pulse. If no pump laser pulse is present, we observe absorption from the ground state (solid triangles). However, a linearly chirped pump pulse drives the system to population inversion. Therefore, we observe stimulated emission and amplification of the probe pulse, i.e. a negative absorption coefficient (open circles).

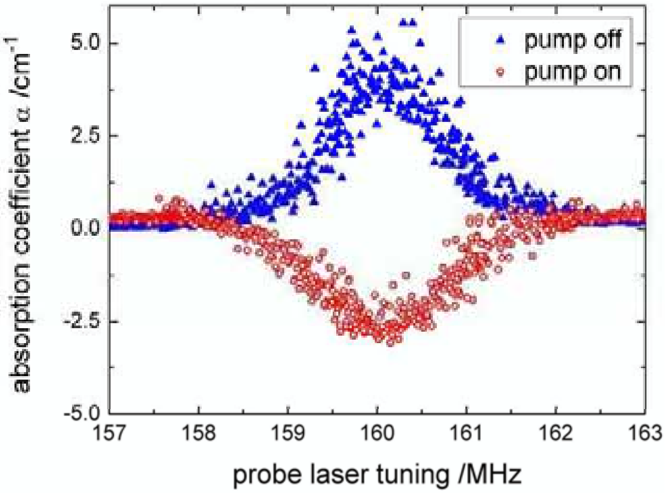

***Figure 1:** Absorption spectrum. By preparation of the medium we obtain absorption from the ground state (solid triangles). After a RAP process we observe stimulated emission (open circles).*

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Mo4-27

COHERENT POPULATION TRANSFER AMONG QUANTUM STATES BY MULTIPHOTON STIRAP

H. K. Avetissian and G. F. Mkrtchian

Department of Quantum Electronics, Yerevan State University,
1 A. Manukian, 375025 Yerevan, Armenia
E-mail: avetissian@ysu.am

The possibilities to control quantum systems, especially to obtain desired coherent superposition states by external electromagnetic fields have been studied intensively during the many decades since the period of development of the nonlinear optics. In particular, it is of interest the robust techniques which allow population transfer between the specified atomic/molecular states in laser fields. However, the control of superposition states by existing laser pulses is problematic in such quantum systems where the energy gap between the states is larger compared with the optical transitions and the multiphoton excitation problem arises. As it has been shown [1-3], the multiphoton resonant excitation of three/four-level atoms subjected to a strong laser field is effective when the atom has a mean dipole moment in the excited states. Otherwise, the energies of the excited states of a three-level atom should be close enough to each other and the transition dipole moment between these states must be nonzero (e.g., hydrogen atom due to random degeneration upon the orbital moment).

In the present work we consider multiphoton adiabatic population transfer process in laser fields that resembles the well known stimulated Raman adiabatic passage (STIRAP) [4]. In considering system the intermediate state has a mean dipole moment, therefore the applied two coupling laser fields induce multiphoton transitions between the initial and desired final states. We consider as lambda as well as a ladder type systems. The time evolution of such systems is found analytically using resonant approximation. The numerical simulations show that by two delayed, overlapping laser pulses it is possible to produce almost complete population transfer. The concrete examples for experimental implementation of considered scheme are suggested.

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Mo4-28

CONTROLLED POPULATION TRANSFER IN INTERSUBBAND TRANSITIONS OF QUANTUM WELL STRUCTURES

E. Paspalakis[1], A. Kanaki[1] and A. F. Terzis[2]

[1]Materials Science Department, School of Natural Sciences, University of Patras,
Patras 265 04, Greece
[2]Physics Department, School of Natural Sciences, University of Patras,
Patras 265 04, Greece

An important problem in the area of intersubband transitions in semiconductor quantum wells is the potential for controlled population transfer between two subbands in a semiconductor quantum well structure, when the many-body effects arising from the macroscopic carrier density of the system are accounted for [1-3]. In this work we study the potential for control of the electron population dynamics in two-subband and three-subband systems in semiconductor quantum wells that interact with strong electromagnetic fields. The inclusion of the electron-electron interactions makes the two-subband or the three-subband system to behave quite differently from non-interacting (atomic-like) two-level or three-level systems. We use the proper density matrix equations, obtained from a time-dependent Hartree approach, for the description of the system's dynamics. Studying specific quantum well structures we show that if decay processes are ignored then complete population transfer in the quantum well system is possible. Significant population transfer can occur in the system even in the presence of decay processes.

Acknowledgments: We thank the European Social Fund (ESF), Operational Program for Educational and Vocational Training II (EPEAEK II), and particularly the Program PYTHAGORAS II, for funding this work.

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POSTERS

Monday 7/5

5. Molecular dynamics

Mo5-1

VACUUM ULTRAVIOLET PHOTODISSOCIATION IMAGING OF HeH$^+$ USING INTENSE FREE ELECTRON LASER PULSES

H. B. Pedersen[1], S. Altevogt[1], B. Jordon-Thaden[1], O. Heber[2], M. L. Rappaport[2],
D. Schwalm[1], J. Ullrich[1], D. Zajfman[1,2], R. Treusch[3], N, Guerassimova[3], M. Martins[4],
J.-T Hoeft[4], M. Wellhöfer[4], and A. Wolf[1]

[1]Max-Planck-Institut für Kernphysik, D-69117 Heidelberg, Germany
[2]Department of Particle Physics, Weizmann Institute of Science, Rehovot, Israel
[3]HASYLAB at DESY, Hamburg, Germany
[4]Institut für Experimentalphysik, Universität Hamburg, Germany

The new Free Electron LASer in Hamburg (FLASH) [1] delivers unprecedented intense light pulses in the VUV and soft X-ray regime that, combined with fast ion beam techniques, allows the regime of valence shell excitation so far inaccessible for molecular ions to be explored by 3D momentum imaging of photofragments. These excitations are of importance in astrophysically occurring radiation fields [2,3] and the fragment momenta reflect the dynamics of the excited quantum chemical system, thus providing a sensitive probe of molecular theory.

We report a first benchmark crossed-beams photodissociation experiment with FLASH, where the photofragment geometry and absolute photodissociation cross section were measured at 38.7 eV excitation energy (32 nm) for HeH$^+$ on the channel H$^+$ + He(1s*nl*). HeH$^+$ is a benchmark case as the ionic analogue of H_2; its excited states have only been addressed theoretically [4] while being of potentially high importance in both astrophysical environments [2,3] and in neutrino mass measurements [5].

The experiment used a novel ion beam infrastructure installed for this purpose at the plane grating monochromator beam line (PG2) [6] at FLASH, performing three-dimensional event-by-event fragment imaging of cold molecular ions in a crossed beams geometry with ~100 HeH$^+$ ions in the interaction region for each FLASH pulse.

The absolute photodissociation cross section at 32 nm into the He-fragment channel was determined to $1.4 \cdot 10^{-18}$ cm^2 with a systematic error of ~50 %. The measured energy release spectrum of HeH$^+$ showed a remarkably large fraction of ~50 % in highly excited states of $n \geq 3$. The angular distributions showed an unexpected dominance of fragmentation transverse to the photon polarization, originating from excitation into curves of $^1\Pi$ symmetry. In contrast, theoretical studies [4] and astrophysical models of the early universe [2] and planetary nebulae [3] have so far emphasized parallel transitions via the low-lying excited states of $^1\Sigma$ symmetry.

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Mo5-2

THE EFFECT OF VIBRATIONAL AND ROTATIONAL EXCITATION OF THE REAGENTS ON DYNAMICS OF THE INTERACTION IN THE SYSTEM CsCl + RbJ

V.M. Azriel, L.Yu. Rusin

Institute of Energy Problems of Chemical Physics RAS,
Leninski prospect 38, Bldg.2, Moscow 119334, Russia
Corresponding author: Azriel_Vladimir@mail.ru

The interaction in the system CsCl + RbJ proceeds via 12 channels [1]:

$\mathrm{CsCl + RbJ} \rightarrow \mathrm{CsCl^* + RbJ^*}$ (1)
$\rightarrow \mathrm{Cs^+ + Cl^- + Rb^+ + J^-}$ (2)
$\rightarrow \mathrm{Cs^+ + Cl^- + RbJ}$ (3)
$\rightarrow \mathrm{Rb^+ + J^- + CsCl}$ (4)
$\rightarrow \mathrm{CsJ + Rb^+ + Cl^-}$ (5)
$\rightarrow \mathrm{RbCl + Cs^+ + J^-}$ (6)
$\rightarrow \mathrm{CsJ + RbCl}$ (7)
$\rightarrow \mathrm{CsClRb^+ + J^-}$ (8)
$\rightarrow \mathrm{CsClJ^- + Rb^+}$ (9)
$\rightarrow \mathrm{CsJRb^+ + Cl^-}$ (10)
$\rightarrow \mathrm{RbJCl^- + Cs^+}$ (11)
$\rightarrow \mathrm{CsClRbJ}$ (12)

Quasiclassical trajectory calculations have been fulfilled at collision energy ($E_{rel.}$) ranging from 4 eV to 17 eV. The choice of initial internal states of interacting molecules on the base of quantum distributions for the temperatures of the nozzles of sources of molecular beams equal 1000K according to experimental conditions shows the following really achieved maximum values of vibration (V) and rotation (J) quantum numbers of the reagents:

$$V_{max}^{CsCl} = 20, \quad J_{max}^{CsCl} = 300, \quad V_{max}^{RbJ} = 30, \quad J_{max}^{RbJ} = 400.$$

In present calculations the initial values of V and J were fixed in turn near left and right boundaries of these ranges this way that the total energy of both molecules was the same in all cases. Thus it was possible at defined value of total energy of the system to ascertain what type of internal excitation of the reagents is more significant for the cross sections of different channels.

The calculations reveal at collision energy 4 eV and low internal values of V and J that vibrational excitation is far more effective in compare to rotational one for all opened at this energy channels. On growth of collision energy the low internal excitation becomes less significant. For high values V and J at $E_{rel.}$= 4 eV this tendency is still more noticeable for channels (4) - (11), but for channel (3) the rotation of any molecule is preferable. At collision energy equal 17 eV the channels (3) and (6) are more sensitive to vibrations of the reagents, while all other channels don’t reveal some preference to define type of internal excitation of colliding partners.

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Mo5-3

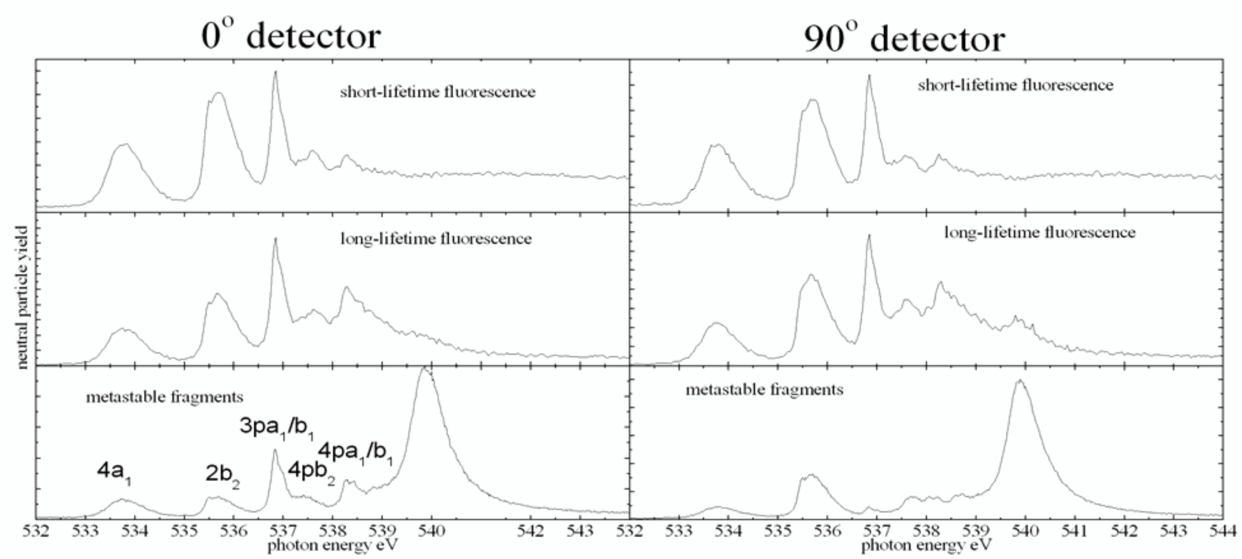
METASTABLE FRAGMENT AND VUV FLUORESCENCE YIELD FOLLOWING O 1s EXCITATION OF H_2O

JR Harries[1], M Iseda[2], T Tamura[2], A Morita[2], M Kuniwake[2], K Honma[2],T Gejo[2]

[1]JASRI / SPring-8, Kouto 1-1-1, Sayou, Hyogo, 679-5198 Japan
[2]University of Hyogo, Koto 3-2-1, Kamigori-cho 678-1297 Japan

We present a study of the neutral particle yield following oxygen 1s photo-excitation/ionisation of H_2O by monochromatised synchrotron radiation of high energy resolution (~50 meV) from BL27SU, SPring-8. Neutral particles produced following the interaction of the incident photons with molecules from an effusive gas jet are detected using micro-channel plate detectors. The pulsed structure of the radiation is used to distinguish between particles in neutral excited states (internal energy of above around 10 eV), and VUV photons, which mostly arise from the decay of excited H atom fragments. An analysis of the arrivals-times spectra of the photons leads to information on the fluorescing states.

The figure shows the VUV fluorescence yield arising from states of differing lifetimes (upper two panels) and the neutral excited H fragment yield (lowest panels) for two detectors mounted at 0 and 90 degrees to the polarisation vector of the linearly polarised incident radiation. The short-lifetime (~1 ns) fluorescence is expected to be mainly due to the production of H atoms in the 2p excited state emitting Lyman-α photons, with more highly-excited states emitting photons on a longer lifetime(~10 ns). Of particular interest is the high yield of metastable particles close to the O 1s threshold – a similar observation has been made near the N 1s threshold of N_2[1]. The fluorescence yield can be compared to the results of [2].



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Mo5-4

OBSERVATION OF CONSECUTIVE PHOTOREACTIONS OF SINGLE ANILINE CATIONS

K. Højbjerre, D. Offenberg[1], A. Mortensen[2], P. Staanum, M. Drewsen

Department of Physics and Astronomy, University of Aarhus, Denmark

klaush@phys.au.dk

Recently, several experiments have proved it feasible to study chemical reactions involving ions co-trapped with laser cooled atomic ions in Paul traps [1-6]. Through sympathetic cooling, this approach provides a way to cool from a single to thousands of molecular ions into the mK-regime and to trap these ions for minutes or even hours. So far, experiments have been focused mostly on simple diatomic ions, but recently large quantities of more complex molecular ions have been sympathetically cooled [6].

With the positively charged aniline molecular ion ($C_6H_7N^+$) as a test molecule, we demonstate the possibility of studying consecutive photodissociations of complex molecular ions at the single molecule level. Exposing a single Aniline cation to light at 397 nm and 294 nm leads to the formation of a broad range of smaller ions like $C_5H_6^+$ and $C_3H_3^+$, either directly or through consecutive photodissociations. Since the technique allows for investigations of a large assortment of molecular ions using various light sources, including free electron lasers or synchrotron radiation beams, it is very versatile and has the potential for studies of, e.g., astrochemical relevant processes.

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[1] Permanent adress: Institut für Experimentalphysik, Heinrich-Heine-Universität Düsseldorf, Germany

[2] Present adress: Physics and Astronomy, University of Sussex, England

Mo5-5

Single Photon-Induced Symmetry Breaking of H_2 Dissociation

F. Martín[1], J. Fernández[1], T. Havermeier[2], L. Foucar[2], Th. Weber[2],
K. Kreidi[2], M. Schöffler[2], L. Schmidt[2], T. Jahnke[2], O. Jagutzki[2], A. Czasch[2],
E. P. Benis[3], T. Osipov[4], A. L. Landers[5], A. Belkacem[4], M. H. Prior[4],
H. Schmidt-Böcking[2], C. L. Cocke[3], R. Dörner[2]

[1] Departamento de Química, C-9, Universidad Autónoma de Madrid, 28049 Madrid, Spain.
[2] Institut für Kernphysik, University Frankfurt, Max von Laue Strasse 1, D-60438 Frankfurt, Germany.
[3] Department of Physics, Kansas State University, Cardwell Hall, Manhattan, KS 66506, USA.
[4] Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA.
[5] Department of Physics, Auburn University, Auburn, AL 36849, USA.

The indistinguishableness of the two protons in the dissociating H_2^+ molecule prohibits the electron to prefer one nucleus for the generation of the neutral hydrogen. In this contribution a method is shown to break this symmetry via the population of doubly excited states. In March 2005 an experiment was performed at the Advanced Light Source in Berkeley to observe the dissociating channels in hydrogen and deuterium molecules. The COLTRIMS method allows a kinematically complete measurement so that a map of all appearing states could be obtained.

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Mo5-6

KINETIC STUDY OF THE REACTION
$H_2O_2 + O(^3P) \rightarrow OH + HO_2$ BY AB INITIO CALCULATION

H. Koussa, M. Bahri, Y. Tarchouna, N. Jaidane
Laboratoire de spectroscopie atomique moléculaire et applications, Département de physique, Faculté des Sciences, université Tunis-El Manar, le belvédère 1060, Tunis, Tunisia
corresponding author:
Present address: Faculté des Sciences de Sfax BP 802 3018 Sfax Tunisie.
E-mail: mohamed.bahri@fss.rnu.tn

Theoretical kinetic study of the $H_2O_2 + O(^3P) \rightarrow HO_2 + OH$ reaction was performed using the ab initio-TST calculation. Tow reaction paths have been considered, the hydrogen abstraction (path1) and the O-O bond destruction one (path 2). (Fig.1)

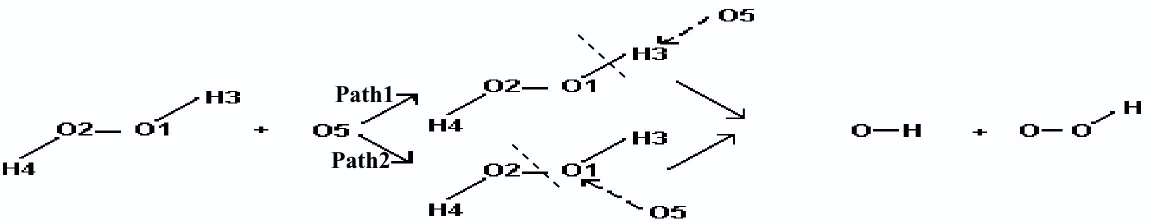

Figure.1.

In the ab initio part of calculation (MP2//CASSCF) [1] method was used with the aug-cc-pVTZbasis set to determine the electronic structure of reactants, products and transition states. The BSSE and ZPE corrected classical barriers height for the two paths were predicted to be, respectively, 6.6 and 18 $kcal.mol^{-1}$.

Electronic structure results were used with the transition state theory (TST) to evaluate the rate constants k_1(path1), k_2 (path2) and $k = k_1 + k_2$ as function of temperature T for $200 \leq T \leq 4000K$. Transmission coefficient was evaluated using the ZCT [2] method. In figure 2 predicted rate constants k_1, k_2 and k (in $cm^3 molecule^{-1} s^{-1}$) are reported and compared to the available experimental results. The reasonable agreement found between predicted and experimental rate constants k shows that for the studied reaction, the path1 is the most likely to occur for $T \leq 1000K$ and at high temperatures the contribution of the path2 to the reaction becomes important and must be taken into account.

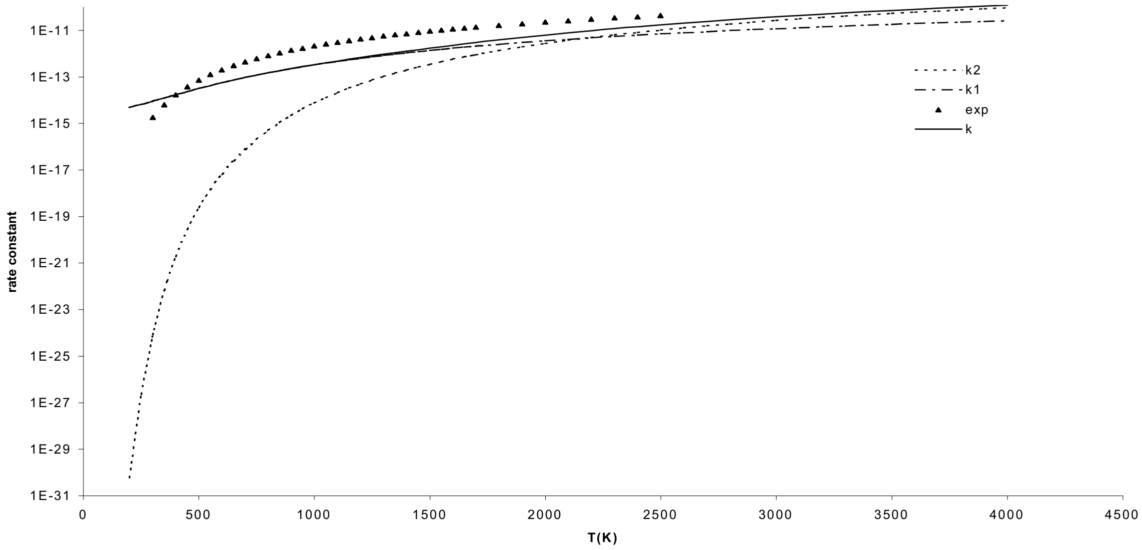

Figure.2.

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Mo5-7

Photofragment Space Distribution in the Photodissociation of NaI in the spectral range 315 - 370 nm: the Role of Molecular Axis Rotation

Konstantin O. Korovin[1], Elke Heinecke[2], Tobias Liebig[2], Alexander Patzer[2], Oleg S. Vasyutinskii[1],
and Dieter Zimmermann[2]

[1]Ioffe Physico-Technical Institute, Russian Academy of Sciences, 19402,1 Saint-Petersburg, Russia
[2]Institute of Optics and Atomic Physics, Technical University of Berlin, D-10623 Berlin, Germany

Vector correlations in photodissociation have been actively studied in recent years as they provide a deep insight into the dynamics of the process and properties of parent molecules.

We report the first determination of translational anisotropy parameters β in the photodissociation of NaI molecules in the spectral range 315-370 nm [1]. The anisotropy parameters were determined by the analysis of Doppler resolved absorption profiles of Na($^2S_{1/2}$) atoms produced in the photodissociation of NaI using two orientations of the linearly polarized photolysis light: parallel and perpendicular to the direction of the probe beam. The value of the parameter β was obtained from a simultaneous fit of the profiles. The parameter exhibits slow decrease from -0.05 at 315 nm down to -0.35 at 345nm and stays at the level around -0.56 in the range of 347.1 nm to 370 nm.

The role of the rotation of the parent molecules on the branching ratio between parallel and perpendicular transitions in NaI during dissociation is discussed.

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Role of symmetry in dissociation of highly symmetric molecules

Vandana Sharma and Bhas Bapat
Physical Research Laboratory, Ahmedabad 380009, India
Email: vandanas@prl.res.in

January 29, 2007

We have probed the unimolecular fragmentation dynamics of tetrahedral (CCl_4) and octahedral (SF_6) molecules, are highly symmetric. The common thread between the dissociation pattern of the two molecules is the formation of an ion which is not 'obvious' (Cl_2^+ from CCl_4 and F_2^+ from SF_6). The ground state geometry of the two does not support the formation of these unusual dissociative products. This implies that the geometry of the dissociating molecular ion is significantly altered from the geometry of the parent neutral. These observations suggest relocation of certain atoms within the molecular ion during dissociation. We have made a successful attempt to determine the geometry of electronically excited dicationic precursor in the centre-of-mass frame by mapping the momenta of all fragments including the neutral arising from the break-up of the precursor. Experimentally determined geometry is in good agreement with the theoretically generated structure.

Another observation which is common between these molecules is that the probability of formation of certain ions is more as compared to others. In dissociative ionisation of CCl_4, CCl^{2+} and CCl_3^{2+} ions are observed whereas CCl_2^{2+} and CCl_4^{2+} are not observed. For the case of SF_6, the probability of formation SF_{2n+1}^+ ions, was observed to be higher than that of SF_{2n}^+ (n =0–2). Similarly, SF_{2m}^{2+} ions, where m =0–2, were found to be more probable than SF_{2m+1}^{2+}. We deduced that a high probability of formation of a certain fragment ion is strongly correlated to its having odd number of electrons for the case of CCl_4 whereas even number of electrons for the case of SF_6. It is still not understood how the symmetry of these molecules plays a role in formation of unusual ion species and the odd-even patterns in the fragment ions.

Mo5-9

ULTRAFAST DISSOCIATION OF $M(CO)_6$: WAVELENGTH-INDEPENDENT COHERENT OSCILLATIONS EXCLUDE A TRIPLET PATH

K. Kosma, W. Fuß, S.A. Trushin, W.E. Schmid, B. Schneider

Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany

Quite a number of electronic states of group-6 metal hexacarbonyls $M(CO)_6$ (M = Cr, Mo, W) is available at energies reached by near-UV wavelengths: the ligand-field (LF or $d \rightarrow d$) excited states that are dissociative and the metal-to-ligand charge-transfer (MLCT) states. It is now believed that the former are higher than the latter in the S_0 geometry, but come down along the dissociation coordinate. There are two intense MLCT transitions (symmetry T_{1u}, the most important one at ≈280 nm) with several weak symmetry-forbidden precursors. Textbooks attribute these precursors to triplets, in particular with the heavier metals, and discussion on the assignment is still going on. In the consecutive reactions, triplets would very much differ from singlets.

We probed the dynamics of photodissociation of $M(CO)_6 \rightarrow M(CO)_5 + CO$ by non-resonant photoionization with time resolution 10-30 fs and found similar results for all wavelengths (270-350 nm) and metals (Cr, Mo, W). The reaction proceeds in several steps, as in part already found previously with lower time resolution and fixed wavelength (267 nm) [1]: After a first relaxation (within 12.5 fs from T_{1u} of $Cr(CO)_6$) probably to an LF state, dissociation takes an additional remarkably short time (18 fs in this example), producing an electronically excited $M(CO)_5$. From there, this unsaturated carbonyl relaxes down through a (Jahn-Teller induced) conical intersection (within 40 fs in $Cr(CO)_5$) and exhibits pronounced coherent oscillations in this lower potential. The oscillations are assigned by the help of DFT calculations to pseudorotation in the S_0 minima of $M(CO)_5$ with square-pyramidal (C_{4v}) structure. The dominant one (95 – 80 cm^{-1} for the three M), with long dephasing time (≈1 ps) is the a_1 component, and the shorter-lived one (42 cm^{-1} for $Mo(CO)_5$) the b_2 component. The vibrations are stimulated by the slope on descending from the conical intersection. Pseudorotation is only possible in the singlet system with the C_{4v} structure; the triplet $M(CO)_5$ would have a trigonal-bipyramidal structure and different vibrational frequencies. In the triplet manifold there would also be no equivalent for the path through a conical intersection. Furthermore, all time constants are longer for the heavier metals than in the later systems, contrary to expectation, if spin-orbit coupling played a role. We conclude that for all metals (Cr, Mo, W) photodissociation proceeds in the singlet manifold, even at the longest wavelengths.

It is also remarkable that we found a coherent oscillation (350 cm^{-1}), excited in the Franck-Condon region and persisting all the way to the product S_0 state, which is assigned to an a_{1g} (breathing) M–C stretch vibration. This seems surprising at first sight, because the M–C dissociation is barrierless, as the short times imply. However, extension of a single M-CO bond results from superposition of several M-CO stretching coordinates including e_g and t_{1u}.

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Mo5-10

APPLICATION OF THE FEW BODY QUANTUM THEORY FOR GUIDED CONTROL OF CHEMICAL REACTIONS AND CREATION OF THE NEW MOLECULAR STRUCTURES

S.A.Pozdneev

P.N.Lebedev Physical Institute, Department Quantum Radiophysics, Laboratory of Photochemical Processes, Leninskiy pr.53, 119924 Moscow, Russia

Guided control of molecular processes and creation of the new molecular structure is a subject of active research in molecular and chemical physics. One of the most natural and general approaches in this area is a quantum few-body theory based on the Faddeev-Yakybovsky equations [1,2]. It is based on the idea, that the possible mechanisms of occurrence of chemical reactions based on a specific multiparticle interaction under condition of low coupling energy between clasters of the system [3,4].

In addition to the quantum approaches classical control theory based on the classical mechanics have also been developed [5]. However phase effects as essential [2-5], and classical treatment cannot be good enough.

Investigation of the methods and tools for creation of the new molecular structures with new properties and control of chemical reaction on the base quantum theory of few-body system are presented.

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Mo5-11

COULOMB EXPLOSION IMAGING OF NEGATIVE MOLECULAR HYDROGEN IONS

Brandon Jordon-Thaden[1], Simon Altevogt[1], Dennis Bing[1], Max Berg[1], Henrik Buhr[1], Robin Golser[2], Hubert Gnaser[3], Oded Heber[4], Jens Hoffman[1], Holger Kreckel[1], Michael Lange[1], Mario Mendes[1], Oldrich Novotny[1], Steffen Novotny[1], Henrik Pedersen[1], Annemieke Petrignani[1], Hillel Rubinstein[4], Dirk Schwalm[1], Dror Shafir[4], Andreas Wolf[1], Daniel Zajfman[4]

[1]Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany
[2]VERA Laboratory, Institut für Isotopenforschung und Kernphysik, Universität Wien, A-1090 Wien, Austria
[3]Department of Physics, University of Kaiserslautern, D-67663 Kaiserslautern, Germany
[4]Department of Particle Physics, Weizmann Institute of Science, Rehovot 76100, Israel

After 40 years of experimental interest, long-lived metastable states of molecular hydrogen anions (H_2^- and D_2^-) were detected with an accelerator mass spectrometer [1]. Subsequent measurements of the lifetimes of H_2^- and D_2^- showed strong disagree with then current theory [2]. Stabilized against autodetachment by large angular momentum, the nonlocal resonance model calculates a molecular bond length of 6 a.u [1].

Fast-beam Coulomb Explosion Imaging (CEI) is a straightforward method to measure the fundamental structure of the molecular anions. The Coulomb explosion is initiated by the sub-femtosecond stripping of the hydrogen anion beam (500 keV/amu) with an 5 nm thick diamond-like carbon foil. The total kinetic energy release (KER) of the fully stripped nuclei is determined on an event-by-event basis. The KER is quantified by measuring the three-dimensional separation of the fragments on a position-sensitive detector 2 m downstream from the stripping foil. The non-negligible effects of the foil and the substantial rotational kinetic energy included in numerical simulations of the measurement as far as possible. A good description of the initial distribution of internuclear distances is found. Results will be presented for measurements of H_2^- and D_2^-.

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Mo5-12

Femtosecond wave packet dynamics in Na_2 revealed by four-wave mixing.

Silvije Vdovic∗

Institute of Physics, Bijenicka cesta 46, HR-10001 Zagreb, Croatia

The propagation of wave packets on the ground and several excited potential energy surfaces of the sodium dimer is investigated in detail by four-wave mixing (FWM) with fs pulses. Dynamics of the ground and A excited state is seen in a simple FWM scheme. Introducing a cw laser, part of the Na_2 population is transferred to the A excited potential surface so that higher potentials became accessible to the 800 nm laser excitation in the FWM sequence.

These higher states are characterized by motion both in nuclear and electronic coordinates. The energetic regions where the two electronic states are excited are thoroughly studied.

∗e-mail: silvije@ifs.hr

Mo5-13

ON THE STABILITY, LIFETIME AND REACTIVITY OF MOLECULAR DICATIONS IN THE GAS PHASE

M. Yáñez and O. Mó

Departamento de Química, C-9, Universidad Autónoma de Madrid, Cantoblanco,
28049-Madrid, Spain

The existence of $[HeNCH]^{2+}$, $[HeCNH]^{2+}$ and $[CuH_2O]^{2+}$, $[CuNH_3]^{2+}$, $[CuHCN]^{2+}$ species formed by the association of alpha particles to HCN and CNH and by the interaction of Cu^{2+} with water, ammonia and hydrogen cyanide, was examined by reliable high-level ab initio methods. It is shown [1] that the former two species are metastable with respect to the proton loss process, but the activation barriers are high enough to accommodate several resonant states. Their lifetimes calculated using the stabilization method are practically infinite for $v < 3$ and never smaller than 1 μs for higher vibrational levels, implying that attachment of alpha particles to HNC and HCN yield kinetically stable dications. This could be an important factor in the cyanide chemistry in interstellar and comets environments. Similarly, although the Cu^{2+} complexes investigated are metastable with respect to their dissociation into $Cu^+ + L^+$ ($L = H_2O$; NH_3, HCN), their lifetimes, obtained using the exterior complex scaling and the semiclassical WKB methods, show that they are kinetically stable [2]. As a matter of fact, if the three complexes are produced in the lowest vibrational levels, they behave as totally bound (with almost infinite lifetime) species. This solves a recent controversy on the existence of monohydrated metal dications in the gas phase. We have also proved that the association of alkaline-earth dications such as Ca^{2+} to neutral systems leads to stable molecular dications which unimolecular reactivity can be followed by suitable mass spectrometry techniques. [3] In these reactions coulomb explosions compete with the loss of neutral fragments so new doubly charged species are generated as primary products of the reactions.

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Mo5-14

INTRAMOLECULAR VIBRATIONAL REDISTRIBUTION IN Ne-Br$_2$: THE SIGNATURE OF INTERMEDIATE RESONANCES

A. García-Vela

Instituto de Matemáticas y Física Fundamental, C.S.I.C.,
Serrano 123, 28006 Madrid, Spain

Wave packet simulations of the Ne-Br$_2$(B,v') vibrational predissociation dynamics in the range v'=16-29 are reported [1]. The aim is to interpret recent time-dependent pump-probe experiments [2]. Good agreement is found between the calculated and the experimental lifetimes corresponding to decay of the Ne-Br$_2$(B,v') initial state and to appearance of Br$_2$(B,v<v') products. The simulations show that up to v' ~22 the dynamics is dominated by direct predissociation, while for higher v' levels an indirect intramolecular vibrational relaxation (IVR) mechanism of dissociation becomes increasingly important. Such a mechanism occurs via coupling of the initial state in the v' vibrational manifold to energetically nearby resonances embedded in the continuum of the lower v<v' manifolds, which act as intermediate doorway states to dissociation. The role of intermediate resonances manifests itself in multiexponential behavior and oscillations in the time-dependent population curves associated with the initial complex state, the final product states, and the Ne-Br$_2$(B,v<v') intermediate complexes. Analysis of the Ne-Br$_2$(B,v<v') intermediate population shows that the continuum resonances are supported by centrifugal barriers involving excitation of the internal rotation of the complex, which confirms their nature of orbiting resonances predicted in previous classical simulations [3]. In the light of the results, a structure of the spectrum of continuum resonances is suggested in which the density of continuum resonances reaches a maximum in the region just above the Ne + Br$_2$(B,v'-1) threshold, and it decreases gradually with increasing energy above this threshold.

In addition, Ne-Br$_2$(B,v') excitation spectra produced after vibrational predissociation have been calculated in the range v'=20-35 [4], in order to investigate the signature of the intermediate resonances lying in the lower v<v' vibrational manifolds, and to elucidate further their role in the IVR dynamics in Ne-Br$_2$. By increasing v', the energy position of the Ne-Br$_2$(B,v') initial resonance state probes the whole range of the spectrum of v'-1 intermediate resonances, from the continuum resonances above the Ne + Br$_2$(B,v'-1) dissociation threshold to the resonances below that threshold. The excitation spectra reveal strong overlapping between spectral features, indicating that the intermediate resonances are coupled and interfere between themselves. This coupling generates an interconnected network of intermediate resonances, through which an efficient flow of the initial population leading to IVR takes place. The results confirm the structure previously suggested for the spectrum of continuum resonances. An upper energy limit for the spectrum of v'-1 continuum resonances has been estimated to be about 23-29 cm^{-1} above the v'-1 dissociation threshold.

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Mo5-15

SOLVENT EFFECT ON THE 0-0 PHOSPHORESCENCE BAND AND CHANGE OF POLARIZABILITY UNDER THE $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ TRANSITION IN MOLECULAR OXYGEN

Vladimir S. Pavlovich

Institute of Molecular and Atomic Physics, 70 Prospect Nezalejnasty, Minsk, 220072, Belarus

In presented work the experimental data from Wessels and Rodgers [1] on solvent effect on the peak position of the 0-0 band ν_{max} of the $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ phosphorescence of molecular oxygen are described through a new relation for solvatochromic shift due to dispersion and induction interactions [2], obtained with help the continuum Onsager's cavity model. Thus

$$\nu_{max} = 7882.4 + \Delta\nu_{rep} + \Delta\nu_{\Sigma} - \frac{\Delta\alpha_{eg}}{a_O^3} P(n,\varepsilon,I_s),\ P(n,\varepsilon,I_s) = \frac{3E_{00}^2 I_s}{I_s^2 - E_{00}^2} P_n + k_B T\, P_\varepsilon$$

where $\Delta\nu_{rep}$ and $\Delta\nu_{\Sigma}$ denote the effect of repulsive and multipole interactions, $\Delta\alpha_{eg}$ is the change of polarizability under $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ transition, a_O is Onsager radius, E_{00}=7882.4 cm^{-1} (energy gap of solute in the gas phase taken from Herzberg), I_s is the ionization potential of solvent molecule, $P_n = \frac{n^2-1}{n^2+2}$, $P_\varepsilon = \frac{\varepsilon-1}{2\varepsilon+1}$ with n and ε being the reflective index and the dielectric constant of solvent. The induction effect arises from the interaction of an induced dipole moment in oxygen molecule with chance electric field produced by the random motion of the solvent dipoles.

The used 35 solvents with known I_s are divisible into three principle groups with virtually alike linear correlation between ν_{max} and the $P(n,\varepsilon,I_s)$ with slope –0.073 ±0.004. Say the first group includes *n*-alkanes, *n*-alcohols (but methanol), benzene and its halogen derivatives, acetone, tetrahydrofuran, C_2Cl_4, toluene and benzonitrile (20 solvents). The second group includes methanol, CCl_4, $CHCl_3$, dioxane and CS_2. The one exception to all solvents is represented by water and acetonitrile. After detail analysis we came to the conclusion that the red shift results in the dipole-dipole, dispersion and induction, interactions as well as from the interactions of multipoles, among which quadrupole-quadrupole interactions play a dominant role. Water, acetonitrile, dioxane, methanol, $CHCl_3$, CS_2 and CCl_4 was shown to have the highest guadrupolarity. The repulsion makes a blue shift of the 0-0 band, which is a more or less alike for all solvents that early pointed by Schmidt [3]. Since $\Delta\alpha_{eg} = 0.073 a_O^3$, it has been found with a_O=1.37 Å that the polarizability in the $a^1\Delta_g$ state is 0.19 ±0.03 Å^3 above than that in the $X^3\Sigma_g^-$ state. There is a need to point that our result for $\Delta\alpha_{eg}$ do not support that of –0.08 Å^3 early obtained by quantum mechanical calculations from Ogilby and co-workers [4].

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Mo5-16

Ejection anisotropy in the Coulomb explosion of some alkyl halides under strong ps laser irradiation

S. Kaziannis, C. Kosmidis
Department of Physics, University of Ioannina, 45110 Ioannina, Greece
*Corresponding author. e-mail address: skaziannis@in.gr, Fax: +30-2651098695

The multielectron dissociative ionisation (MEDI) of C_2H_5X, 1-C_3H_7X, 1-C_4H_9X, where X=I, Br, Cl, following their interaction with strong (1×10^{13}-2.0×10^{15} W/cm^2) 35ps laser pulses at 1064nm is studied by means of time-of-flight mass spectrometry. The multiple molecular ionization is found to take place at elongated C-X bond distances for the studied molecules. By combining the intensity dependence of the ion yields, the estimated kinetic energies of the released fragment ions and their angular distributions, different Coulomb explosion channels of the transient multiply charged parent ions have been identified.

The angular distributions of the MEDI halogen fragment ions are indicative of the dynamic alignment of the corresponding multiply charged precursors. The alignment mechanism has been verified by comparing the ionisation yields of the fragment ions for linearly and circularly polarized laser pulses [1] and, also, by the dependence of their angular distributions' characteristics on the irradiation intensity [2]. The latter indicates that the majority of the molecular alignment under ps laser irradiation takes place at lower laser intensities than the required for the multiple molecular ionization and that the 'post-ionization alignment' mechanism does not contribute to the final degree of alignment [3], in agreement with that reported for diatomic molecules previously [4].

Finally, from the comparison of the angular distributions' widths of the halogen fragment ions originating from multiply charged molecular ions it is concluded that the degree of alignment is strongly depended on the size of the molecular alkyl chain, especially for the case of the alkyl chloride molecules. Particularly, a broadening of the angular distributions' widths from ethyl- to butyl-halide molecules is observed, which is consistent with an increasing moment of inertia and with an enhanced multiple ionization probability as the size of the molecular alkyl chain increases [5]. However, the moment of inertia is clearly not the only parameter determining the effectiveness of the molecular alignment since the degree of alignment is only weakly depended on the mass of the halogen atom for molecules of the same molecular chain.

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Mo5-17

THEORETICAL STUDY OF THE PHOTOIONIZATION CROOSS SECTION NEAR THE C*K*-IONIZATION THRESHOLD OF THE C_2H_2 MOLECULE

V.A.Yavna, A.M.Nadolinsky, A.N.Hopersky

Rostov State University of Transport Communication, Rostov-na-Donu, 344038
Russia, amnrnd@mail.ru

The absolute values of the cross sections and the shape of the *K*-absorption spectrum of the carbon atom in the acetylene molecule C_2H_2 are calculated with the one-electron wave functions of occupied and free states calculated with the one-centre method [1,2] using the theory of non-orthogonal orbitals. Considered are the processes of single and double excitation/ionization.

Comparison of the theoretical spectrum with the experiment [3] shows that the process of single photoabsorption accounts for about 70% of the experimental spectrum intensity and for one weakly expressed photoabsorption resonance at 308 eV.

In order to perform a detailed comparison with the experimental [3] and theoretical [4] results, we consider the processes of double excitation/ionization with the additional ejection of the 1π-electron into the 2π-state. The comparison of the spectra makes it possible to conclude that the resonances observed in the spectrum in the immediate vicinity of the 1σ-molecular orbital threshold are due, in the first place, to the states of double photoexcitation.

Calculation results for the single photoexcitation oscillator strengths are predictions.

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Mo5-18

VALENCE SHELL DOUBLE PHOTOIONIZATION OF ALKALINE-EARTH ATOMS

A. S. Kheifets[†] and Igor Bray[⋆]

[†]Research School of Physical Sciences, The Australian National University
Canberra ACT 0200, Australia

[⋆]ARC Centre for Matter-Antimatter Studies, Murdoch University, Perth, 6150
Australia

We apply the convergent close-coupling (CCC) formalism to describe direct double photoionization (DPI) of the valence ns^2 shell of alkaline-earth atoms: beryllium ($n = 2$), magnesium ($n = 3$) and calcium ($n = 4$). We consider the range of photon energies below the onset of resonant and Auger ionization processes where the subvalent and core electrons can be treated as frozen. Our model comprises the multiconfiguration Hartree-Fock expansion of the valence shell of the target atom and the CCC expansion of the two electron continuum in the Hartree-Fock field of the ionized target. Both in the ground state and the final ionized state, the core (and subvalent) electrons are kept frozen.

As a test bench, we use the recent accurate measurement of the single and double photoionization cross-sections in Be [1]. Our data are in a reasonable agreement with experiment. For the single photoionization cross-section, the theory is about 10% below the experimental data near the DPI threshold, but comes into better agreement further away from the threshold. For double photoionization, our CCC calculation in the velocity gauge is about 20% higher than the experiment near the threshold. Agreement is somewhat better at excess energies above 10 eV.

Having tested our model and gotten indication of its accuracy, we proceed with calculations for other atoms, Mg and Ca. We use the notion of the reduced excess energy measured in units of the ionization potential of the singly ionized target. This allows us to bring alkaline earth atoms and He on the common scale. On this scale, the double-to-single photoionization cross-sections ratio in all the targets follows a universal shape function. This is related to the fact that DPI process near threshold in all two-electron targets is dominated by the electron impact ionization of the corresponding singly charged ion.

As compared with He, we observe significantly stronger angular correlation in the two-electron continuum of the alkaline earth atoms. We attribute this reduction to the narrowing width of the momentum profile of the bound electron attached to the corresponding singly charged ion. This effect has been reported earlier in DPI of various excited states of He and other two-electron targets [2].

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Mo5-19

ISOTOPE EFFECTS IN THE $Mg^+(3p)$ + HD → MgD^+ (MgH^+) + H(D) REACTION

K. Højbjerre, P. Staanum, R. Wester[1], M. Drewsen

Department of Physics and Astronomy, University of Aarhus, Denmark

klaush@phys.au.dk

A common way to gain insight into chemical reactions is to conduct experiments with various isotopologues. Such laboratory studies are also carried out to better understand the chemical evolution of inter-stellar clouds and other astronomical objects. In particular, isotopologues including Deuterium are interesting. Reactions of atomic ions with different isotopologues of molecular hydrogen have been studied extensively in guided beam experiments [1,2,3] as well as recently in Paul traps with samples of trapped and laser cooled ions [4,5].

Here, we present the results of $Mg^+(3p)$ + HD → MgD^+ (MgH^+) + H(D) reactions studied on the single ion level in a Paul trap. Through a non-destructive mass measurement [6], we are able to detect a single ion-molecule reaction and determine the reaction product with nearly 100% efficiency. In the reaction of Mg^+ with HD at room temperature, we find that the production of MgD^+ is strongly preferred over MgH^+. Assuming a Langevin capture process, a simple model enables us to deduce the relative probabilities for forming the two possible products. We find that the formation rate for MgD^+ is $\simeq 10$ times higher than that of MgH^+.

The general nature of the technique to investigate single ion reactions can be applied to a broad selection of molecules, and hence could in the future be a useful tool for studying reactions of fundamental interest and of relevance to astrochemistry.

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[1] Permanent address: Physikalisches Institut, Universität Freiburg, Germany

Mo5-20

TIME-RESOLVED STIMULATED EMISSION SPECTROSCOPY THROUGH SUB-PICOSECOND PUMP-PROBE EXPERIMENTS

L.Guidoni[1], S. Orlando[2], A. Paladini[2], G. P. Parisi[2], A. Santagata[2], R. Teghil[3], , A. De Bonis[3], A.Giardini[2,4], P. Villani[2,3] , S. Piccirillo[5]

[1] CNRS, Matériaux et Phénomènes Quantiques UMR 7162, Université Denis Diderot - Paris 7, Paris, France
[2] CNR - Istituto Metodologie Inorganiche e Plasmi, I-85050 Tito Scalo (Pz), Italy
[3] Dipartimento di Chimica, Università degli Studi della Basilicata, I-85100 Potenza, Italy
[4] Dipartimento di Chimica, Università di Roma "La Sapienza", I-00185 Roma, Italy
[5] Dipt. di Scienze e Tecn. Chimiche, Università di "Tor Vergata", Roma, Italy

contact details: anna.giardini@uniroma1.it, tel. +39 06 49913358, fax +39 06 490324

The photoemission properties of fluorescent chromophores have a widespread application in many fields ranging from chemical–physics and biology to organic light emitting devices. They usually display high fluorescence conversion efficiency, which make them suitable for transient/gain experiments also in liquid solutions, thin films and eventually in protein environments [1]. Pump and probe methods have been widely employed for wavelength resolved spectroscopy in the subpicosecond time scale. The dynamic response of photoinduced changes in the chromophore induced by suitable solvent molecules has been studied with a time resolution of 300 fs.

The pump-probe experiments have been performed using a Nd:glass laser (Light Conversion) emitting 10 Hz pulses of 250 fs duration at 527 nm. The laser beam has been splitted into two parts, one focused directly into a quartz cuvette containing the liquid solution (rhodamines, coumarines, DCM, etc. dissolved in methanol, ethanol and acetone), the other used to generate a broad spectral continuum by a sapphire plate. This continuum spectrum is temporally squeezed and used as probe of the induced optical changes in the 0-300 ps time range. The obtained spectral data have been recorded through a 500 mm monochromator coupled with a fast ICCD detector. In order to optimize the experimental setup two tests on Rhodamine B in ethanol and acetone have been performed and the process of amplified spontaneous emission centred at 612 nm has been recorded.

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Mo5-21

High-resolution slice imaging of quantum state-to-state photodynamics

M. Laura Lipciuc [a], T. P. Rakitzis [b] and M .H. M. Janssen [a]

[a] Laser Centre and Department of Chemistry, Vrije Universiteit, de Boelelaan 1083, 1081HV Amsterdam, The Netherlands
[b] Department of Physics, University of Crete and IESL-FORTH, 711 10 Heraklion-Crete, Greece

High-resolution slice imaging experiments are reported for the quantum state-to-state photodissociation dynamics of OCS, CH_3Br and CD_3I. We present data using our recently developed large frame CCD centroiding imaging detector, and have implemented a new high speed MCP high voltage pulser with an effective slice width of only 5 ns [1-3]. Slice images are presented for quantum state-to-state photolysis of vibrationally excited OCS(υ_2=0,1,2). Two-laser pump-probe experiments show a dramatic change in the β-parameter for the same final rotational state of CO(J) when the photolysis energy is reduced by about 1000 cm^{-1} [3]. The quantum state-to-state cross section for the photodissociation of selected rovibrational bending states of OCS (v_2=0,1,2|J) is presented. The photodissociation cross section is strongly enhanced by the excitation of the bending vibration in OCS. Depending on the CO rotational state, the cross section for OCS(υ_2=1) is about 20 times stronger than for OCS(υ_2=0), and for OCS(υ_2=2) about 55 times stronger than for OCS(υ_2=0) [4]. Strong polarization effects of the probe laser are observed, both in the angular distribution of the intensity of single $S(^1D_2)$ rings and in the resolution of the radial velocity distribution [5]. We present results from rotationally state-selected photolysis of both CH_3Br and CD_3Br at 212.8 nm and into the red wing of the absorption band. The photodissociation leads to the population of several vibrational modes in the methyl fragment, especially in the case of the deuterated methyl bromide photolysis. Angular and translational energy distributions of state-selectivity detected CH_3/CD_3 fragments are presented [6].

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Mo5-22

Dissociation dynamics of small molecules under strong laser field

A. Diner[1,5], A. Natan[2], U. Lev[1], I. Ben-Itzhak[1,3], O. Heber[1], D. Schwalm[4], Y. Silberberg[2], D. Zajfman[1]
[1]*Department of Particle Physics*
[2]*Department of Physics of Complex Systems*
Weizmann Institute of Science, Rehovot, 76100 Israel
[3]*J.R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas 66506, USA*
[4]*Max-Planck Institut für Kernphysik, Heidelberg, Germany*

Dissociation under ultrashort intense laser fields differs from the process occurring in the presence of a weak field by two main characteristics. In the strong field regime, the force exerted by the laser on the molecule is comparable to the inter-molecular forces. In addition, this force is varying on a time scale comparable to that of the molecular vibration. The combination of these two effects results in "Dynamic potential energy curves".

In recent years, a few groups investigated the dissociation of H_2^+-beam targets experimentally (see, for example, [1-3]) to complement the numerous studies using H_2 [4]. These experiments used different pulse durations and intensities in order to investigate the effect of these parameters on the kinetic energy release and angular distribution of the dissociating fragments.

In the current work we present a new experimental system which enables further the investigation of the dynamics of the dissociation process. Our experimental setup includes an amplified Ti-Sapphire femtosecond laser [intensity range of 10^{13} -10^{15} W/cm^2], a 4-f pulse shaper, and a fast (keV) ion beam with a coincidence three-dimensional momentum imaging system.

The use of a pulse shaper opens new possibilities for controlling the laser pulse both in the frequency and in the time domain. Using this, we measured the dissociation of H_2^+ by an intense laser pulse with a spectral π phase step located at the centre of its spectrum. In the time domain, applying a π phase step at the central wavelength results in the fastest transient available, producing a narrow zero intensity dip in the centre of the pulse envelope, the time duration of which is of the order of a vibration time of H_2^+ (~14fs).

By comparing the energy release profile and the angular distribution of the fragments of H_2^+ to that of its isotope D_2^+, where the later differ only in mass, hence in the vibration period but not in the potential energy curves, we gain insight to the dissociation dynamics of H_2^+ in particular, and of small molecules in general.

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[5] email:adi.Diner@weizmann.ac.il

Mo5-23

HIGH-ORDER HARMONIC GENERATION IN LASER-IRRADIATED LIGHT MOLECULAR DIMERS

Vladimir I. Usachenko[1], Pavel E. Pyak[1] and Shih-I Chu[2]

[1] Institute of Applied Laser Physics UzAS, Tashkent, 100185, Uzbekistan.
[2] Department of Chemistry, University of Kansas, Lawrence, KS 66045-7582, USA

The highly multiphoton process of high-order harmonic generation (HHG) in light molecular dimers (H_2^+, H_2, N_2 and O_2) irradiated by a strong linearly polarized laser field of low fundamental frequency $\omega << I_p$ (I_p is the molecular ionization potential and the *atomic system of units* is used) is considered. The incident laser field is generally supposed to be of very high intensity $\boldsymbol{I}$, such that the HHG process under study can not be adequately described yet by a perturbation expansion with respect to the electromagnetic (EM) interaction. The applied approach based on the *velocity-gauge* version of *strong-field approximation* (SFA) [1] (alternatively developed to adequately incorporate *rescattering* effects beyond the quasiclassical *saddle-point approximation*) is currently extended to molecular case [2] by means of supplementing the standard *linear combination of atomic orbitals* (LCAO) and *molecular orbitals* (MO) method. The associated molecular HHG model proved to adequately reproduce a general shape and detailed structure of molecular harmonic spectra, which demonstrate a number of remarkable distinctive differences from respective spectra of atomic counterparts (of nearly equal ionization potential) calculated under the same laser pulses. The revealed differences as well as other generic features (such as the extent of the high-frequency *plateau* and harmonic emission rates) are found to be strongly dependent on internuclear separation R_0 and also very sensitive to the orbital and bonding symmetry of the contributing molecular valence shell. In particular, for sufficiently large R_0, the molecular harmonic spectra demonstrate a plateau of a noticeably longer extent and significant enhancement (up to 2÷3 orders of magnitude) in harmonic emission rates compared to spectra corresponding to equilibrium internuclear separation and calculated under the same laser pulses. In addition, for some group of high harmonics within the plateau *cutoff* domain, the harmonic emission rates were ascertained to dominate by contribution from inner molecular shells (such as $3\sigma_g$ in O_2 and/or $2\sigma_u$ in N_2 of higher binding energy and different orbital symmetry) compared to the outermost molecular orbital (such as $1\pi_g$ in O_2 and/or $3\sigma_g$ in N_2) normally predominantly contributing. Finally, due to a high suppression in ionization of O_2 relative to counterpart atomic *Xe*, the harmonic spectrum calculated for O_2 proved to demonstrate a noticeably longer plateau extending far beyond the harmonic cutoff in HHG spectrum of atomic counterpart *Xe*, in a fairly good accordance with relevant experiments [3].

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Mo5-24

SINGLE PHOTON–INDUCED SYMMETRY BREAKING IN H_2 DISSOCIATIVE IONIZATION

F. Martín,[1] J. Fernández,[1] T. Havermeier,[2] L. Foucar,[2] Th. Weber,[2] K. Kreidi,[2]
M. Schöffler,[2] L. Schmidt,[2] T. Jahnke,[2] O. Jagutzki,[2] A. Czasch,[2] E. P. Benis,[3]
T. Osipov,[4] A. L. Landers,[5] A. Belkacem,[4] M. H. Prior,[4] H. Schmidt-Böcking,[2]
C. L. Cocke,[3] R. Dörner[2]

[1]Departamento de Química, C-9, Universidad Autónoma de Madrid,
28049 Madrid, Spain.
[2]Institut für Kernphysik, University Frankfurt, Max von Laue Strasse 1,
D-60438 Frankfurt, Germany.
[3]Department of Physics, Kansas State University, Cardwell Hall, Manhattan,
KS 66506, USA.
[4]Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA.
[5]Department of Physics, Auburn University, Auburn, AL 36849, USA.

H_2, the smallest and most abundant molecule in the universe, has a perfectly symmetric ground state. What does it take to break this symmetry? We have found [1] that the inversion symmetry can be broken by absorption of a linearly polarized photon, which itself has inversion symmetry. In particular, the emission of a photoelectron with subsequent dissociation of the remaining H_2^+ fragment shows no symmetry with respect to the ionic H^+ and neutral H atomic fragments (see figure). This lack of symmetry results from the entanglement between symmetric and antisymmetric H_2^+ states caused by autoionization. The mechanisms behind this symmetry breaking are general for all molecules.

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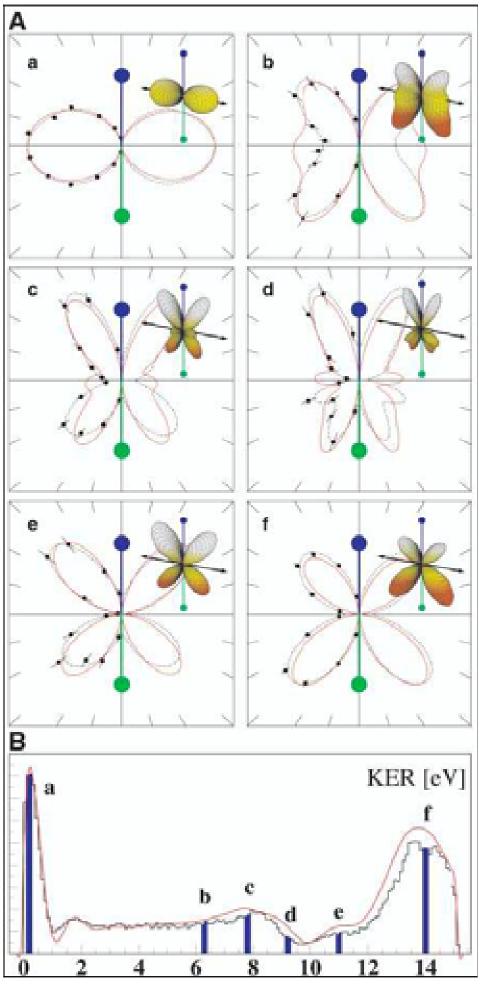

Figure. **(A)** Angular distribution of the electrons as a function of KER for dissociative ionization of D_2 at a photon energy of 33.25 eV, linearly polarized light. The orientation of the molecule at 90° to the polarization (theory) and 90° ± 10° (experiment) is indicated by colored circles (blue, deuteron; green, deuterium). The (horizontal) polarization vector and the molecular axis define a common plane. The electron is restricted to this plane by ±45°. Solid red line, theory; circles with error bars (where error is SD), experiment; dotted line, fit of the experimental data with spherical harmonics. The theoretical results have been integrated over the experimental acceptance angles and KER resolution as well as electron resolution. Infinite resolution theoretical results are shown by the small three-dimensional plots in the upper right: KER = 0.2 (a), 6.3 (b), 7.8 (c), 9.2 (d), 11 (e), and 14 eV (f). Units are arbitrary units. **(B)** The angle-integrated KER spectrum. Red line, theory; black line, experiment; letters a to f correspond to a to f in **(A)**; KER intervals are ±0.1 eV. The x-axis shows KER in eV. The y-axis shows a cross-section in arbitrary units.

Mo5-25

High-resolution UV-Laserspectroscopy on jet-cooled 9-Cyano-Anthracene in electric fields

Markus Glugla, Elke Heinecke

Institute of Optics and Atomic Physics, Technical University of Berlin, D-10623 Berlin, Germany

The analysis of high-resolution spectra of large organic molecules can be a difficult procedure. Still their jet-cooled rotational spectra consist of thousands of overlapping lines caused by small rotational constants. The experimental determination of electrical properties of large molecules by Stark-effect measurements requires the analysis of such spectra further complicated by line shifts and splittings. We present the results of our investigation of the vibrationless S_1 - S_0 transition of 9-cyano-anthracene at 382 nm in static homogeneous electric fields. We recorded the high-resolution zero-field spectrum and determined rotational constants for the ground and excited state of 9-cyano-anthracene as well as Stark-shifts and Stark-splittings of single rotational lines for various electric field strengths. From these data we determined the electric dipole moment of the ground and excited state.

Mo5-26

Can 2D photon echo spectroscopy distinguish electronic and vibrational coherences in molecular systems?

Dassia Egorova, Maxim Gelin[1] and Wolfgang Domcke
Department of Chemistry,
Technical University of Munich,
Lichtenbergstr, 4, D-85747 Garching, Germany
[1] present address: *Department of Chemistry and Biochemistry, University of Maryland,*
College Park, MD 20742-4454

Ultrafast photon-echo (PE) spectroscopy belongs to the realm of the four-wave mixing techniques. If a density-matrix description is employed for system dynamics, PE spectroscopy reflects both populations and coherences of the density matrix in real time (as distinct from the pump-probe and fluorescence spectroscopy, which primarily deliver information about population dynamics only).

The so-called two-dimensional (2D) or Fourier-transformed PE has gained especially much attention in the recent years. This approach, which has proven invaluable for determining intervibrational couplings in the infrared, has recently been successfully implemented in the optical domain, gaining a direct information on electronic couplings in the seven-chromophore Fenna-Matthews-Olson protein [1].

Electronic couplings are expected to manifest themselves as cross peaks in 2D electronic spectra. However, as we have recently demonstrated [2], Franck-Condon activity of vibrational modes can lead to detection of cross peaks as well. It is thus desirable to determine some criteria which would allow us to distinguish between different mechanisms giving rise to cross peaks in 2D electronic spectra.

The calculations within an underdamped harmonic oscillator model [2] suggest that the wave-packet motion induced in the excited electronic state (i.e., vibrational coherences) can be visualized by 2D PE spectroscopy. On the other hand, simulations for a dimer model, which explicitly consider only electronic degrees of freedom [3], predict a possibility of detection electronic coherences by this technique. The present contribution aims to clarify the difference between manifestations of vibrational and electronic coherences. Our novel numerically efficient method for the computation of four-wave mixing signals within the density-matrix formalism [4] is employed for this purpose. The method is valid for any pulse durations and automatically accounts for pulse-overlap effects.

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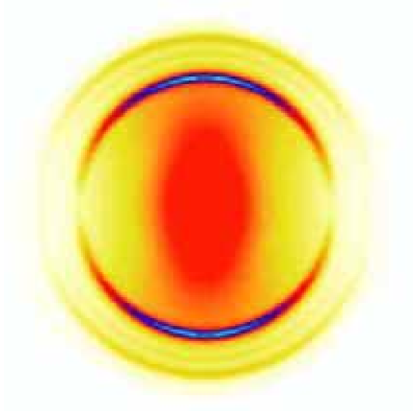
Mo5-27

A FEMTOSECOND IMAGING STOPWATCH FOR THE BOND BREAKAGE OF A POLYATOMIC MOLECULE

R. de Nalda[1], J.G. Izquierdo[2], J. Durá[2], L. Bañares[2]

[1]Instituto de Química Física Rocasolano, Consejo Superior de Investigaciones
Científicas, Serrano 119, 28006 Madrid, Spain
[2]Facultad de Ciencias Químicas, Universidad Complutense de Madrid, Avda.
Complutense s/n, 28040 Madrid, Spain

We demonstrate that the combination of velocity map imaging and femtosecond pump-probe technology for the observation of ground-state neutral fragments allows the measurement of the reaction times of several well-defined channels in the bond breakage of a polyatomic molecule. By using resonant detection, we have been able to clock the C-I bond rupture of methyl iodide, CH_3I, from the *A* band, which involves non-adiabatic dynamics yielding ground-state I($^2P_{3/2}$) and spin-orbit excited I*($^2P_{1/2}$) and ground and vibrationally excited CH_3 fragments. The reaction times found for the different channels are directly related with the non-adiabatic dynamics of this multidimensional photodissociation reaction. Once the wave packet is formed in the $^3Q_0$ potential surface, the dynamics is probed by a time-delayed femtosecond pulse. Results obtained with both resonant and non-resonant probing will be presented and discussed in relation to the observation of transition states.



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Contact: r.nalda@iqfr.csic.es, lbanares@quim.ucm.es

Singly differential cross section for Ps-fragmentation with exchange

Hasi Ray
Institute of Plasma Research, Bhat, Gandhinagar, Gujrat, India
E-mail: *hasi_ray@yahoo.com*

Projectile ionization in Ps-atom scattering is of fundamental importance [1-7]. We study Ps-H and Ps-He systems. We evaluate singly differential cross sections for Ps-ionization in Ps-He scattering to compare them with the recently available experimental data. These provide more accurate test of a theory than integrated or total ionization cross sections due to the fact that the energy averaging is relaxed in the former case. The agreement of our integrated ionization cross sections with experiment in Ps-He scattering and the available data using a coupled-pseudostate R-matrix theory for Ps-H scattering impose the success of our theory and importance of exchange at lower incident energies which are incorporated in the comparison of singly differential cross sections with experimental data.

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Mo5-29

Transition State Spectroscopy of open shell systems: angle-resolved photodetachment spectra for the adiabatic singlet states of OHF.

Susana Gómez-Carrasco

Instituto de Matemáticas y Física Fundamental, C.S.I.C.,

Unidad Asociada UAM-CSIC, Serrano 123, 28006 Madrid, Spain.

Alfredo Aguado, Miguel Paniagua

Unidad Asociada UAM-CSIC. Departamento de Química Física,

Facultad de Ciencias C-XIV, Universidad Autónoma de Madrid, 28049, Madrid, Spain

Octavio Roncero

Inst. de Matemáticas y Física Fundamental, C.S.I.C.,

Unidad Asociada UAM-CSIC, Serrano 123, 28006 Madrid, Spain.

Abstract

In this work three-dimensional potential energy surfaces of the first five singlet states of OHF are developed based on fits of more than 10000 highly accurate *ab initio* points. An approximate treatment is presented for the calculation of the anisotropy parameter describing the electron angular distribution photodetached from a molecular anion. This method is used to calculate the angle-resolved photoelectron spectra in the photodetachment of OHF^-. The wave packet formed in the neutral OHF system is placed at the transition state region, and yields the formation of OH+F and HF+O products. The results are compared with the recent experimental measurements published by Neumark(Phys. Chem. Chem. Phys. **7**, 433 (2005)). The intensity found at low electron kinetic energy including these 5 states and the three lower triplet states is found to be low. To analyze the effect of higher electronic states more excited $^1\Sigma^-,^3\Sigma^+$ and $^3\Delta$ states are calculated at collinear geometry. The agreement with the experimental data improves, thus demonstrating that the correct simulation of the photodetachment spectrum at 213 nm involves at least 12 electronic states. All the structures of the experimental spectra are semiquantitatively reproduced finding an overall good agreement. It is concluded that the main problem of the simulation is in the intensity and anisotropy parameters. An alternative to their calculation would be to fit their values to reproduce the experimental results, but this would require to separate the contribution arising from different final electronic states.

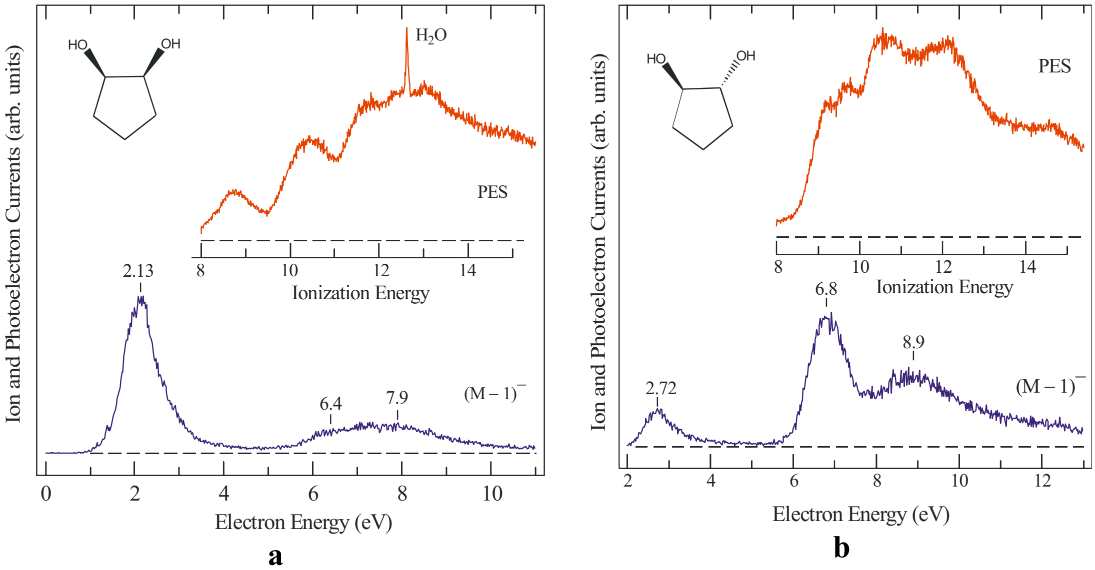
Mo5-30

Dissociative electron attachment of some cyclic diols

Bogdan Catalin Ibanescu, Olivier May, Michael Allan

Department of Chemistry, University of Fribourg, Switzerland

We studied the dissociative electron attachment of several compounds containing hydroxyl groups motivated by their importance in biologically relevant processes [1-3].



a **b**

Fig 1. Yield of the $(M\text{–}1)^-$ fragment and the HeI photoelectron spectrum of:
a) *cis*-1,2 cyclopentanediol and b) *trans*-1,2 cyclopentanediol

It has been shown that in the case of monoalcohols the DEA spectrum reveals a shape resonance around 3 eV[4] and several Feshbach resonances at higher energies [4,5]. While in monoalcohols the low energy band is substantially weaker than the Feshbach resonances, in 1,2 cyclopentanediols it is comparable to, and even higher than, the high energy bands. Another striking feature is the decrease of the energy of the shape resonance, due to the increase of electron affinity of the fragments.

There are other more 'complex' fragmentations present in the Feshbach resonance range. The loss of an H atom and one H_2 molecule indicate that the initially formed resonance may be first stabilized by a relaxation of the molecular frame and H atom loss, followed by more complex chemical changes. This complex fragmentations show that low energy electrons can cause dramatic damage to alcohols.

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POSTERS

Monday 7/5

6. Plasma

Mo6-1

COLLISIONAL-RADIATIVE MODELS FOR DIAGNOSIS OF Xe PLASMAS

K. Katsonis[1], Ch. Berenguer[1], R.E.H. Clark[2], M. Cornille[3], M. Ganciu [1]

[1] *Lab. de Physique des Gaz et des Plasmas, UMR 8578, Université Paris-sud 91405 Orsay, FRANCE*

[2] *Nuclear Data Section, IAEA, Vienna, AUSTRIA*

[3] *LUTH, UMR 8602, Observatoire de Paris, Meudon, FRANCE*

Although a rare element in nature, Xe has a number of interesting properties such as high atomic weight, low ionization potential and chemical inertness, due to the outer shell consisting of two *s* and six *p* electrons. These outer electrons are easily ionized due to the presence of ten 4*d* electrons lying just lower in energy, a structure which is absent from the Ar atom. Therefore, Xe has been used in a number of applications, including adoption as a plasma thruster propellant (note the parallel use of In as a propellant, with an isoelectronic sequence to which Xe VI belongs, see [1]), as a buffer gas in fusion reactors plasmas (more promising than the currently used Ar because of the enhanced reaction with the target surface), in lighting (because of the rich $5s^2p^6$ spectrum), as a puffing gas for diagnostics in Tokamaks (especially in the divertor region) and many other uses.

Considerable amounts of Xe atomic data are required for modeling and optical diagnostics. Non-intrusive emission spectroscopy plasma diagnostics allows for the evaluation of the local temperature and density [2], and provides information on the constituents and most important processes encountered in the plasma. The satisfactory application of such diagnostics requires a full Collisional–Radiative (C-R) model that takes into account all of the species present, both neutral and ionized, together with their excited state level structure and transition probabilities between the levels; all contributing processes need to be taken into account through their respective reaction rates. We have evaluated a large amount of such data, which we have subsequently used in building a C-R model for the optical diagnostics of various Xe plasmas, as reported previously [3]. During the course of this evaluation, we have made extensive use of the set of codes developed at Los Alamos National Laboratory [4] to help resolve choices between various values of structure, transition probabilities and excitation cross sections. A Maxwellian distribution was used throughout this work as a first approximation for the calculation of the reaction rates.

We report here on the characteristics of this model as applied to the diagnostics of the plasmas, notably a relatively low temperature Xe plasma produced in a hollow cathode with dielectric barrier available at the LPGP laboratory. For higher ionization stages, calculations and measurements of more atomic data are necessary. Validation experiments are under way (see [5]). Comparisons of the theoretical spectra generated from our model with the experimental data obtained at LPGP have been used to validate the Xe I and II atomic data and the theoretical approaches adopted [6].

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Mo6-2

Imaging and spectroscopy of collisions between hot dense plasmas

J. Dardis[1], C. L. S. Lewis[2], J. T. Costello[1]

[1]National Centre for Plasma Science and Technology (NCPST) and School of Physical Sciences, Dublin City University, Dublin 9, Ireland

[2]International Research Centre for Experimental Physics (IRCEP) and School of Physics and Mathematics, Queens University Belfast, Belfast BT7 1NN, Northern Ireland

When two counter-propagating plasmas collide, two extremes of behaviour are observed: they may simply interpenetrate and binary collisions will constitute the main interaction or they may stagnate at the collision interface leading to the formation of a tightly defined plasma layer. The rate of flow and density of this layer can be controlled by the laser pulse energy and laser wavelength used to initially produce the 'seed' plasmas. One may also alter the target configuration to control their separation and mutual angle of approach, two parameters which also affect layer formation and parameters (ion and electron density etc.). Colliding laser plasmas play a key role in areas such as pulsed laser deposition [1], inertial confinement fusion [2], X-ray lasers [3] and laboratory-scale astrophysical simulations [4].

We investigate here the specific case of the collision of a pair of opposing hot dense plasmas generated by a short pulse laser system. Briefly a pair of point plasmas are formed by splitting in two and focussing the 250mJ/ 170ps/ 1064nm output from an EKSPLA 312P Nd-YAG laser on a solid surface. Following formation, the two plasmas expand and collide along a plane parallel to the target surface. The collisionality of the system depends on the ion-ion mean free path (mfp) and the plasma geometrical scale length. At power densities close to 10^{13} W.cm^{-2}, the seed plasmas will possess relatively high temperatures ($T_e \sim 200$ eV) leading to ion-ion mfps that are quite large. As a result the interaction is characterised by low collisionality and we expect to observe a fair degree of interpenetration occurring between the two plumes. Given the high temperatures of the seed plasmas in this case, we have used soft X-ray spectra of the individual source plasmas obtained using a system described in [5] to identify dominant ion stages. We have also measured the soft x-ray emitting size of each plasma using a pinhole camera coupled to an Andor in-vacuum CCD camera. In order to track both the hydrodynamics and the plasma parameters (density and temperature) we have employed time resolved UV/Vis imaging and spectroscopy respectively using an Andor Shamrock 173i spectrometer with ICCD readout. Colliding plasmas generated on various target materials in different configurations (flat, wedge) will be presented. Collisionality is varied by changing the plasma-plasma separation in these cases and the interaction will be discussed in terms of the associated time-space plasma parameter sets.

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Mo6-3

AN INDIUM COLLISIONAL-RADIATIVE MODEL FOR DIAGNOSTICS OF PLASMA THRUSTERS

K. Katsonis[1], J. Bonnet[2], D. Packan [2] , Ch. Berenguer[1], A. Ndiaye[1]

[1] *Lab. de Physique des Gaz et des Plasmas, UMR 8578, Université Paris-sud*
91405 Orsay, FRANCE.

[2] *ONERA/DMPH, 91761 Palaiseau, FRANCE.*

Plasma thrusters are taking more and more importance in space propulsion, as they are efficient and allow for using a reduced mass in a given mission, due to the high velocity of the expelled ions. We are interested here in Field Emission Electric Thrusters (FEEP) in which molten Indium at the tip of a needle is ionized and accelerated to high velocity (100 km/s) in the very high electric field of a small gap between the needle polarized at 8 kV and a surrounding cathode. Indium is preferred due to his low melting temperature and high atomic mass. The thrust is controlled by the ion current, between 0.1 and 20 Micro-Newton. In this context, a detailed analysis of the plasma parameters near the tip, where it is not possible to introduce a probe, is of paramount importance. The density in the region of interest is low and the number of collisions severely reduced, which means that a model is necessary to interpret the spectra.

Indium has some interesting atomic properties: high atomic weight and a low ionization potential which is due to the two *s* and one *p* electron of the external part of its outer $n = 5$ shell. These are easily ionized because of the presence of ten 4*d* electrons just lower. We remind also that the In isoelectronic sequence belongs to Xe VI which is present in the plasma of thrusters using Xe as propellant, see [1].

As it is well known, besides providing information on the constituents and on the most important processes encountered in the plasma, non-intrusive emission spectroscopy plasma diagnostics allows primarily for the evaluation of the local temperature and density which are needed here. For a satisfactory application of such diagnostics a full **C**ollisional – **R**adiative (C-R) model is necessary [2], taking into account all of the species present, both neutral and ionized, together with their excited state level structure and transition probabilities between the levels. In this model, all contributing processes are taken into account through their respective reaction rates. For the moment being, calculation of the reaction rates has been made on the basis of a sole Maxwellian distribution for each species; a second distribution could be also added later if necessary.

In view of the plasma modeling and optical diagnostics of FEEP, we have evaluated a large amount of atomic data, which we have subsequently used in building a C-R model. For this evaluation, structure, transition probabilities and excitation cross sections of In and In^+ ion coming from the set of codes developed at LANL [3] has been extensively used.

We report here on the characteristics of a C-R model taking into account only neutral and once ionized In and on its application on the diagnostics of the relatively low temperature In plasmas present in the In FEEP thruster. Comparisons of the theoretical spectra generated from our model with those obtained experimentally at ONERA/DMPH from the In plasma will be used both for optical diagnostics and for validation of the atomic data and of the theoretical approaches used throughout. All the atomic data used will be available in due time from the GAPHYOR Atomic Data Center [4].

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Mo6-4

ANGLE-RESOLVED ABSOLUTE OUT-OF-BAND RADIATION STUDIES OF TIN-BASED LASER-PRODUCED PLASMA SOURCES.

O Morris*, P Dunne, F O'Reilly, G O'Sullivan, and P Hayden

School of Physics, University College Dublin, Belfield, Dublin 4, Ireland.

*Electronic address: Oran.Morris@ucd.ie

Out-of-band (OOB) radiation has been measured from a laser plasma EUV source formed on a solid tin planar target for a range of angles between 20 and 90 degrees to the target normal. The measurements were made over six spectral bands centered between 200 and 1000 nm. The plasma was formed in a custom made chamber which facilitated target rotation with respect to a diode/filter combination, which acted as an OOB detector. The laser power density was set so as to yield the optimum in-band radiation at 13.5 nm. The plasma OOB emission was found to be dominated by the radiation in the band centred on 214 nm, and a significant contribution from scattered Nd:YAG laser light was observed. The data was analyzed using an $I(\theta) \propto \cos^{\alpha}(\theta)$ approximation with a value for α of 0.229 ± 0.022 and a correlation coefficient of 0.99 with the experimental data recorded.

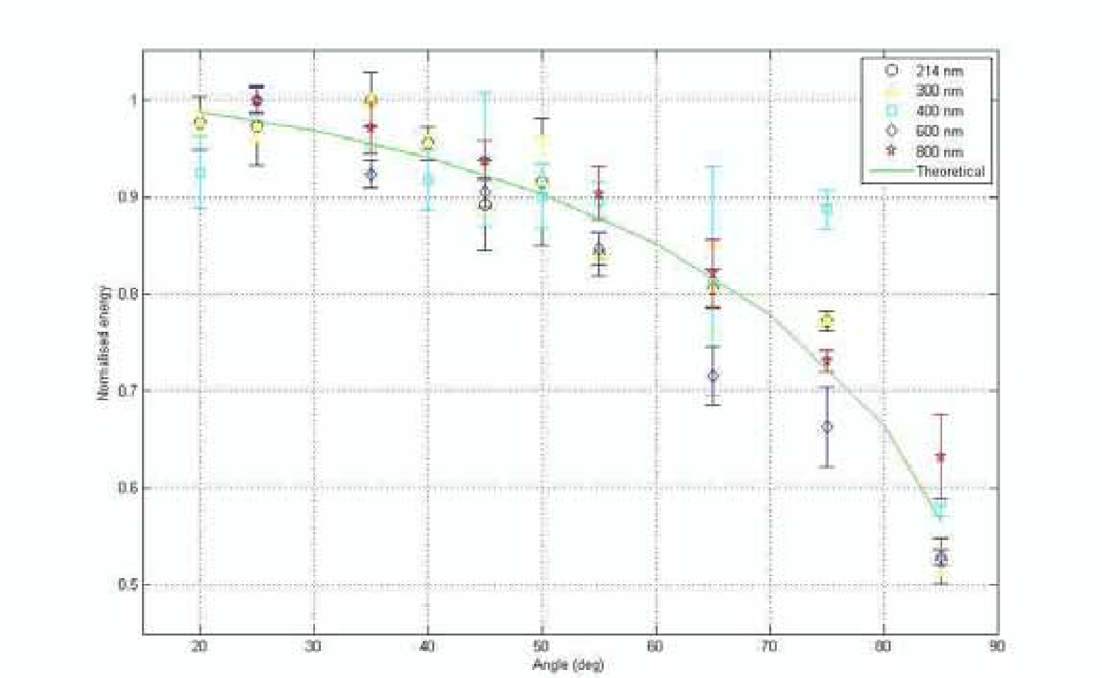

Fig 1: Angular distribution of normalised energies for the bands centred at 214, 300, 400, 600 and 800 nm, including the $I(\theta) \propto \cos^{\alpha}(\theta)$ approximation.

Mo6-5

PLASMA CHARACTERISTICS COMPARISSON OF N_2 AND (N_2+HE) HOLLOW CATHODE GLOW DISCHARGES

V.Gencheva and R. Djulgerova

Institute of Solid State Physics, 1784 Sofia, Bulgaria
veselina@issp.bas.bg

Hollow cathode glow discharges with working gases N_2 and a mixture (N_2+He) are compared. The often used in the technologies nitrogen plasma has disadvantages as instability in time and low range of discharge current. The aim of our study is to improve the characteristics of the nitrogen plasma without changing the typical plasma conditions for N_2 gas
To compare N_2 and mixture (N_2+He) plasmas the current-voltage characteristics and the main plasma parameters as electron temperature and electron concentration are measured. Another feature of the plasma is the measured change in plasma conductivity when the plasma is illuminated with laser light, resonance to the certain optical transition, i.e. so called optogalvanic effect. The advantage of the optogalvanic spectrum in comparison with absorption spectrum is much better signal/noise ration [1].

The experimental set-up contains a glow discharge lamp with an Al hollow cathode. The working pressure is 2.5 Torr, the range of the discharge current is from 3mA to 20 mA. The optogalvanic signals (OGS) are registered from nitrogen molecule transition ($B^3\Pi_g$-$C^3\Pi_u$) by using a pulse nitrogen laser, generating at wavelength of 337,1 nm. For measuring of the electron temperatures and concentrations the Langmuir's probe is applied.

The obtained current-voltage characteristics and electron temperatures and concentrations present increase of ionization efficiency and discharge stability when He is added to the working gas N_2. It can be explained by the 6 times bigger thermal conductivity of He. The optimal mixture for our discharge conditions is (He+5%N_2).

The registered dynamic OGS show the following advantages when working gas (He+5%N_2) instead of pure N_2 is used:
-the OGS amplitude in the mixture becomes one order of magnitude higher than in nitrogen,
-the working discharge current range increases from (8-15) mA to (3-18) mA.

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Mo6-6

IMPOSSIBILITY OF IONIZATION EQUILIBRIUM IN SWIFT HEAVY ION TRACKS

A.E. Volkov*, N.A. Medvedev

Russian Research Centre 'Kurchatov Institute', Kurchatov Sq.1, Moscow, 123182, Russia, (*)
volkov@dni.polyn.kiae.su

The energy deposited during 10^{-17} s by a swift heavy ion (SHI) into the electronic subsystem of an irradiated solid can achieve extremely high values up to 50-70 keV/nm. The temporal difference between the temperatures of exited electrons and atoms is usually assumed in order to describe subsequent energy transfer to the lattice resulting in structure and phase transformations in the nanometric vicinity of the projectile trajectory (“two temperatures” model, [1]).

The conception of the single temperature of the excited electronic subsystem and the forms of equations used in this model are based on the assumption of the local equilibrium including the ionization equilibrium in SHI tracks.

We demonstrate that the ionization equilibrium can not appear during subpicosecond cooling down of delocalized electrons in SHI tracks even when no gradients and radiation generated by electronic transitions are taken into account. A lack of the ionization equilibrium results in a temporal dependences of the density of delocalized electrons, their heat capacity and thermodiffusion coefficient crucially affecting the model equations. Moreover, the single temperature can not describe the state of the electronic subsystem as well as energy transfer to the lattice in this case. This conclusion is positioned on the framework of the general approach describing nonequilibrium plasma [2-3].

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Mo6-7

REACTIVE INTERACTIONS OF SMALL HYDROCARBONS WITH FUSION RELEVANT MATERIALS

N. Endstrasser[1], B. Rasul[1], W. Schustereder[2], F. Zappa[1], P. Scheier[1], T.D. Märk[1]

[1]Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstr. 25, A-6020 Innsbruck, Austria
[2]Max-Planck Institut für Plasmaphysik, EURATOM Association, Boltzmannstr. 2, D-85748 Garching, Germany

In order to understand the role of the collision processes in the plasma edge region of fusion reactors and their use for controlling the plasma conditions, it is essential to have a detailed and quantitative knowledge on the elementary processes in gas-phase, such as reaction rate coefficients (S, γ,. . .), and on the interaction of the gas phase particles with the plasma facing walls. These data are necessary as input parameters for edge plasma modelling and various diagnostic techniques.

Molecular fragmentation and reactive collisions of fusion fuel present in the scrape-off layer as hydrogen isotopes of different molecular composition X_n^+ (X= D, T, n=1-3) lead due to plasma-wall interactions to the production of ion and neutral species that were previously not present in the plasma performing effective chemical and physical sputtering due to their high mass numbers. The erosion of graphite used in future ITER design for covering the strike-point regions of the divertor leads to subsequent formation of small hydrocarbons performing further ion-surface collisions with the plasma-facing
materials like tungsten.

Vacuum plasma spraying of tungsten on graphite tiles would be a feasible and cost effective method to provide the large tungsten areas of more than 100 m^2 shielding parts of the divertor region in ITER. Systematical investigation of ion-surface collisions of hydrocarbons with fusion-relevant materials has been started with the investigation of ion-surface collisions of CD_3^+ on plasma-sprayed tungsten samples provided by IPP Garching in the hyperthermal energy range of 0 - 100 eV.

In order to allow a quantitative investigation of surface induced dissociation (SID) and surface induced reaction (SIR) processes it is important to control and determine accurately the collision energy and to achieve collision energy spreads as small as possible. The presently used apparatus is the tandem mass spectrometer set-up BESTOF (consisting of a B-sector field combined with an E-sector field, a Surface and a Time-Of-Flight mass spectrometer). This set-up allows the investigation of ion-surface reactions with high primary mass resolution and an energy resolution smaller than 1 eV.

Different mechanisms leading to the production of secondary ions under CD_3^+ impact were identified by the analysis of secondary ion mass spectra. Further investigations of fusion-relevant surfaces with small hydrocarbon species are ongoing.

Mo6-8

Time Resolved Study of Low Temperature Colliding Line Plasmas

J. Pedregosa-Gutierrez, K. D. Kavanagh and J. T. Costello.

NCPST and School of Physical Science, Dublin City University, Dublin , Ireland
E-mail: jofre.pedregosa@dcu.ie

We will present measurements on the evolution of a stagnated layer which can grow at the collision front between two counter-propagating line plasmas. Each of the 'seed' plasmas was formed by splitting a laser beam and focussing the two resultant beams onto a flat calcium target using a cylindrical lens. The study of colliding plasmas is a topic of interest to number of communities such as those working on fusion energy generation and x-ray lasers. Hence, most work to date on them to date has involved high temperature (0.1 - 3KeV) plasmas. However, 'technological' laser produced plasmas, such as those used in pulsed laser deposition of materials [1], are usually of a much lower temperature (<5eV). So the motivation for our current study is to explore the dynamics of such 'cool' laser plasmas in a counter-propagating colliding plasma geometry, with a view to developing the layer formed at the collision interface as a potentially novel materials deposition source [2] or even as a beam-like source of atoms, ions, molecules, clusters etc..

The weakly ionized plasmas were studied using both time-space resolved spectroscopy [3,4] as well as with VUV absorption imaging [5] to study ground state species. In addition, Thompson scattering [6] measurements were also performed. The line plasmas were formed by focussing 15ns pulses of 250-270mJ at 1064nm on a flat Ca target to produce focal footprints of 8mm x 0.1mm, while the Thompson Scattering signal was generated by crossing the stagnation layer with a 9ns laser pulse at 355nm with 80mJ of energy per pulse. These techniques helped to track the evolution of neutral and singly charged calcium species in the plumes and at the stagnation layer of the collision interface. They also provided information on the time-space evolution the electron density and temperature of the layer which indicate quite a homogeneous system likely to aid controllable PLD.

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Mo6-9

ELECTRICAL AND OPTICAL CHARACTERIZATION OF PULSED PLASMA OF $N_2 - H_2$ MIXTURE

H. Martínez[1] and F. B. Yousif[2]
[1]*Centro de Ciencias Físicas, UNAM, Apdo. Postal 48-3, 62210, Cuernavaca Morelos, México*
[2]*Facultad de Ciencias, UAEM, Cuernavaca,Morelos, México.*
fbyousif@servm.fc.uaem.mx

This abstract considers the electrical and optical characterization of glow discharge pulsed plasma in N_2 / H_2 mixtures at pressures of 0.5-4.0 Torr and discharge current between 0.2 and 0.6 A. The total discharge current and the applied voltage are measured using conventional techniques. The emission from the pulsed plasma of a steady-state electric discharge in a N_2 / H_2 mixtures within the wavelength range 200-600 nm is investigated. It is shown that, at total pressures of 0.5 to 4.0 Torr, the discharge mainly emits within the range 280-500 nm. The emission consists of $N_2(C-X)$ 316, 336, 358 nm narrow peaks and a broad band with a maximum at $\lambda_{\max} = 427 nm$. Also lines of N_2, N_2^+ and NH excited states were observed. All lines have their maximum intensity at the discharge current of 0.417 A. The intensities of the main band and spectral lines are determined as functions of the total pressure and discharge current.

Mo6-10

APPLICATION OF COLLISIONAL-RADIATIVE MODELS TO SPECTROSCOPIC DIAGNOSTICS OF WEGA

K. Katsonis[1], D. Zhang[2], R. König[2], WEGA Team[2], Ch. Berenguer[1], R.E.H. Clark[3], M. Cornille[4]

[1]*Laboratoire de Physique des Gaz et des Plasmas, UMR 8578, Université Paris-sud 91405 Orsay Cedex, FRANCE*

[2] *Max-Planck-Institut fuer Plasmaphysik, EURATOM Ass., Wendelsteinstr. 1, 17491 Greifswald, GERMANY*

[3] *Nuclear Data Section, IAEA, Vienna, AUSTRIA*

[4] *LUTH, UMR 8602, Observatoire de Paris, Meudon, FRANCE*

The local electron temperature T_e and density n_e of a plasma can, in principle, be obtained by non-intrusive emission spectroscopy diagnostics, from which information on the other constituents and the most important processes encountered in the plasma can be derived. A full Collisional-Radiative (C-R) model is required that takes into account all the species, both neutral and ionized, together with their excited states (including atomic structure and transition probabilities) as well as rate coefficients. We have developed such a model for Ar plasmas, valid for T_e from a fraction of an eV up to 40 eV [1]. The higher limit corresponds to a temperature sufficient to remove all six outer 3p electrons of the Ar atom. This model, has been previously used to diagnose and model Ar plasmas in various devices, and is used here for emission spectroscopy diagnostics at argon plasmas in the WEGA stellarator. Results of this application have been presented previously [2].

WEGA is a medium sized classical stellarator operated at IPP Greifswald for basic plasma research, educational training and for testing of diagnostics foreseen for W7-X being under construction [3]. The plasmas are generated by a microwave heating system operating at a frequency of 2.45 GHz and a maximum power of 26 kW. Emission spectroscopy diagnostics has been extended to discharges of Xe and Ar+Xe mixtures. These measurements permit comparisons of the T_e, n_e values derived from the Ar C-R model with those given by the Xe model, and thus test the Ar and Xe atomic data used in the C-R models and verify both models. Application of rare gas C–R models to spectroscopic diagnostics of WEGA takes advantage of a general study on the characterization and optimization of the plasmas [4] and bolometric results [5]. Probe measurements show an electron temperature T_e of about 10 eV and a density n_e of about 10^{12} cm^{-3} for Ar discharges. Preliminary calculations based on a simple coronal model predict that Ar I to Ar V spectra and partial radiation from Ar^{5+} should be present. Although rather faint, the Ar IV spectrum has been shown to be clearly present. All ions can not be simultaneously present in homogeneous plasma with a single T_e. However, probe measurements give hint to a small fraction of high temperature electrons with an energy of a few hundred eV that may explain the simultaneous detection of signatures for all of the ionized Ar species as well as the neutral, possibly altering the total radiated energy. Accordingly, more than one Maxwellian distribution may prevail for some or all of the present species. Typical Ar I-IV spectral lines have been now identified in various WEGA discharges. The main features of the relevant spectra will be shown and discussed. A detailed comparison with the theoretical spectra derived from the Ar C-R model is also underway.

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Mo6-11

QED EFFECTS IN INTERACTION OF ENERGETIC ELECTRONS AND PHOTONS WITH STRONG PLASMA FIELDS

I. Kostyukov and E. Nerush

Institute of Applied Physics RAS, Uljanova 46, 603950 Nizhny Novgorod, Russia

Crystalline fields along with laser fields are now the most important tools in laboratory strong-field physics [1]. Another example of a strong field, that is achievable under laboratory conditions, is a strong plasma field. Such plasma fields can be generated by short intense laser pulse or by short and dense electron bunch propagating in a plasma. The plasma electrons can be completely expelled from interaction region leaving behind a plasma cavity [2]. The huge space charge formed due to the electron evacuation generates strong electromagnetic field. The strong plasma field is now considered as a key element of plasma-based accelerators [3], laser-plasma x-ray radiation sources [4], etc.

Radiation spectrum of extreme relativistic electrons and a probability of electron-positron pair production by energetic photons in a strong plasma field generated by ultrahigh intensity laser pulse are derived in the framework of a semiclassical approach. It is shown that that the radiation losses of the relativistic electron scale as $\varepsilon^{2/3}$ in the quantum limit when the energy of the radiated photon becomes close to the electron energy, ε. In the classical limit (the photon energy is much less than electron energy) the radiation losses scale as ε^{2} [5]. The quantum effects will play a key role in future plasma-based accelerators operating at ultrahigh energy of the electrons.

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Mo6-12

KINETIC ENERGY DISTRIBUTIONS OF IONS PRODUCED BY LASER ABLATION OF METALS

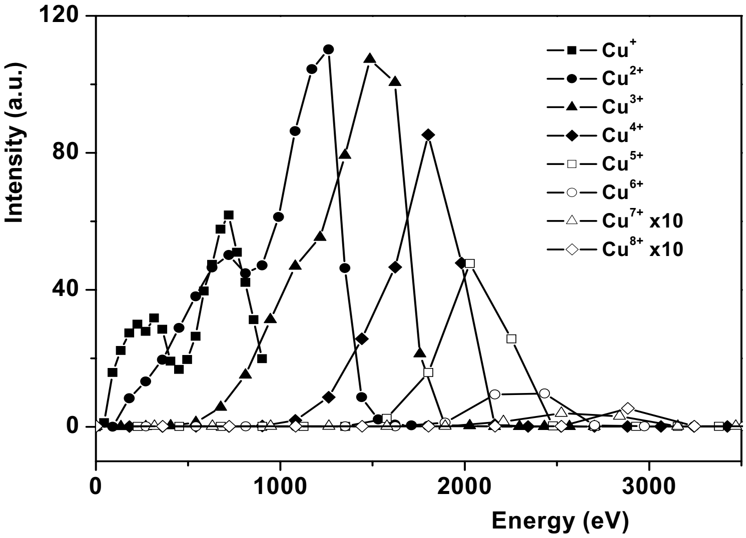
Borja Sierra[1], Jon I. Apiñániz[1], Roberto Martínez[2], Fernando Castaño[1]

[1]Facultad de Ciencia y Tecnología, Departamento de Química Física. Universidad del País Vasco, Apdo. 644. 48080 Bilbao. Spain
[2]Facultad de Farmacia, Departamento de Química Física, Universidad del País Vasco, Paseo de la Universidad, 7. 01006 Vitoria. Spain.

Phenomena associated with laser interaction on materials give rise to powerful techniques in applied physics and chemistry [1]. Moreover, not only the target material itself but the extracted one has properties and characteristic energies making it useful for applied purposes. A good understanding of these phenomena is of great interest for the success and optimization of any laser-based application.

Pulsed laser deposition (PLD), nanoparticles and clusters production, material sampling, etc. are a small part of techniques have been worked out with laser ablation [2]. In spite that the mentioned applications are of technological interest, few information about mechanisms of ion formation and acceleration has been published.

In this work, ions produced by laser ablation of metallic targets are focussed towards an electrostatic ion energy analyzer (EEA, Comstock AC-901) where they are energetically selected. A tube-of-flight allocated after the EEA allows a definitive separation of ions according to their mass/charge relation.



Kinetic energy distributions of ions produced by laser ablation of a Cu target

Ion kinetic energy distributions are fitted to Maxwell-Coulomb distributions [3] and parameters such as the expansion velocity, the Coulomb velocity or the ion temperature KT can be determined. Fluences higher than 1 J/cm^2 show a contribution to the kinetic energy distribution in the M^{Z+} ion due to electron impact ionization of $M^{(Z-1)+}$ ions. Such mechanisms will be exposed and discussed.

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Mo6-13

LASER PULSE INTERACTION WITH INHOMOGENEOUS CYLINDRICAL PLASMA

N. Mirnes and A. H. Belbachir
Laboratory of Analysis and Application of Radiation (LAAR)
Physics Department, University of Sciences and Technology of Oran
M. B. (USTO)
P. O. Box: 1505, El-M'Nouar, Oran, Algeria
e-mail: nawel002002@yahoo.fr

Abstract:

On the basis of the collisional Boltzmann equation for an unmagnetized plasma, the interaction of a laser pulse with a cylindrical plasma has been studied using the P_1 approximation of Spherical Harmonics Expansion.

Our model leads to two coupled and nonlinear differential equations for the electrons temperature θ_e and electrons density n_e. Two approximations are introduced to solve these equations which are the adiabatic plasma heating and the isobar heating.

The obtained results show that the electronic temperature profile in inhomogeneous plasma has a weak variation in the laser axis directions (z axis), and the temporal variation of the temperature electrons has similar pattern to the laser temporal profil.

We are now working to find the numerical solution for the coupled equations in the general case.

Keywords : Laser pulse interaction, Boltzmann equation, plasma temperature, plasma density, coupled and nonlinear differential equations

Mo6-14

CORRECTION OF MEASURED EMISSION SPECTRA OF LASER INDUCED PLASMA

K. Yu. Catsalap[1], E. A. Ershov-Pavlov[1], Yu. A. Stankevich[2], K. L. Stepanov[2]

[1]Institute of Molecular and Atomic Physics, National Academy of Sciences, 70
Nezavisimosti, Minsk, Belarus, e-mail: catsalap@imaph.bas-net.by

[2]Institute of Heat and Mass Transfer, National Academy of Sciences 15 Brovka str.,
Minsk, Belarus

Laser induced plasma (LIP) is nowadays considered to be one of the most promising light sources in applications related to elemental analysis by the atomic emission spectroscopy. The possibility of remote probing and in-situ analysis are most important advantages of LIBS methods. However, erosion plasma plumes have rather complicated structure and time behavior. As a sequence, recorded spectra differ significantly from local ones directly related to the measured elemental content. In the scope of the express-analysis and remote probing the detailed spatial and temporal diagnostics of LIP is not reasonable due to high cost and technical problems. One of possible solutions is preliminary numerical modeling of LIP emission spectra. The modeling data can help to learn the spectra forming and to work out a method accounting for the LIP inhomogeneity and instability.

In the paper, results of the numerical modeling of emission line spectra of laser-induced plasma are reported. It is supposed that the laser beam falls normally to the sample (pure aluminum) surface. Erosion plume parameters are calculated by a numerical solution of the thermal and gas dynamics problems. Spectral intensity is calculated by a numerical solution of the plasma radiation transfer equation. The modeling has resulted in the spatial and temporal distributions of atomic and ionic aluminum line emission. The analysis of line intensity distribution is performed. The relations between the recorded spectra parameters and the local ones are proposed. Its accounts for inhomogeneity, instability of laser induced plasma. Also self-absorption rate of a spectral line can be estimated. The use of relations significantly increases an accuracy of spectral line parameters measurement.

Mo6-15

3D SIMULATIONS OF LASER ELECTRON ACCELERATION

Michael Geissler[1),2)], Sergey Rykovanov[2)], Jörg Schreiber[2)]
and Jürgen Meyer-ter-Vehn[2)]

[1)]Department of Physics and Astronomy, Queen's University Belfast
Belfast BT7 1NN, UK
[2)]Max-Planck Institute for Quantum Optics, Hans-Kopfermann Str.. 1 D-85748,
Garching, Germany

In recent years some milestones where achieved for laser based electron acceleration. Following theoretical predictions, experiments where performed indicating that the so called bubble acceleration regime is one of the most promising way for a tunable, stable and reproducible laser driven electron source with a quasi-monoenergetic energy distribution. This is in strong contrast to temperature like spectra from classical wakefield acceleration schemes and represents the most important feature of bubble acceleration. Further the electrons, which are accelerated directly out of the background plasma, are highly localized within a few µm comprising a bunch with unique properties in terms of duration and number of electrons (10^9/bunch). Simulations indicate that the most efficient energy transfer to mono-energetic electrons appears for sub10-fs pulses. Although a 5fs 100mJ laser system is under construction at MPQ, the shortest current available high intensity pulses are about 30fs long.

We present here studies obtained with the 3D-PIC code ILLUMINATION for several aspects of bubble acceleration:

First of all the differences in the plasma interaction of few cycle pulses compared to longer pulses are studied revealing that the these pulses undergo strong nonlinear modification finally a small fraction of the initial pulse end up as a single sub-10fs pulse.

So far only constant plasma density profiles are considered in simulations. Here we will show how the rising and falling edge of the density, which is unavoidable in real experimental setups, will influence the electron bunch properties. Although long gradients will change substantially the bunch properties, we will show how to use the gradient to tune the bunch properties in a controlled way.

One major problem for efficient bubble acceleration is to achieve long interaction distances at high laser intensity. Resent experiments using guiding inside a preformed plasma channel overcome this limitations and led to the highest ever reported laser produced bunches energies. We will present here some aspects of channel guiding and compared them to constant plasma densities.

Mo6-16

Investigation of x-ray and high energy ions produced by laser-generated plasma in H2- and He-droplets

Nikos Petridis, Rui A. Costa Fraga, Robert E. Grisenti and Reinhard Dörner

Institut fuer Kernphysik
Johann Wolfgang Goethe Universitaet
Max-Von-Laue-Str. 1
60438 Frankurt am Main
Germany

petridis@atom.uni-frankfurt.de

We present novel cryogenic H2- and He- microjets which can be used as liquid droplet targets. They offer the possibility of a debris-free, one-component, self-replenishing and high-density light element target for laser-induced plasma-generation, used as a table top, continuous source of high energy α-particles, protons and x-rays with widespread applications. This experiment will also provide new insight into the non-linear electron dynamics responsible for ion acceleration in laser-driven plasmas.

Mo6-17

MEASUREMENTS OF ELECTRON TEMPERATURE AND DENSITY, IN AN AC PULSED OXYGEN PLASMA DISCHARGE

H Martínez[1], F. B. Yousif[2] and F Castillo[3]
[1]Centro de Ciencias Físicas, Universidad Nacional Autónoma de México,
Apartado Postal 48-3, 62210, Cuernavaca, Morelos, México.
fbyousif@servm.fc.uaem.mx
[2]Facultad de Ciencias, Universidad Autónoma del Estado de Morelos (UAEM).
[3]Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México,
México.

Emission and analytical spectroscopy was applied to investigate O_2 plasma, which was generated by an AC discharge between 0.15 and 0.5 Torr pressure. For the diagnostic study, a double Langmuir probe was employed. The derivation of plasma parameters is based on a theoretical description of the double-probe current-voltage characterization in the Thick Sheath Limit (TSL) region [1]. In the TSL the plasma sheath, which is characterized by the Debye length $\lambda_D = (\varepsilon_0 kT_e/e^2 n_e)^{1/2}$ is small relative to the probe dimensions (ε_0 is the permittivity of free space, T_e electron temperature, n_e electron density, k Boltzmann's constant and e the electron charge). In this case, the probe current (I) as a function of voltage (V) is given [1] by

$$I = I_{\infty} \tanh({}^{eV}\!\big/_{2kT_e}) \qquad (1)$$

with the saturation current (I_{∞}) being dependent on ion density (n_i), ion mass (m_i), electron temperature (T_e) and probe area (A): $I_{\infty} = Aen_i(kT_e/2\pi m_i)$ (2)

Theoretical curve was fitted to the measured current-voltage characteristic curve using equation (1) and by adjusting the ion density (n_i) and the electron temperature (T_e). Electron temperature of T_e = 1.09 eV and an ion density of n_i= 2.08 x 10^{10} cm^{-3} were evaluated. As both probes have equal area, the electron temperature (T_e) can also be calculated from the slope of the log-plot of the *I-V* curve at the origin, using the equation

$$In(\frac{I_{p1}+I_{p2}}{I_{e2}}-1)=\frac{eV}{kTe} \qquad (3)$$

where I_{p1} and I_{p2} are the ionic saturation currents of the two probes, and I_{e2} is the electronic current at the second probe [2,3]. From equation (3), the slope of the logarithmic plot will give an electron temperature that is expected to be insensitive to small variations of ionic saturation current. The electron density (n_e) was also evaluated from the following equation [4,5]

$$I_{0e} = -en_e r_p \sqrt{\frac{2\pi kT_e}{m_e}} \qquad (4)$$

where I_{0e} is the thermal electron current; r_p is the probe radius; and m_e is the electron mass. That method gave an ion density of n_e= 1.93 x 10^{10} cm^{-3} .

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Mo6-18

APPLICATION OF A LASER-INDUCED-PLASMA TO THE STUDY OF STARK WIDTHS OF Pb III SPECTRAL LINES

A.Alonso-Medina[1] and C. Colón[1]
[1]Dpto. Física Aplicada, EUIT.Industrial, Universidad Politécnica de Madrid (UPM), Madrid, Spain
e-mail. aurelia.alonso@upm.es cristobal.colon@upm

The application of laser ablation for chemical element analysis of solid sample is one of the most important applications of Laser Induced Plasma (LIP) in science and technology. Stark broadening data for a large number of transitions in many atomic and ionic spectra are needed not only for atomic structure research, but also for applications to astrophysics and analytical techniques. LIP is one of the habitual methods for the experimental determination of different atomic and molecular parameters and in particular of the Stark broadening parameters.

From the experimental point of view, LIP has proved to be a valuable source of spectroscopic data on neutral and ionized species (e. g. Radziemski and Cremers). These authors have been working in this technique from several years ago.

In this work, Stark widths of 10 spectral lines corresponding to the 7s-7p, 6d-7p and $6ps^2$-7p transitions of Pb III have been measured. These values are the first experimental data in the literature.

The studied plasma has a temperature of about 25 200 K and an electron density of about 10^{17} cm^{-3}. Local Thermodynamic Equilibrium conditions and plasma homogeneity has been checked. Special attention was paid to the possible self-absorption of the different transitions.

Plasma was generated by focusing a laser beam at a sample lead surface. A chamber, filled with argon and maintained at a constant pressure of 12 Torr was used.

Samples were located inside the chamber, on top of a device capable of moving it horizontally with respect to the laser beam. The laser beam used to generate the plasma was produced by a Q-switched Nd:YAG laser (Quantel YG585),that generates 290mJ pulses of 7 ns duration at a frequency of 20 Hz and 10640 Å wavelength. Its beam was focused on the sample by a lens of focal distance of 12 cm. The spatial width of the focused laser beam was measured by recording its image with a 1024-element linear silicon diode array. The light emitted by the LIP was transmitted, through a sapphire window, to the input slit of a 1 m Czerny Turner spectrometer.

Each observed spectrum was adjusted, taking in mind the instrumental profile, using Voigth profiles. The profile area of each line studied were recorded in order to obtain their total intensity and the contribution of Lorentz profile to their HWHM was obtained.

The population levels distribution and the corresponding temperatures for each considered atomic species were obtained using Boltzmann plots.

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Mo6-19

ATOMIC DATA FOR FUSION REACTOR IMPURITIES

K. Katsonis[1], R.E.H. Clark[2], M. Cornille[3], Ch. Berenguer[1], D. Humbert [2], A. Ndiaye[1], G. Maynard [1]

[1] Lab. de Physique des Gaz et des Plasmas, UMR 8578, Université Paris-sud 91405 Orsay, FRANCE

[2] Nuclear Data Section, IAEA, Vienna, AUSTRIA

[3] LUTH, UMR 8602, Observatoire de Paris, Meudon, France

We report on atomic data for radiative and collision processes involving medium to heavy fusion reactor impurities. This work is in progress at the GAPHYOR Atomic Data Center of the LPGP Laboratory, in collaboration with the Atomic and Molecular Data Unit of the IAEA Nuclear Data Section in Vienna and the LUTH Laboratory of the Observatory of Paris in Meudon [1]. Atomic data characterize the behavior of the impurities encountered in the edge and the core regions of fusion reactors, and cover both radiative (energy levels and transition probabilities $A_{i,j}$) and collisional processes (involving electron and heavy particle collisions). The important electron collision processes are excitation, ionization and recombination (radiative, dielectronic, three-body), while the main heavy particle collisions processes are excitation and charge exchange.

We have recently evaluated the structure and $A_{i,j}$ values of a number of multiplets for Ar and Xe ions, including low radiative and metastable levels of the multiplets 3*p* - 4*s*,5*s*; 3*p* - 3*d*,4*d*,5*d*; 4*p* - 4*s*,5*s*; 4*p* - 3*d*,4*d*,5*d* for the Ar ions and the corresponding 5*p* - 6*s*,7*s*; 5*p* - 5*d*,6*d*,7*d*; and 6*p* - 6*s*,7*s*; 6*p* - 5*d*,6*d*,7*d* multiplets for the Xe ions. These multiplets contain the most prominent lines in the Ar and Xe ion spectra. Excitation cross sections (σ_e) for the aforementioned multiplets were evaluated at the same time, together with σ_e for multiplets which contain only forbidden optical transitions (notably 3*p* – 4*p*, 3*d* - 4*d* for Ar and 5*p* – 6*p*, 5*d* – 6*d* for Xe). Evaluations of the cross sections for other processes are also underway [2]. This work is part of an ongoing IAEA Coordinated Research Project on "*Atomic data for heavy elements impurities in fusion reactors*" [3].

The evaluated data will be used in the modeling of plasmas in fusion and in optical diagnostics, which are two basic tools for theoretical studies of plasmas. Non-intrusive emission spectroscopy permits the evaluation of the local temperature and density of the plasma if a full Collisional–Radiative (C-R) model is available. Information is also generated on the constituents and on most important processes encountered in the plasma. As an example we mention the optical diagnostics of the WEGA Stellarator [4]. The evaluated data have been stored in XML form and passed on to the CHLOEO-06 code that supports C-R models of rare gases through Python scripts. Data validation experiments in the UV region are under way [5].

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POSTERS

Tuesday 8/5

1. Electron, atom, molecule and ion collisions

Tu1-1

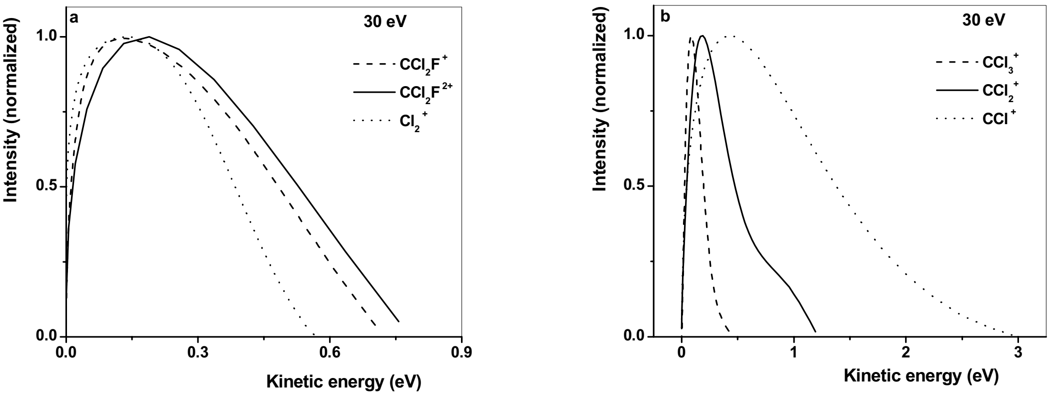
ELECTRON-IMPACT DISSOCIATIVE IONIZATION OF $CClF_3$ AND CCl_3F

Borja Sierra[1], Roberto Martínez[2], Fernando Castaño[1]

[1]Facultad de Ciencia y Tecnología, Departamento de Química Física. Universidad del País Vasco, Apdo. 644. 48080 Bilbao. Spain
[2]Facultad de Farmacia, Departamento de Química Física, Universidad del País Vasco, Paseo de la Universidad, 7. 01006 Vitoria. Spain.

The knowledge of electron-impact dissociative ionization processes is crucial for the simulation of industrial and low temperature plasmas and their properties. High concentrations of some of the reactive ions and/or neutrals are essential for plasma processing and other applications, such as etching in the semiconductor manufacture [1]. The ions created in the electron-molecule collisions are released with characteristic kinetic energy distributions (KEDs), the knowledge of which is of substantial assistance in the understanding of the dissociative ionization mechanisms and their control influences further the rate of the processes [2,3].

This work reports the experimental determination of KEDs and appearance energies (AEs) of the ions produced by electron impact on chlorofluoromethanes $CClF_3$ (freon 13) and CCl_3F (freon 11). Both molecules have the same symmetry in the ground and excited states, yield halogen atoms (both neutrals and ions), (inter)halogen molecules, as well as other C-halogen species, but CCl_3F has more electrons, a larger volume and hence sizeable excitation and ionization cross sections (ICS). The processes involved also correlate with the initial electronic state of the precursor. In consequence, a study of the influence of the fragment size and the electronic structure on the KED and AE of the ions produced in the dissociative ionization is of fundamental interest.



Relative KED of CCl_2F^+, CCl_2F^{2+}, Cl_2^+, CCl_3^+, CCl_2^+ and CCl^+ following 30 eV electron impact on the CCl_3F molecule

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Tu1-2

ELECTRON IMPACT EXCITATION OF THE INITIALLY EXCITED ATOMS: A FULLY RELATIVISTIC APPROACH

Rajesh Srivastava*, Lalita Sharma* and A. D. Stauffer#

*Department of Physics, Indian Institute of Technology, Roorkee, 247667, India
#Department of Physics and Astronomy, York University, Toronto, Canada M3J 1P3

There has been little work, either experimental or theoretical, on electron impact transitions between excited states of atoms. Sufficiently large populations of excited states can be produced by laser irradiation to allow for the measurement of inelastic and superelastic scattering processes. Pioneering measurements on such transitions were carried out by Johnson et al [1] for barium and by Boffard et al [2] for inert gases.

We have previously applied fully relativistic distorted-wave (RDW) method to calculate electron impact excitation from the ground state of various atoms and obtained results, which gave good agreement with experiment and other theoretical work. In the present work, we apply the RDW method to study the electron excitations from the excited states of alkaline earth atoms and inert gases.

We have carried out relativistic distorted-wave calculations for inelastic electron scattering from the 6s5d $^{1,3}D_2$ and 6s6p $^1P_1$ excited states of barium in the energy range from 20 to 40 eV. Results are presented for the differential cross sections and electron impact coherence parameters and compared with experimental measurements and other theoretical calculations for these quantities [3].

We further extended our RDW method to study the excitation from the initially excited metastable states of calcium and inert gases for which some experimental and scarce other theoretical results are available [2,4]. We have carried out calculations for electron scattering from the 4s4p $^3P_{0,2}$ excited states of calcium to its various excited fine structure states. For inert gases viz. neon, argon, krypton and xenon, the excitation of the J = 0, 2 levels of the np^5(n+1)s configuration to the ten higher-lying fine-structure levels of the np^5(n+1)p configuration have been considered. We present and compare our results with experimental measurements of the integrated cross section at energies up to 100 eV and with other theoretical calculations for these cross sections [5].

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*rajsrfph@iitr.ernet.in

Tu1-3

EFFECT OF FINITE DETECTION EFFICIENCY ON THE OBSERVATION OF DIPOLE-DIPOLE INTERACTION OF A FEW RYDBERG ATOMS

I.I.Ryabtsev, D.B.Tretyakov, I.I.Beterov, and V.M.Entin

Institute of Semiconductor Physics
Pr. Lavrentyeva 13, 630090 Novosibirsk, Russia, e-mail: ryabtsev@isp.nsc.ru

We have developed a simple theoretical model describing multi-atom signals that could be measured in the experiments on resonant collisions of a few Rydberg atoms [1]. Such collisions occur due to strong dipole-dipole interaction and lie at the heart of the dipole-blockade effect and other related schemes of quantum information processing with neutral atoms. We have shown that finite efficiency of the selective field-ionization detector leads to the mixing up of the spectra of resonant collisions registered for various numbers of Rydberg atoms. This may impede possible observations of dipole blockade or coherent two-atom interactions required to perform quantum gates. The formulae are presented, which help to estimate an appropriate mean Rydberg atom number for a given detection efficiency. On the other hand, we have found that a measurement of the relationship of the amplitudes of collisional resonances observed in the one- and two-atom signals provides a straightforward determination of the absolute detection efficiency and mean Rydberg atom number. This novel method is advantageous as it is independent of the specific experimental conditions.

We have also performed a testing experiment on the resonant collisions Na(37S)+Na(37S)→Na(36P)+Na(37P) in a small excitation volume of a sodium atomic beam [1]. The energy resonance was tuned by the electric field [Fig.1(a)]. In Fig.1(b) the fine-structure resonances observed in the one-atom signal are presented. The resonances obtained for 1 to 4 of detected Rydberg atoms have been analyzed and compared with the theoretical predictions. An agreement between experiment and theory in the width and amplitudes of the resonances has confirmed the validity of the simple approximations used in the theoretical model.

This work was supported by the Russian Foundation for Basic Research, Grant No.05-02-16181, by the Russian Academy of Sciences, and by INTAS, Grant No.04-83-3692.

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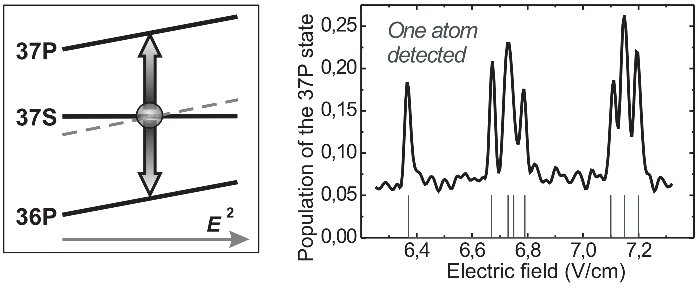

Fig.1. (a) Sodium energy levels for the resonant collisions Na(37S)+Na(37S)→Na(36P)+Na(37P) tuned by the electric field *E*. (b) An example of the experimental spectrum of collisional resonances in the velocity-selected atomic beam for the case of one sodium Rydberg atom detected. Vertical lines indicate the calculated positions of resonances for various fine-structure components of P-states.

A high resolution study of the $N_2^-(^2\Sigma_g^+)$ resonance in electron scattering

T. H. Hoffmann[1,2], M. Allan[2], G. Sauter[3], W. Meyer[3], K. Franz[1], M.-W. Ruf [1], H. Hotop[1]

[1] *Fachbereich Physik, Techn. Universität Kaiserslautern, 67653 Kaiserslautern, Germany*
[2] *Department of Chemistry,University of Fribourg, 1700 Fribourg, Switzerland*
[3] *Fachbereich Chemie, Techn. Universität Kaiserslautern, 67653 Kaiserslautern, Germany*

The narrow $N_2^-(^2\Sigma_g^+)$ Feshbach resonance (estimated width 0.6 meV [1]) is formed in electron scattering from the ground state $N_2(X, v = 0)$ at an electron energy close to 11.5 eV, about 0.37 eV below the excited $N_2^*(E\ ^3\Sigma_g^+, v = 0)$ state which can be regarded as the neutral parent state. Using two different experimental setups, we reinvestigated this resonance in both elastic and vibrationally inelastic electron scattering with high energy resolution.

Combining a laser photoelectron source with a triply differentially pumped supersonic beam target and five electron multipliers for simultaneous detection of elastically scattered electrons at the angles 22.5°, 45°, 90°, 112.5°, and 135° [2], the resonance profiles have been measured with an unprecedented resolution of 5 meV. The resonance energy has been determined as 11.497(2) eV with reference to the position of the lowest Feshbach resonance in Ar, using a mixed Ar-N_2 target beam. An independent set of elastic scattering measurements has been obtained with an optimized apparatus with hemispherical monochromator and energy analyzer [3], which moreover allowed an observation of the resonance at 180° scattering angle with help of a specially designed magnetic angle changer [4]. The combined elastic scattering data yield a resonance width of 1.0(2) meV.

The resonance is even more prominent in vibrational excitation spectra of the electronic ground state which have been recorded up to $v = 2$ with about 13 meV energy resolution in incident and scattered electrons by means of the electrostatic analyzer apparatus. These spectra were recorded at the same angles as in the elastic channel. The inelastic data will be analyzed using our new *ab initio* potential energy curves for the neutral $N_2(X)$ and $N_2^*(E)$ states as well as for the $N_2^-(^2\Sigma_g^+)$ resonance, calculated with a coupled-cluster method.

Electron impact excitation of nitrogen molecules to metastable states has been measured, again with unprecedented resolution of 5 meV, over the range 11.3 - 13.3 eV using the photoelectron source apparatus by detecting the deflected long-lived excited molecules with a channel electron multiplier at the kinematically appropriate position. The spectrum is dominated by excitation to the $N_2^*(E\ ^3\Sigma_g^+)$ state with an onset at 11.87 eV and a peak at 11.918 eV.

This work has been supported by the Deutsche Forschungsgemeinschaft (HO 427/28), by the Swiss National Science Foundation, and by the European Science Foundation via the network EIPAM through grant 1288.

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Tu1-5

INTRAMOLECULAR BOND REARRANGEMENT IN CH_3OH

Jyoti Rajput [1], Sankar De [1,2], A. Roy [1], P. N. Ghosh [2] and C. P. Safvan [1]

[1] Inter-University Accelerator Centre, Aruna Asaf Ali Marg, Post Box – 10502,
New Delhi–110067, India
[2] Dept. of Physics, University of Calcutta, 92, A. P. C. Road, Kolkata–700009, India
Email : jyoti@iuac.res.in

We report here results of time-of-flight (TOF) multi-hit coincidence experiments [1] that provide evidence for intramolecular reactions involving proton coagulation in methanol [2] after interaction with 1.2 MeV Ar^{8+} projectiles produced from an ECR ion source in the LEIBF laboratory of Inter-University Accelerator Centre, India. Quite remarkably, we have found formation of bonds due to movement of protons within the multiply charged parent molecular ion formed due to ion-induced ionization and such bond formation occurs much before the Coulomb repulsion makes the fragment ions to fly apart. The fast rearrangement leads to formation of H_2^+ and H_3^+ ions and they are formed with substantial kinetic energy release (KER) in the center-of-mass (CM) frame of the molecule. Analysis of the fragmentation pattern of the doubly charged methanol has been carried out using *ab initio* quantum chemical techniques. Structural calculations indicate that the formation of H_3^+ is the preferred pathway in the overall fragmentation dynamics of the ground state of this alcohol. The field generated from HCI induces the system to rearrange its structure following a minimum energy pathway and form hydrogen molecular ions.

From the TOF spectrum of methanol molecules, we observed a wide range of dissociation products starting from undissociated molecular ions (CH_3OH^+), fragments losing a hydrogen atom due to breakage of C-H and O-H bonds (CH_2OH^+, $CHOH^+$, COH^+, CO^+) to complete rupture of C-O skeleton producing charged atomic species like C^{q+} and O^{q+} (q = 1 - 3). From the offline analysis of the acquired multihit data, we have generated a coincidence map, which is a 2D spectrum of the TOF of the first fragment ion versus that of the second. A specific area of the coincidence map shows that H_3^+ is ejected from doubly charged methanol ions through two-body process ($CH_3OH^{2+} \rightarrow H_3^+ + COH^+$) after rearrangement has taken place. But H_2^+ is formed due to both two-body ($CH_3OH^{2+} \rightarrow H_2^+ + CHOH^+$) and three-body ($CH_3OH^{2+} \rightarrow H_2^+ + COH^+ + H$) dissociation pathways. We have also noted that as soon as the O-H bond is disrupted and CO^+ is formed neither of H_2^+ and H_3^+ is recorded. Repeating the experiment with CH_3OD confirm our bond rearrangement phenomenon and establish that H_3^+ formation occurs only within the methyl group of the alcohol. Since organic molecules like methanol and highly charged ions (HCI) are found in dense and diffuse interstellar media, the collision of HCI with organic molecules is suggested as an alternate mechanism for the formation of H_3^+ in space.

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Tu1-6

DOUBLE IONIZATION OF HYDROGEN MOLECULE BY FAST ELECTRON IMPACT: CALCULATION USING EXACT WAVE FUNCTIONS OF TWO-CENTER CONTINUUM

V. V. Serov, V. L. Derbov, B. Joulakian and S.I.Vinitsky

Saratov State University, 83, Astrakhanskaya st., Saratov 410026, Russia
E-mail: vladislav_serov@mail.ru

The differential cross-section of the double ionization of the hydrogen molecule by a fast-electron impact is calculated using the expansion of the solution in terms of exact one-electron two-Coulomb-centers spheroidal functions [1]. The calculation of the cross-section is reduced to the calculation of a set of one-dimensional integrals of the spheroidal functions which is a substantial advantage of the method. Calculations based on different approximate models of electron-electron correlation in the final double continuum state and shielding of the nuclear charge are compared with each other and with the experiment [2].

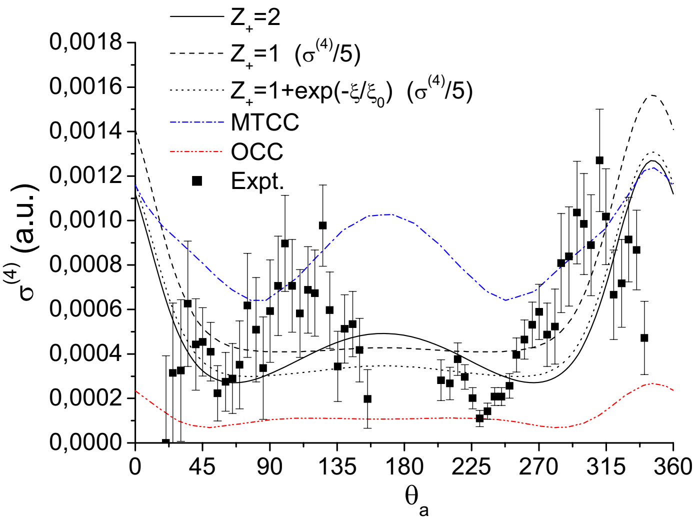

Fig. 1. The differential cross-section of (e, 3 - 1e) process on H_2 versus the angle of ejection θ_a measured [2] and calculated using different approximations: no screening (solid line), full screening (dashed line), partial screening (dotted line). The results of other authors: MTCC [3] (dashdot line), OCC [4] (dashdotdot line)

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Tu1-7

SIGNATURE OF TARGET EXCITATION IN NITROGEN FRAGMENTATION

Jyoti Rajput [1], Sankar De [1, 2], A. Roy [1] and C. P. Safvan [1]

[1] Inter-University Accelerator Centre, Aruna Asaf Ali Marg, Post Box – 10502,
New Delhi - 110067, India
[2] Dept. of Physics, University of Calcutta, 92, A. P. C. Road, Kolkata - 700009, India
Email : jyoti@iuac.res.in

Target excitation following ion-impact has been observed to play a significant role in multi-electron capture studies in ion-atom collision experiments [1] but not many reports exist for similar studies in ion-molecule collision experiments. To the best of our knowledge this is the first report on the role of target excitation in ion-induced N_2 fragmentation.

The multiple ionization and fragmentation of N_2 induced by ion impact is studied using the technique of time-of-flight mass spectrometry employing time and position sensitive detectors in multi-hit coincidence mode. The experiment was carried out at the ECR ion source based Low Energy Ion Beam Facility (LEIBF) of the Inter - University Accelerator Centre (IUAC), New Delhi, India. The details of the experimental setup can be found in reference [2]. With Ar^{9+} projectiles at a velocity of 1 atomic unit we observe a total of seven fragmentation channels originating from multiply charged transient molecular ions. The kinetic energy release (KER) spectra of all the observed fragmentation pathways was extracted from analyzing the data on an event by event basis. *Ab initio* calculations were done for determining the potential energy curves for multiply charged nitrogen molecular ions to account for the observed KER using the quantum chemistry package GAMESS [3]. The preference of symmetric charge breakup channels over the asymmetric ones is clearly observed. A signature of core excitation of the target molecule followed by Auger emission is observed in the kinetic energy spectra of the N^{3+} - N^{3+} fragmentation channel [4] in the form of a clear distinct peak at 72 eV, this value being very close to the most probable kinetic energy release in the case of N^{2+} - N^{3+} fragmentation channel.

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Tu1-8

RELATIVISTIC CALCULATION OF THE EMISSION SPECTRA OF W IONS AND ELECTRON IMPACT IONIZATION OF W/W$^+$

Yong-joo Rhee, Duck-hee Kwon
Laboratory for Quantum Optics, Korea Atomic Energy Research Institute
P.O.BOX 105 Yuseong, Daejeon 305-600 Korea
yjrhee@kaeri.re.kr
and
(late) Yong-ki Kim
National Institute of Standards and Technology
Gaithersburg, MD 20899 U.S.A.

The importance of the spectroscopy data of highly charged tungsten (W) ions and the electron-impact ionization cross section data of W has increased considerably for their applications to plasma diagnostics and a divertor modeling as a plasma facing material by considering the specific characteristics of its being a high refractory material.

We report on the calculation of emission spectra of the W^{33+}, W^{34+}, W^{35+}, W^{36+} ions and the electron impact ionization cross sections of W and W$^+$ calculated by using the relativistic MCDF code. For the electron impact ionization schemes, the binary-encounter Bethe (BEB) model [1] and a scaling of the Coulomb and/or Born cross section [2] have been adapted. These methods have been successfully applied to Mo (Z=42) and Mo$^+$ [3], which have a half-filled 4d valence shell similar to W and W$^+$. We calculated the total ionization cross sections of W and W$^+$ for the ground, first and second metastable levels individually [4] and compared our results with experiments and other theories.

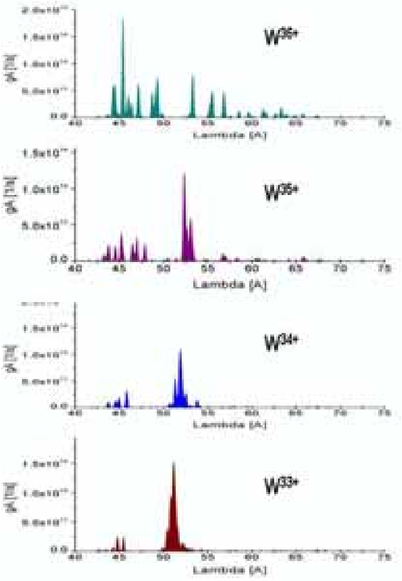

Fig 1 Spectra of highly charged W ions calculated by using MCDF code

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Tu1-9

LOWLY IONIZED Xe SPECTRA IN THE UV REGION

K. Katsonis[1], E. Biémont[2], H.-P. Garnir[2], M. Cornille[3], Ch. Berenguer[1], R.E.H. Clark[4]

[1]*Laboratoire de Physique des Gaz et des Plasmas, UMR 8578, Université Paris-sud 91405, Orsay Cedex, FRANCE*

[2] *IPNAS, Université de Liège, Sart Tilman B15, B-4000 Liège, BELGIUM*

[3] *LUTH, UMR 8602, Observatoire de Paris, Meudon, FRANCE*

[4] *Nuclear Data Section, IAEA, Vienna, AUSTRIA*

Study of the spectra emitted by low charge-state Xe ions requires both advanced experimental techniques for the confinement of the ions in conditions minimizing the collision effects and the sophisticated analysis of the observed spectra. We report on Xe III and Xe IV observed in a beam-foil experiment. A 1 µA beam of Xe^+ ions, produced by the Van de Graaff accelerator IPNAS (Liege, Belgium), was passed through a thin carbon foil. After exiting the foil, the light emitted in the far UV by the excited and ionized ions was analyzed with a CCD-equipped spectrometer. Spectra of Xe in the 30-100 nm wavelength region have been recorded at different beam energies corresponding to different excitation energies.

Collisional-**R**adiative (C-R) models are required to model spectroscopic measurements in plasmas outside local thermodynamic equilibrium. Development of such models calls for the collection and evaluation of atomic data for the coefficients of the second member of the relevant Boltzmann equations, leading to the formulation of a system of statistical equations. Once these coefficients have been validated in the steady state condition, extension to the transient, non stationary case can be conceptually reduced to the solution of a set of differential equations, with the first members accounting for the temporal and spatial variation of the distribution functions. We have developed a C-R model [1,2] for Xe plasma spectroscopy, using evaluated atomic data whenever possible. Transition probabilities (A_{ij}) and electron collision excitation are the main parameters defining the relative intensities within a given multiplet. When the necessary A_{ij} of the Xe III and IV were missing, we performed calculations in intermediate coupling, in collaboration with the LUTH Laboratoire de Meudon, Observatory of Paris, using the SUPERSTRUCTURE code. We have also calculated *ab initio* the Xe ions structure and A_{ij} by using the CATS [3] code in collaboration with the IAEA and Los Alamos National Laboratory (LANL).

Our evaluation of electron collision ionization and excitation cross sections of the Xe species involves the use of a calculational package of few body CTMC type codes [4] and the ACE [5] code of LANL. The spectra of various multiplets belonging to Xe III and IV have been analyzed, and will be presented at the conference.

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Tu1-10

Rotational energy transfer efficiency for neutral and ionic molecular targets: $Li_2(^3\Sigma)$ and $Li_2^+(^2\Sigma)$ in collision with ^4He at low temperatures.

M. Wernli*, E. Bodo and F. A. Gianturco

Dipartimento di Chimica and CNISM, Università "la Sapienza", P.le Aldo Moro 5, 00185 Rome, Italy

The lithium dimer, although being the second simplest homonuclear molecule (after H_2), has received great interest, since a lot of its properties are still to be studied regarding its chemistry, spectroscopy and inelastic collisional properties. Notably, lithium-bearing species may have played an important role as coolers (through rotational transitions) in the young universe (see [1] for a detailed review on the topic). Two states of the dimer are studied here in collisions with ^4He atoms: $Li_2(^3\Sigma)$ and $Li_2^+(^2\Sigma)$. As homonuclear species, they do not have permanent dipole moments (as H_2) and will not be observable through dipolar rotational transitions ($\Delta J = 1$). But a challenging point in studying the two systems is to see weather the polarisability of the ion, chiefly responsible for a deep van der Waals minimum, could also induce sufficiently strong quadrupolar ($\Delta J = 2$) transitions.

Here, we first give a description of the potential energy surfaces for both systems, and show the huge difference between the neutral and ionic lithium (see figure). The neutral species presents a negligible vdW minimum (~ -3 cm^{-1}), whereas it is much larger (~ -380 cm^{-1}) for the ionic system. We then present results for low-temperature rotational excitation of both species, in the domain 10-100 K, using these two surfaces. Results for both species are compared. Then, for both systems, the Wigner regime down to 10^{-6} cm^{-1} is also discussed. For $Li_2(^3\Sigma)$ – a Hund's case b system – calculations are carried both with and without the spin-rotation coupling. Influence of the latter on the rotational rates is discussed.

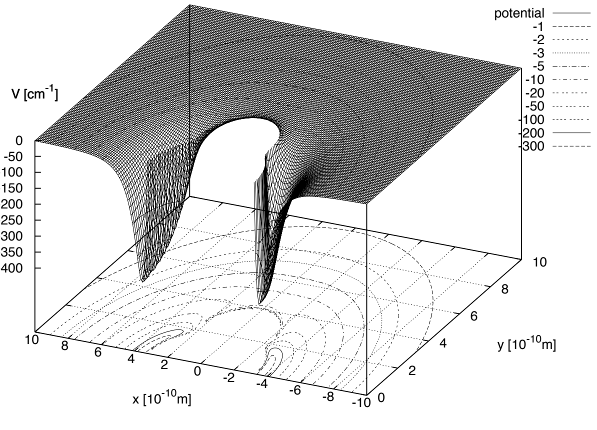

Figure 1: Potential energy surface for the ionic lithium ($Li_2^+(^2\Sigma)$) interacting with ^4He.

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* wernli@caspur.it

Tu1-11

THE IONIZATION OF MG 3s AND 2p ORBITALS BY ELECTRON IMPACT

P. Bolognesi[1], G. Bogachev[2], V. Borovik[2], S. Veronesi[1], R. Flammini[1], E. Fainelli[1] ,
A. Borovik[2], C:T. Whelan[3], H.R.J. Walters[4] and L. Avaldi[1]

[1]CNR-IMIP, Area della Ricerca di Roma 1, Monterotondo Scalo, Italy
[2] Institute of Electron Physics, National Academy of Sciences, Uzhgorod, Ukraine
[3] Old Dominion University, Department of Physics, College of Sciences, Norfolk,USA
[4] Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast, Northern Ireland

The most suited way to fully characterize the dynamics of the ionization process of an atom by electron impact is to detect in coincidence the scattered and ejected electrons. These experiments, named (e,2e) experiments, have been successfully performed in several rare gases under different kinematical conditions. The comparison of their results with theoretical predictions has provided valuable information to the present understanding of electron impact ionization [1]. In recent years some results on both valence and inner shell in Mg have been reported in the literature [2, 3]. These works investigated either the role of the two step mechanism in the ionization at large momentum transfer [2] or in the near threshold region [3]. Here we present the results of recent measurements at about 1000 eV incident energy, in unequal energy sharing (E_1=1000 eV, E_2=20 eV) and momentum transfer K≤2 a.u.. The experiments have been performed using the (e,2e) apparatus of the CNR-IMIP institute [4], which to the purpose has been equipped with an inductively heated oven.
Together with the Mg TDCS also the He TDSC in the same kinematical conditions have been measured, in order to identify difference that can be ascribed to 3s,2p initial state. The results of both He and Mg experiments will be compared with DWBA predictions.

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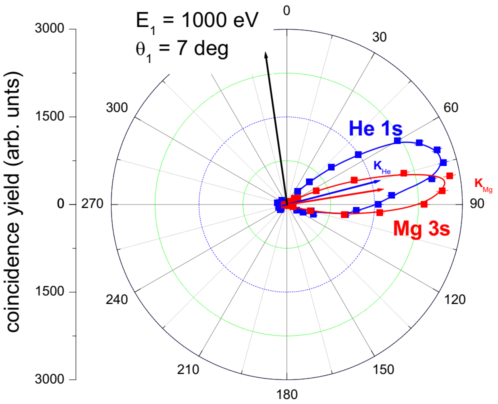

Figure 1. A comparison between the TDCS of the He1s and Mg3s shells measured in the same kinematic conditions (see text).

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Tu1-12

BREMSSTRAHLUNG IN INTENSE LASER-ASSISTED ELECTRON SCATTERING

Erik Lötstedt, Stephan Schnez, Ulrich D. Jentschura, and Christoph H. Keitel

Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg
Erik.Loetstedt@mpi-hd.mpg.de

We present calculations of the cross section for laser-assisted bremsstrahlung [1], the first concrete evaluation of a second-order quantum electrodynamic process with the Dirac-Volkov propagator in a strong laser field [2, 3]. In this process an electron in a strong laser field collides with a nucleus and emits a non-laser mode photon. The electron-laser interaction is treated exactly by using the analytical solution and propagator of the Dirac equation in an external plane-wave field, while the interaction with the nucleus and the emitted photon is taken into account perturbatively. Numerical results are presented for laser intensities of order 10^{21} W/cm^2, for both circular and linear polarization of the laser. In particular we show that this process is resonant for certain values of the emitted bremsstrahlung frequency, and we explain the physical origin and the numerical treatment of these resonances. This resonant behavior is absent in the non-relativistic treatment of the problem [4]. Finally, we discuss pair creation by photon absorption in the field of a nucleus and a laser, which is related to laser-assisted bremsstrahlung by a crossing symmetry.

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Tu1-13

TOTAL CROSS SECTION FOR DOUBLE IONIZATION OF HELIUM BY ELECTRON IMPACT

Z. S. Machavariani[1], T. M. Kereselidze[1], I. L. Noselidze[1], P. Defrance[2]

1Department of Exact and Natural Sciences, Physics Division, Tbilisi State
University, Chavchavadze Av. 3, Tbilisi 0128, Georgia
zaalmachavariani@hotmail.com
[2]Department de Physique, Universit´e Catholique de Louvain, Chemin du Cyclotron
2, B-1348 Louvain-la-Neuve, Belgium

Total cross sections (TCS) for double ionization (DI) of helium by electrons are calculated at intermediate and high incident energies in the first Born approximation (FBA). The radial and angular correlations between the bound electrons and repulsion between the ejected electrons are accounted [1,2].

Comparing of the calculated TCS with measured TCS shows that theory underestimates the TCS at the intermediate energies and overestimates the TCS in the high energy region.

One of the main shortcoming of theory may be attributed to the restriction of the theoretical treatment in the intermediate and low energy region by the first Born approximation (FBA). Remaining within the framework of the shake-off (SO) mechanism we made an attempt to go beyond the FBA and described the scattered electron by means of Coulomb continuum wavefunction with screened effective charge [2]. Such a simple inclusion of the non-FBA effects and improvement of the wavefunctions revealed the following tendency in the TCS behaviour: (i) the overall magnitude of the cross section increases and approaches the measured TCS, (ii) maximum of the cross section shifts to the left and approaches the experimental ones. In spite of improvement the substantional disagreement between theoretical and experimental TCS still exist in the high energy region. Namely, while theory predicts possitive slope experiments exhibit a negative slope in the Bethe plot of data (see figure 1).

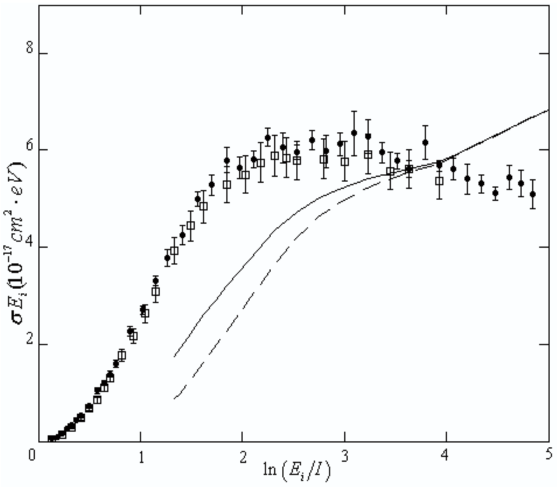

Figure 1. The Bethe plot for double ionization of *He*: dashed curve – FBA calculation. solid curve – FBA calculation with effective charges. □ ● – experiments (see references for details).

The obtained results stimulated us to develop the screened effective charge approach for calculation the TCS in the high energy region. For this we have utilized the dynamical variation principle. These calculations now are in progress.

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ABSOLUTE CROSS SECTIONS FOR ELECTRON IMPACT IONIZATION AND DISSOCIATION OF CD^+

J. Lecointre[1], J.J. Jureta[1, 2], D.S. Belic[3], Becker[4], H. Deutsch[5], T.D. Märk[6], M. Probst[6], R.K. Janev[7] and P. Defrance[1]

[1] Département de Physique-PAMO, Université Catholique de Louvain,
Chemin du Cyclotron 2, B-1348 Louvain-la-Neuve, Belgium
[2] Institute of Physics, P.O. Box 68, Belgrade, Serbia
[3] Faculty of Physics, P.O. Box 386, Belgrade, Serbia
[4] Department of Physics and Center for Environmental Systems, Stevens Institute of Technology, Hoboken, NJ 07030, USA
[5] Institut für Physik, Ernst Moritz Arndt Universität Greifswald, Domstr. 10a, D-17487 Greifswald, Germany
[6] Institut für Ionenphysik und Angewandte Physik, Leopold Franzens Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria
[7] Macedonian Academy of Sciences and Arts, 1000 Skopje, Macedonia.

Electron impact ionization and dissociation of hydrocarbon ions (for example the methane family CD_n^+) are very important processes in any laboratory plasma, astrophysics and thermonuclear fusion.

We report on results of absolute cross section measurements for electron impact ionization and dissociation of CD^+ to the different fragments: C^+, D^+, C^{2+} and C^{3+}. Measurements are performed by using the animated electron-ion crossed beams experiment. The electron energy range extends continuously from the threshold of the initial reaction (excitation or ionization) up to 2.5 keV. In the case of dissociation processes, substantial internal energy may be transferred to the dissociation fragments, inducing important broadening of both the angular and the velocity distributions in the laboratory frame. Usually, only a fraction of them is detected, so that absolute values of the cross section are obtained after the determination of the product ion transmission [6].

Individual contributions of dissociative excitation and dissociative ionization processes are estimated separately. Present results are compared with the experimental data of Djuric et al [1, 2] and with the semi-empirical results of Janev and Reiter [3]. The results obtained by application of the Deutsch-Märk model [5] are found to be in satisfactory agreement with corresponding experimental results, which are estimated by summing all the dissociative ionization contributions.

In addition, a magnetic field scan allows the determination of the kinetic energy release (KER) distribution of fragments for a given incident electron energy. For singly charged products, the comparison of the present energy thresholds and kinetic energy release with published data allows the identification of states contributing to the observed processes. At fixed electron energy, the cross sections for the various ionization channels are seen to reduce exponentially with the potential energy of each dissociated ion pair [5, 6].

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Tu1-15

DYNAMIC POLARIZATION EFFECTS IN INTERACTIONS OF FAST MOLECULES WITH GRAPHENE

I. Radović[a], Z.L. Mišković[b,*], Lj. Hadžievski[a] and N. Bibić[a]

[a]VINČA Institute of Nuclear Sciences, P.O. Box 522, 11001 Belgrade, Serbia
[b]Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

Although graphene can be considered as building material for fullerene molecules, carbon nanotubes, and the highly-oriented pyrolytic graphite (HOPG), single sheets of graphene have been isolated only very recently. Nevertheless, this simple planar structure of carbon atoms, with its unique electronic properties, is already placed in the focus of research due to its promise in a variety of applications [1]. From a theoretical point of view, graphene can serve as a relatively simple testing filed for development of various models to be used in studies of other carbon nanostructures.

In the present contribution, we investigate the stopping force (or the energy loss per unit path-length), as well as the dynamic image forces on fast molecular ions moving parallel to a graphene sheet, which are caused by the polarization of carbon valence electrons. Using a two-dimensional hydrodynamic model for the graphene dielectric response [2], we obtain both the first– and second–order perturbation results for these forces. Thus, e.g., the second-order results for energy loss amount to the well-known Barkas effect in stopping power of energetic particles. Moreover, special emphasis is paid to an analysis of the so-called vicinage effects in energy losses due to spatial correlation between the constituent ions in an incident molecular projectile.

The results obtained in this contribution will be of interest in studies of ion irradiation effects on graphene, with specific applications to Coulomb explosions of molecular ions and the accompanying secondary electron emission during grazing scattering from a HOPG surface [3] or during channelling through the inter-graphene regions in HOPG [4].

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[*] E-mail address: zmiskovi@math.uwaterloo.ca. Phone: +1 (519) 888-4567 / x 35463

Tu1-16

ELECTRON IMPACT IONIZATION AND DISSOCIATION OF NeD$^+$

J. Lecointre[1], J.J. Jureta[1, 2], J.B.A. Mitchell[3] and P. Defrance[1]

[1] Département de Physique-PAMO, Université Catholique de Louvain,
Chemin du Cyclotron 2, B-1348 Louvain-la-Neuve, Belgium
[2] Institute of Physics, P.O. Box 68, Belgrade, Serbia
[3] PALMS, 'Equipe d'astrochimie expérimentale', UMR N°6627 du CNRS, Université de Rennes I, F-35042 Rennes, France.

Electron-ion collision is one of the fundamental processes in fusion research. Data are needed for modeling the structure and dynamics of high-temperature plasmas. Neon is frequently introduced in tokamaks as a diagnostic of the hot plasma in the divertor region. Furthermore, ion-molecule reactions involving H$^+$ or D$^+$ with noble gas atoms and ions are of great interest: the NeD$^+$ molecular ion plays a role in the plasma chemistry of the future thermonuclear reactor [1, 2].

We report on results of absolute cross section measurements for electron impact ionization and dissociation of NeD$^+$ to the different fragments: Ne$^+$, D$^+$, Ne^{2+} and Ne^{3+}.

Measurements are performed by using the animated electron-ion crossed beams experiment. The electron energy range extends continuously from the threshold of the initial reaction (excitation or ionization) up to 2.5 keV. Usually, only a fraction of the signal is detected, so that absolute cross sections are obtained after determination of the product ion transmission. Individual contributions of dissociative excitation and dissociative ionization processes are estimated separately [3].

At the maximum, i.e. for an electron energy around 35 eV, absolute cross sections for dissociative excitation are found to be $(3.6\pm0.5)\times10^{-17}$ cm^2 and $(6.3\pm0.8)\times10^{-17}$ cm^2 for Ne$^+$ and D$^+$, respectively, and the corresponding appearance energies are (9.1±0.5) eV and (10.0±0.5) eV. In the very low energy region, dissociative excitation leading to the D$^+$ formation dominates over the Ne$^+$ one. The absolute cross section for dissociative ionization (Ne$^+$+D$^+$ formation) is found to be $(8.2\pm1.6)\times10^{-17}$ cm^2, around 135 eV, and the corresponding threshold energy is (25.1±0.5) eV. Moreover, absolute cross sections for the multiply charged fragments are found to be $(5.4\pm0.5)\times10^{-18}$ cm^2 and $(18.2\pm2.6)\times10^{-20}$ cm^2 for Ne^{2+} and Ne^{3+}, respectively, and the associated appearance energies are (53.1±1.0) eV and (132±2) eV.

In addition, a magnetic field scan allows the determination of the kinetic energy release (KER) distribution of fragments for a given incident electron energy. For singly charged products, the comparison of the present energy thresholds and kinetic energy release with published data allows the identification of states contributing to the observed processes. At fixed electron energy, the cross sections for the various ionization channels are seen to reduce exponentially with the potential energy of each dissociated ion pair [3, 4].

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Tu1-17

CORRECTION OF FRINGING FIELD EFFECTS IN HEMISPHERICAL DEFLECTOR ANALYZERS USING BIASED PARACENTRIC ENTRY

Omer Sise[1], T.J.M. Zouros[2,3], Melike Ulu[1], Mevlut Dogan[1]

[1]Department of Physics, Science and Arts Faculty, Kocatepe University, 03200 Afyonkarahisar, Turkey
[2]Department of Physics, University of Crete, P.O. Box 2208, 71003 Heraklion, Crete, Greece
[3]Institute of Electronic Structure and Laser, P.O. Box 1527, 71110 Heraklion, Crete, Greece

Hemispherical deflector analyzers (HDAs) are certainly today the most widespread electron energy analyzers. Simulations of electron trajectories within the field of the two concentric hemispheres assume ideal fields. However, in a real analyzer, the ideal radial field has to be suddenly terminated, usually by the mounting plate of the HDA at ground potential. This introduces departures from ideal field behavior leading to distorted trajectories, the degradation of 1rst order focusing and corresponding loss in energy resolution and/or transmission. This is one of the main disadvantages of this type of analyzer. The commonly used fringing field correctors such as Herzog [1], Jost [2], tilted input lens [3], and equipotential rings [4] mounted at the entrance and exit of the hemispheres reduce the effect of the electrostatic fringing field, but do not solve the problem, especially for spheres with a large interradial distance. Our concept is quite different. In a previous paper [5], we have shown in simulation that a simple repositioning of the HDA entry when appropriately biased results in the effective utilization of the intrinsic lensing properties of the fringing fields to restore and even improve 1rst order focusing. This arrangement has been referred to as “biased paracentric entry” HDAs [6].

In our present work, we report on a detailed comparison of the spectroscopic characteristics between commonly used fringing field corrector methods and the biased paracentric entry HDAs. This novel design does not require any fringing field correction systems and provides improved high-energy resolution capability (first-order focusing) and transmission. Furthermore, the use of fewer electrodes in a paracentric HDA will not only lower the overall cost of power supplies and construction, but will also reduce its operational complexity and weight. These features make such an HDA particularly attractive in the technical challenge to perform high-resolution experiments.

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Tu1-18

DISSOCIATIVE ELECTRON ATTACHMENT TO NITROTOLUENE ISOMERS

P. Sulzer, S. Denifl, A. Mauracher, F. Zappa, N. Wendt, A. Aleem, F. Rondino*,
S. Jaksch, A. Bacher, V. Grill, S. Ptasinska, S. Matejcik, P. Scheier, T.D. Märk

Institut für Ionenphysik und Angewandte Physik, Leopold-Franzens Unversität
Innsbruck, Technikerstr. 25, 6020 Innsbruck, Austria
*Universita di Roma, La Sapienza, Dipartimento di Chimica, Rome, Italy

The present work studies dissociative electron attachment to 2-, 3- and 4-nitrotoluene (NT). In extension to former publications (e.g. [1]) we investigated all measurable fragment anions and recorded the resulting anion yield as a function of the incident electron energy with 80-100meV electron energy resolution.

Our measurements were performed utilizing a hemispherical electron monochromator. After crossing the electron and the neutral beam, the product ions are analysed with a quadrupole mass filter and detected by a channeltron type secondary electron multiplier operated in the pulse counting mode. In the past this experimental setup was successfully used to investigate inelastic interactions of free electrons with gas phase molecules of biological relevance, such as DNA bases [2,3,4], fructose [5], etc. Nitrotoluenes show a sufficient vapour pressure so that head space vapours could be used for analysis without further heating of the samples.

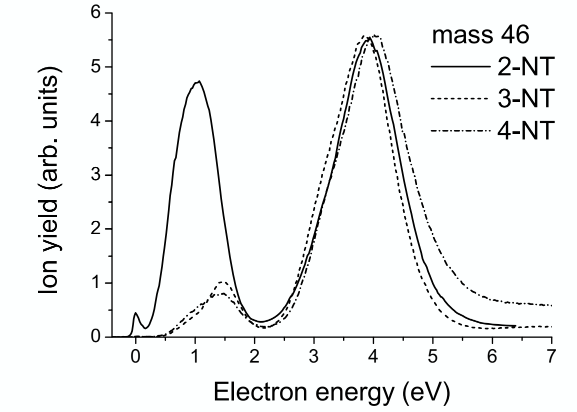

Fig. 1: NO_2 anion yield for all NT-isomers (normalized on the second peak)

Fig. 1 shows the anion yield for the fragment NO_2^- for all three NT-isomers. All isomers are easily distinguishable by the anion efficiency curves of this fragment which was also discovered recently by Harvey et al. [6]. Furthermore, there seems to be a strong correlation between the distance between the methyl- and the nitro-group and the height of the 1 eV resonance. This relation is also observable for the complementary channel (mass 91m/z; loss of neutral NO_2). Nearly all measured fragments show significant differences for the different isomers.

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Tu1-19

QUENCHING OF ^{3}He EXCITED STATES (n>2) BY COLLISIONS WITH NEON ATOMS

E. Dimova

Institute of Solid State Physics, BAS, 72 Tzarigradsko Chaussee,
1784 Sofia, Bulgaria
edimova@issp.bas.bg

Helium is one of the most used elements as a buffer gas for cooling and trapping of atoms or in light sources and in particular to create inversion population in some gas-discharge lasers (He-Ne, He-Cd, He-Zn, etc.). The interaction processes are mainly investigated for processes with participation of ^{4}He, while for ^{3}He isotope there is no data.

The aim of our work is to investigate the processes leading to quenching of helium excited states (n>2) by collisions with neon atoms in the ground state.

The energy levels of ^{3}He excited states (^{3}He*) with n>2 are higher than the ionization potential energy of all elements and particularly for neon. The interaction between ^{3}He* atom and Ne_0 atom is assumed to be a Penning ionization:

$$^3He^*(n>2) + Ne_0 \rightarrow {}^3He_0 + Ne^+ + e^-$$

The quenching process of ^{3}He* (n>2) by collisions with Ne atoms in the ground state at low pressure is experimentally investigated by a time - resolved spectroscopy method. The delay coincidence method is used for observation of the kinetic of the population of He excited states. The decay of He* excited states is observed in the afterglow as a consequence of a pulse electron excitation of the ^{3}He-Ne mixture. The concentration of He atoms is kept constant during the experiment and correspond to 0,5 Torr pressure at room temperature. The variation of effective lifetimes of the investigated He* states, when the concentration of Ne atoms is changed, allows to determine the corresponding quenching cross sections. The experimental setup is described in [1]

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Tu1-20

TREATMENT OF CLOSE COUPLING APPROXIMATION IN ALLOWED ATOMIC TRANSITION

Smail Bougouffa[1], Saud AL-Awfi

Department of Physics, Faculty of Science, Taibah University,
P.O. Box 344, Madinah, Saudi Arabia.
[1]sbougouffa@hotmail.com

The problem of excitation of the 3^2P state of sodium has been treated by several authors [1]. Calculations have been made for Na $3s \rightarrow 3p$, which is an excellent example of a near resonance and strong coupling, with an energy separation $\Delta E = 2.104\ eV$ and a rather large line strength $s^2 = 19$. We use a Numerov technique for calculations of electrons scattering on atomic sodium. We show that the results are in good quantitative agreement with those of the previous work [2], and the difference can be assigned to the use of the set of three-channel differential equations in the $3^2S \rightarrow\ 3^2P$ transition of sodium, while in the last works [2, 3] the two-channel problem are considered. It is found that the three-channel problem results are typically in reasonably good agreement with experiment and previous 2-channel calculations [4] for intermediate energy range. we shall concerned with the special class of electron-atom collisions which induced transitions of the type $n, l, m \rightarrow n,\ l\pm 1,\ m$, where the interaction potentials can be calculated using the wave functions of the one-electron orbital of the excited electron. It has been demonstrated in the close-coupling calculations that the contribution of the 3-channel on the excitation cross sections of the 3^2P state in the low and intermediate energy range is very important. In this energy range the exchange electron effect is important and must be taken in consideration. While in high range of energy, it is sufficient to consider just the initial and final states and the coupling through the intermediate states can be neglected. Nevertheless in the intermediate and high energy range the method of close coupling in the 2- or 3-channel approximation proves to be a useful tool for calculating excitation cross sections of dipole -allowed states.

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Tu1-21

Low-energy electron collisions with CH_3Br: the dependence of elastic scattering, vibrational excitation, and dissociative attachment on the initial vibrational energy

M. Braun [1], I. I. Fabrikant [1,2], M.-W. Ruf [1], and H Hotop [1]
[1] *Fachbereich Physik, Technische Universität Kaiserslautern, D-67653 Kaiserslautern, Germany*
[2] *Department of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588-0111, USA*

Using the Laser Photoelectron Attachment (LPA) method at an energy width of 1 – 2 meV, the Br^- yield due to dissociative electron attachment to the molecule CH_3Br has been measured over the energy range 1 – 180 meV at a gas temperature of 600 K [1]. The data clearly exhibit the vibrational Feshbach resonance predicted by Wilde *et al.* [2] and associated with the $v_3 = 4$ vibrational level of the C – Br stretch mode in the neutral molecule. We also report the dependence of the rate coefficient for Rydberg electron attachment (measured at high principal quantum numbers $n \approx 150$) on gas temperature over the range $T = 300 - 600$ K and find an Arrhenius-type behaviour [1] compatible with the results of the R-matrix calculations and with earlier findings of electron swarm experiments [3 – 7].

With the aim to stimulate experiments, we report absolute cross sections for elastic scattering and vibrationally inelastic scattering involving the C – Br stretch mode v_3 of CH_3Br for several initial vibrational levels in the range $v_3 = 0 - 4$. They were obtained with R-matrix calculations based on the same potential input as that involved in the computations of the cross sections for dissociative attachment. Depending on the initial vibrational level, these cross sections show more or less clear structure at the vibrational thresholds (especially at the $v_3 = 3, 4$ onsets) [1].

This work has been supported by the Deutsche Forschungsgemeinschaft (HO 427/29), by the Forschungsschwerpunkt *Optische Technologien und Lasergesteuerte Prozesse* and by the US National Science Foundation (PHY - 0354688.)

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Tu1-22

DIELECTRONIC RECOMBINATION OF PARTIALLY-FILLED M-SHELL IONS

D. Nikolić[1], S.A. Abdel-Naby[1], J. Fu[1], T.W. Gorczyca[1], N.R. Badnell[2], and D.W. Savin[3]

[1] Department of Physics, Western Michigan University, Kalamazoo, MI 49008, USA
[2] Department of Physics, The University of Strathclyde, Glasgow, G4 ONG, UK
[3] Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027, USA

Dielectronic recombination (DR) is the important process in modeling the ionization-recombination balance of multiply-charged atomic ions in low-density high-temperature plasmas. For that purpose, we have carried out systematic calculations of the total DR rates for selected low-charged M-shell ions.

First, we will present the results for Al-like S^{3+} using the level resolved distorted-wave AUTOSTRUCRE program package. In addition to previous results [1], our present analysis of the total DR rate coefficients is carried out in both the LS and IC-coupling schemes including $\Delta N = 0$ ($3\rightarrow3$) and $\Delta N = 1$ electron core excitations and further expanded by $3s^2n\ell$ and $3s3pn\ell$ (n =4 and 5) configurations.

Second, the long standing discrepancies (low-lying resonance positions and asymmetry profiles, as well as the overestimation by factor 1.6 at the highest Rydberg limit) between the experimental and theoretical [2-4] DR rate coefficients for Ar-like Sc^{3+} and Ti^{4+} ions are resolved.

Our new approach enables us to treat accurately DR for open M-shell ions in computationally feasible manner, and at the same time to achieve a good agreement with the available storage-ring experiments.

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Tu1-23

H + He$^+$ ELECTRON TRANSFER CROSS-SECTIONS FOR PLASMA PHYSICS

J. Loreau[1], F. Rosmej[2], M. Desouter Lecomte[3] and N. Vaeck[1]

[1] Service de Chimie Quantique, ULB, Brussels, Belgium
[2] PIIM, Université de Provence, France
[3] LCP, Université de Paris XI, Orsay, France

Charge transfer mechanisms during collision processes between ions and neutral atoms or molecules have recently received renewed attention, due to their role in the analysis of laboratory and astrophysical plasmas.

To understand the physical processes that underlie plasma transport in torodially confined plasmas and more specifically the anomalous plasma transport induced by Coulomb collisions, spectroscopic methods have turned out to be very effective. One of the most powerful spectroscopic methods is based on the space and time resolved observation of line emission from impurity ions. The optical helium line emission has been simulated from an atomic physics model with given temperature and density profiles and contrasted with the experimental data. However, under real experimental conditions of fusion plasmas, the impurity ions do interact with the plasma background H/D which leads to a change of the radial distribution of the impurity ions due to charge exchange processes. An important point in the present work is to calculate the respective charge exchange cross sections for low energies because the electron temperature of divertor plasmas is much below an atomic unit. However, at present the complete set of data required are neither available in the literature nor in data bases to perform the requested coupling [1]. The difficulties for typical conditions of divertor plasmas are connected with the fact that the widely applied Born approximation is highly invalid. Moreover, for low Z-elements like H/D and He the classical approximation is also highly invalid due to the strong influence of the molecular band formation.

We have used a quasi-molecular approach of the ion-atom collision based on the use of conventional quantum-chemistry *ab initio* methods to obtain the potential energy surfaces as well as the radial coupling matrix elements of the quasi-molecule HeH$^+$. The main problem encountered in this work is the large number of excited molecular states that need to be taken into account, necessitating the introduction of a new basis of molecular orbitals.

A wave packet method is used to treat the curve-crossing dynamics resulting from the failure of the Born-Oppenheimer approximation. A Gaussian wave packet is prepared in the entrance channel and propagated on the coupled effective channels. The post-collisional amplitudes of the wave packets are recorded in the asymptotic region and the collision matrix is extracted after Fourier transforming these asymptotic amplitudes, giving access to the charge exchange cross-section [2].

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Tu1-24

Complex electron dynamic in He^+-He-collisions at 60 keV/u

M. S. Schöffler[1*], J. Titze[1], L. Ph. H. Schmidt[1], O. Jagutzki[1], T. Jahnke[1], S. Otranto[2],
R. Olson[2], R. Dörner[1] and H. Schmidt-Böcking[1]

[1] Institut für Kernphysik, Universität Frankfurt, 60486 Frankfurt, Germany
[2] University of Missouri, Rolla, USA

At high projectile velocities ($v_P > 3$ a. u.) the dynamic of transfer ionization (TI) processes is nearly independent of the projectile. This approximation is also valid for lower velocities, except some post collision effects (PCI). The final state of a transfer ionization leads to a less charged projectile and a continuum electron ($P^{q+} + He \rightarrow P^{(q-1)+} + He^{2+} + e^-$). In general this approximation is also valid for lower projectile velocities (1.5 a. u.), if the projectile is bare (proton, He^{2+}). In the case of He^+, where an electron originating from the projectile is involved the collision dynamics change conspicuously. We have used the COLTRIMS technology (COLd Target Recoil Ion Momentum Spectroscopy) [1] to determine the momentum vectors of all final state products to investigate the influence of the projectile electron.

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* electronic address: schoeffler@atom.uni-frankfurt.de

Tu1-25

Collisional depolarization and polarization transfer for molecular and atomic lines. Astrophysical applications

Moncef Derouich

Institut d'Astrophysique Spatiale, Batiment 121, F-91405 Orsay, France

Symmetry-breaking processes such as anisotropic radiation pumping and anisotropic collisions could create the so-called atomic polarization. This atomic polarization reflects the fact that the Zeeman sublevels of the atomic system are unevenly populated and there are quantum coherences among them. The atomic polarization leads to selective emission and/or selective absorption processes and thus to polarization in atomic/molecular spectral lines. It is important, however, not to confuse this atomic polarization with the more familiar Zeeman polarization which due to the magnetic fields.

With the development of a new generation of very accurate spectro-polarimeters, the spectrum of the atomic polarization open a new window for the diagnostics of magnetic fields and physical conditions of the astrophysical mediums. The most known example is the "second solar spectrum", which is the spectrum of the linear atomic polarization observed close to the solar limb. This spectrum is as rich in spectral structures as the ordinary intensity spectrum, but is governed by different physical processes and differs in appearance and information content.To correctly interpret the spectrum of the polarization, it is necessary to know the (de)polarizing rates due to the collisions of the emitting atomic systems with nearby perturbers.

In this contribution: 1) We present our collisional semi-classical theory developed over the last few years and applied for all simple/complex atoms. For solar conditions, a fundamental result which justifies our approach is that the collisional depolarization process depends strongly on the intermediate regions of collisions which are accurately described by our semi-classical approach. 2) We give the first results obtained for the collisional depolarization and polarization transfer for rovibrational levels of diatomic molecules. 3) We report a recent theoretical investigation which has been carried out in order to quantify the influence of the polarization transfer rates by collisions on the linear polarization amplitudes of several lines. 4) We establish the real contribution of the anisotropic and isotropic collisions in the polarization for the so-called multiterm atoms, i.e. where in particular the coherence between the different *j*-levels (the so-called superinterferences) are taken into account. We show an application of our collisional rates calculations by determining very week unresolved magnetic fields in the solar photosphere by their Hanle effect on the linear polarization of the lines. 5) Finally, we draw attention to various still open problems in the solar physics because of the luck of collisional data (e.g. MgH and C2 solar lines; Halpha line...): much important work still remains to be done and we would surely see a number of surprising results in the years to come.

Tu1-26

Plateau and cut-off in the electron energy spectrum from ionization in laser-assisted ion-atom collisions

M. F. Ciappina[1] and L. B. Madsen[2]

[1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38,
D-01187, Dresden, Germany
[2]Lundbeck Foundation Theoretical Center for Quantum System Research,
Department of Physics and Astronomy, University of Aarhus, 8000 Aarhus C,
Denmark

We study single ionization in laser-assisted high-energy non-relativistic ion-atom collisions and show that the low-energy electron spectrum is enhanced by 5 orders of magnitude by an external field of strength less than 1/100 of a typical atomic field. With increasing strength of the assisting field, the energy spectrum is characterized by the emergence of a plateau extending to a cut-off at a position where the photon exchange balances the change of kinetic energy of the projectile. In the plateau region a startling multiphoton effect appears: despite projectile-induced ionization, the final energy of the projectile is higher than its initial energy. This effect can be considered as a *multiphoton induced speed-up* of the incoming heavy ion [1]. The dressing by the external field gives rise to two characteristic regimes. A weak-coupling regime with photon exchanges that do not alter the overall field-free energy balance and a strong coupling regime, where so many photons are exchanged that we predict *multiphoton induced* speed up of the ion and the projectile emerges from the collision with higher kinetic energy than it originally had. In the strong coupling regime, we predict an enhancement by up to 5 orders of magnitude compared with the field-free cross section for moderate laser intensities. Experimental investigations of the predicted effects are entirely possible with current laser, beam and detection technologies. As an alternative to heavy-ion projectiles one could consider fast electrons (v~10 a.u.) and study the effect in laser-assisted (e-2e) experiments.

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Tu1-27

MECHANISMS OF MULTIPLE AUGER DECAY FOLLOWING SINGLE PHOTON IONISATION OF THE n=4 SHELL IN XENON.

F. Penent[1], P. Lablanquie[1], Y. Hikosaka[2], T. Kaneyasu[2], E. Shigemasa[2],
J.H.D. Eland[3], T. Aoto[4] and K. Ito[4]

[1] LCP-MR, UPMC and CNRS, 11 rue P. et M. Curie, 75005 Paris, France
[2] UVSOR Facility, Institute for Molecular Science, Okazaki 444-8585, Japan
[3] P.T.C.L., South Parks Road, Oxford, OX1 3QZ, UK
[4] Photon Factory, I.M.S.S., Oho, Tsukuba 305-0801, Japan

Inner-shell ionisation followed by (multiple) Auger decay can produce multiply charged ions when the process is energetically allowed. However, Auger spectroscopy alone may be unable to disentangle complex spectra involving different inner-shell vacancies and cascade or direct multiple Auger decay. The n=4 shell in xenon is particularly complex in this sense due to many body effects [1]: the $4p^{-1}$ hole is, for instance, strongly mixed with $4d^{-2}nf$ and $4d^{-2}\varepsilon f$ configurations and presents abnormal photoelectron spectra [2].

Our experiment uses a Magnetic Bottle Time of Flight (TOF) spectrometer and allows the efficient detection in coincidence of **all** the electrons analysed in energy and is able to reveal mechanisms leading to multiply charged ions. The initial inner-shell ionisation is induced by a VUV-XUV photon provided by synchrotron radiation (from Photon Factory, Tsukuba, Japan) during single bunch operation (624 ns period) to allow TOF measurements.

Following the observation of double Auger decay after Xe(4d) ionisation [3], we have studied here xenon ionisation at 220 and 300 eV photon energy, i.e. above “4p” inner-shell ionisation limit.

Coincidence electron spectroscopy (2, 3 or 4 electrons detected in coincidence) reveals many different processes in that case with all the ionisation mechanisms, the decay channels and the branching ratio to final ionic states:

1) “$4p_{3/2}$” inner-shell ionisation is mainly followed by Coster-Kronig decay to $4d^{-1}5p^{-1}$ states that further decay by single or double Auger processes to Xe^{3+} or Xe^{4+} [4].

2) In the energy region where “$4p_{1/2}$” photoelectron could be expected (if many body effects were not so strong), the initial and prominent ionisation process consists in fact in the simultaneous ejection of two 4d electrons sharing continuously the available energy (that can only be revealed by coincidence spectroscopy). The $4d^{-2}$ Xe^{2+} states undergo cascade Auger decay through the successive filling of the two 4d vacancies by 5p or 5s electron leading to Xe^{4+} ($5p^{-4}$ or $5s^{-1}5p^{-3}$) ions [5].

3) The spectroscopy of Xe^{4+} ion is directly achieved.

This shows the efficiency (and the need) of high resolution multicoincidence experiments to disentangle complex mechanisms where strong many body effects make the single electron picture almost meaningless.

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Tu1-28

Low energy electron interactions with molecules in the condensed phase

R. Balog[1], P. Cicman[1], N.C. Jones[1], K. Høydalsvik[1], D. Field[1], L. Feketeová[1]
T.A. Field[2], K.Graupner[2], J.-P. Ziesel[3]

[1]Department of Physics and Astronomy, University of Aarhus, Ny Munkegade, Aarhus, 8000 C, Denmark

[2]Department of Physics and Astronomy, Queen's University Belfast, Belfast, BT7 1NN, United Kingdom

[3]Laboratoire Collisions Agrégats Réactivité (CNRS UMR5589), Université Paul Sabatier, Toulouse, 31062, France

Using a new apparatus, we report the first data for low energy electron collisions with solid material. We find that polycrystalline water ice at 130K is effectively transparent to electrons for energies between a few tens of meV and few hundred meV. Higher energies up to 8 eV display structure and are in part reflected from the material. There is no evidence of charging. This behaviour is in contrast to propanoic acid, for example, which charges strongly and shows relatively low effective electron transmission at all energies up to 7 eV. The electron source is a synchrotron radiation photoionisation source, using the ASTRID storage ring at ISA, Aarhus, with a typical resolution of 1 meV in the incident beam [1]. The beam of electrons is focused onto a thin film of material deposited on tantalum. Films are prepared in a separate chamber using standard dosing techniques. The entire apparatus is UHV.

The transmitted current is measured as a function of electron energy. At present the energy scale is assigned by assuming that the onset of electron current is at zero energy. This may be in error by tens of meV.

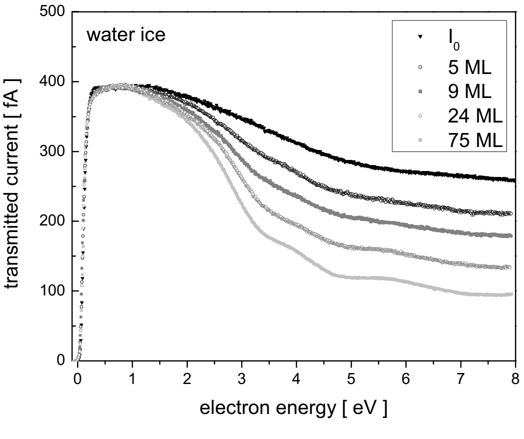

Fig. 1 Transmitted current vs electron energy for polycrystalline water ice at 130K. The top curve is for bare tantalum, and the curves refer successively to 5, 9, 24 and 75 monolayers.

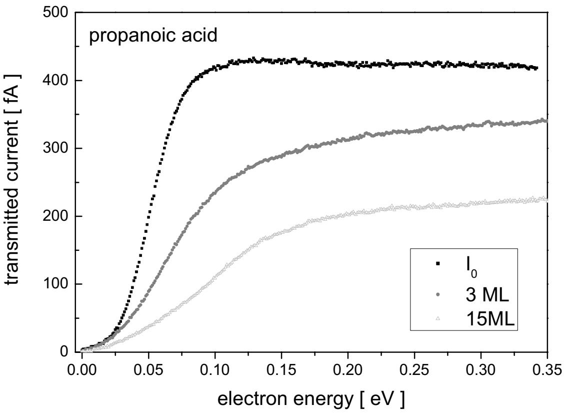

Fig. 2 Transmitted current vs electron energy for propanoic acid at 130K. The top curve is for bare tantalum, and the curves refer successively to 3 and 15 monolayers.

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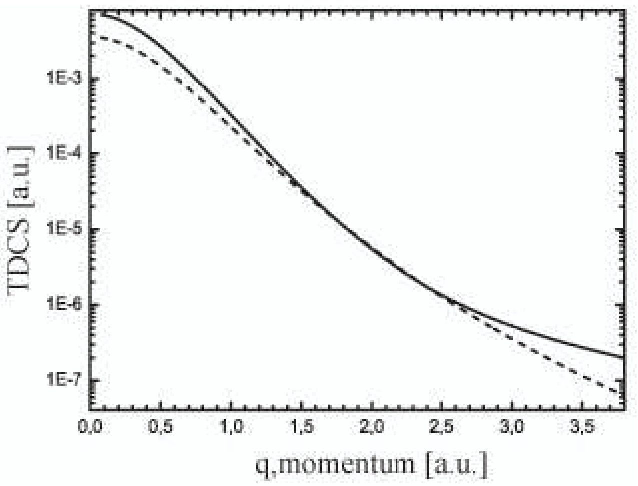
Tu1-29

HIGHER-ORDER BORN CALCULATIONS FOR (E,2E) REACTIONS AT LARGE MOMENTUM TRANSFER

P.S. Vinitsky*, K.A. Kouzakov*, Yu.V. Popov #

* Faculty of Physics, Moscow State University, Moscow 119899, Russia
# Nuclear Physics Institute, Moscow State University, Moscow 119899, Russia



A method of exploring the electronic structure of an atomic target in electron impact single and double ionization processes at large momentum transfer [1] is based on domination of a first Born approximation (FBA) in the corresponding ionization amplitudes. However, contributions of higher-order Born terms, such as the second Born approximation (SBA), have not been seriously studied so far. We consider such impact energies [2] that the contribution of higher-order effects can be not small. To estimate the validity of the first-order treatments, it is necessary to calculate the second- and third-order terms. But these are given by divergent integrals due to infinite range of Coulomb potentials. For their calculations a renormalization procedure [3] is used, i.e., certain separation and truncation of divergent expressions.

As a result of the carried out calculations, it was shown that at inspected impact energies the second-order Born treatment is worse than the first-order one. Performed analytical estimates of some third-order Born terms also indicated insufficiency of the second-order treatment. For domination of the FBA contribution, which provides direct information about a target wavefunction, it is necessary to increase the impact energy value at least by three times. But this would considerably decrease the cross section values and thus would lead to experimental difficulties.

Fig. 1 shows the triple differential cross section (TDCS) of the H(e,2e)H^+ reaction within FBA (dashed line) and SBA (solid line).

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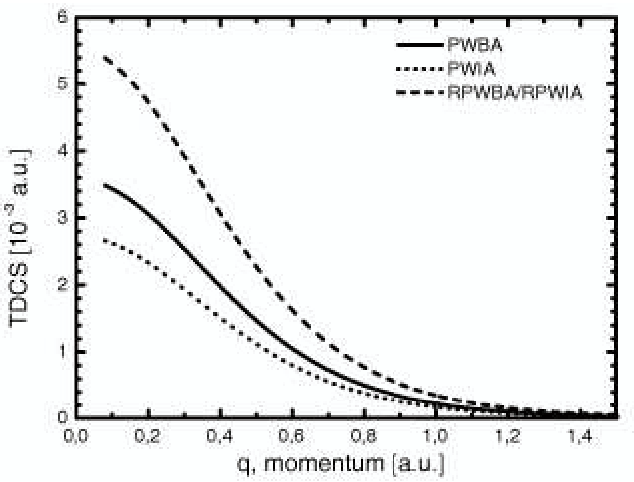
Tu1-30

(E,2E) REACTIONS NEAR THE BETHE RIDGE: AN ANALYSIS OF FIRST-ORDER MODELS

P.S. Vinitsky[*], K.A. Kouzakov[*], Yu.V. Popov [#] , C. Dal Cappello [§]

[*] Faculty of Physics, Moscow State University, Moscow 119899, Russia
[#] Nuclear Physics Institute, Moscow State University, Moscow 119899, Russia
[§] Université Paul Verlaine-Metz, LPMC, ICPMB (FR 2843), Institut de Physique,
1 rue Arago, 57078 Metz Cedex, France



We consider electron impact single ionization (the (e,2e) process) of an atom in the Bethe-ridge kinematics, where the momentum of the residual ion is small compared with the transferred momentum. Such a method is powerful for exploring the electronic structure of atomic systems [1]. Theoretically, it exploits dominance of the first-order term in the ionization amplitude, such as plane wave Born and/or impulse approximations (PWBA and/or PWIA), employing plane waves for the incident and outgoing electron states. Contributions of the higher-order plane wave terms are thus neglected. However, these terms are described by divergent integrals, which typically occur in perturbative approaches to Coulomb breakup scattering.

In this work, we revise the traditional PWBA and PWIA approaches, in the light of the aforementioned deficiency of the corresponding perturbation series. We employ a renormalization procedure proposed in [2] and results of a regularized multi-channel scattering theory for Coulomb potentials developed in [3]. Proceeding from the Lippman-Schwinger plane wave amplitude we regularize the corresponding Born series. A renormalized PWBA/RPWIA (RPWBA/RPWIA) model, depending on the employed regularization procedure, is introduced.

Fig. 1 shows the triple differential cross section (TDCS) for electron-hydrogen ionization in symmetric noncoplanar kinematics as a function of the recoil-ion momentum value [1] in the first-order models.

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Tu1-31

EXPLORING NUCLEAR STRUCTURE AND DYNAMICS BY ELECTRON CAPTURE

A. Pálffy, Z. Harman, A. Surzhykov, U. D. Jentschura, W. Scheid*

Max-Planck-Institut für Kernphysik, Heidelberg, Germany
(*) Institut für Theoretische Physik, Justus-Liebig-Universität Giessen, Germany

We investigate the resonant process of nuclear excitation by electron capture (NEEC), in which a free electron is trapped into a bound atomic shell with the simultaneous excitation of the nucleus. NEEC is a process analogous to dielectronic recombination (DR), and when followed by the radiative decay of the nucleus, is a competing resonant channel of radiative recombination (RR). Similar to other resonant recombination channels, NEEC can occur in highly-ionized plasmas with heavy ions and, therefore, might have relevant applications in astrophysical processes. Partly due to the RR background, NEEC has not been observed experimentally yet, although other experimental observations of atomic physics processes with regard to the internal structure of the nucleus have been reported, such as bound internal conversion [1] and nuclear excitation by electron transitions [2]. Theoretical studies of NEEC occurring in scattering measurements are therefore particularly useful in finding candidate isotopes with nuclear transitions suitable for experiments. In Refs. [3,4], total cross sections for NEEC followed by the radiative decay of the nucleus are presented. NEEC is expected to allow the determination of nuclear transition energies and probabilities, the study of atomic vacancy effects on nuclear lifetimes and population mechanisms of excited nuclear levels.

The measurement of the angular distribution of the emitted photons in the recombination process offers a useful method of discerning NEEC from RR [5]. With the help of a density matrix formalism, the angular distribution of the photons emitted in the radiative decay of the nucleus is derived. We present anisotropy parameters and angular distributions of the photons emitted in a radiative E2 decay of a nuclear state excited by the capture of the electron into the K shell of several bare ions. The angular pattern of the photon emission for NEEC can serve as a signature for the occurrence of this process.

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Tu1-32

ISOTOPICAL EFFECTS IN ELECTRON AND ATOM MOLECULE SCATTERING

S.A.Pozdneev

P.N.Lebedev Physical Institute, Department Quantum Radiophysics, Laboratory of Photochemical Processes, Leninskiy pr.53, 119924 Moscow, Russia

The principal difficulties in the investigation of the fundamental dynamic characteristics of few-body systems with three or more particles are associated with the multidimensionality of the problem and with the fact that real systems and processes do not agree with the approximations of well-known theories (perturbation theory, strong coupling, adiabatic theory, etc.). Thus, it is important to understand the physical meaning of numerous approximations applied to the few-body problem and their limitations. The following questions arise in this way.

1. What formalism should be used in investigation of the dynamics of a few-body system? It could be classical or quantum-mechanical equations of the motion, empirical or semi-empirical models, and so on.

2. What is the aim of the simulation? It can be a study of dynamic or static characteristics of a few-body system, calculations of the binding energy, cross sections, rate constants, thermodynamic features, etc.

3. Are the considered models adequate to real physical systems?

Answers to many of these questions can be found within the framework of the rigorous mathematical theory suggested by L.D.Faddeev, O.Ya.Yakubovsky and S.P.Merkuriev [1] which describes the dynamics of a few-body system using the correct mathematical basis.

For this reason we applied this formalism for the investigation of the different few-body processes based on the treatment of collision processes as many body processes, using Faddeev-Yakubovsky equations (FYE) in integral and differential forms[1-3].

In particular techniques based on FYE have been used successfully in studies of the dynamics of few-particle systems (bound-state properties and elastic, reactive and breakup scattering [2]. This is partly due to the increasing need for these cross sections in fields of pure and applied science.

The theoretical investigation of the collision of low energy electrons and atoms with diatomic molecules has emerged as a particulary rewarding field for the application of fundamental scattering theory as well as the common existence of strong threshold phenomena caused by the effect of long range electron molecular intersection potentials.

Investigation isotopical effects and resonant collisions of slow electrons and atoms with molecules set an urgent and challenging problem for contemporary theory [2-4].

The principal difficulty of this problem is due to two reason: strong interaction between the electron trapped in the intermediate resonance state and the heave particles motion, and the essentially multidimentionality character of this motion. Some of the most interesting phenomena arise from the connection of the electronic scattering dynamics with dynamics of nuclear motion in particular in processes rovibrational excitation, fragmentation and dissociation of the molecule.

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Tu1-33

FEW-BODY THEORY OF ELECTRON MOLECULE COLLISION

S.A.Pozdneev

P.N.Lebedev Physical Institute, Department Quantum Radiophysics, Laboratory of Photochemical Processes, Leninskiy pr.53, 119924 Moscow, Russia

The theoretical investigation of the collision of low energy electrons with diatomic molecules has emerged as a particulary rewarding field for the application of fundamental scattering theory as well as the common existence of strong threshold phenomena caused by the effect of long range electron molecular interaction potentials.

Investigation of resonant collisions of slow electrons with molecules set an urgent and challenging problem for contemporary theory. Some of the most interesting phenomena arise from the connection of the electronic scattering dynamics with dynamics of nuclear motion in particular in processes rovibrational excitation and dissociation of the molecule.

The collision processes in electron scattering with an initially rovibrational excited diatomic molecules H_2, HD, D_2, HCl, F_2, Cl_2, Br_2, I_2, DCl, HBr, N_2, Li_2, Na_2 are considered. Theoretically investigated the role of initially rovibrationally excitation of the diatomic molecules in the processes on the base of the quantum theory of few body scattering [1-2] are presented. Besides importance of the investigation of the DA of the lithium molecule are especially appropriate now due to several reasons:

- recent experimental observation reveal that the rate of Li^- formation by thermal electron impact on highly vibration exited Li_2 is $\sim 310^{-8} cm^3/sec$;

- the Li^- ions could possibly play, in the future, the same roles as have played by H^- ions for neutral beam formation;

- since lithium dimers are isovaleric with H_2, an investigation of the dependence of the DA to Li_2 on the initial rovibrational excitation of the molecule would be similar to the DA on H_2 [2,4].

The principal difficulty of this problem is due to next reasons:

- strong interaction between the electron trapped in the intermediate resonance state of the heavy particles;

- multidimensional character of the motion of the electrons and nucleus. That is why a method based on the treatment of the collision electron with the two-atom molecule as a three-body process again proposed for calculating the cross sections of the processes electron-molecule scattering. The interaction of the electron with each atom of the molecule as if they are simple field centers [2-4].

This approximation seems reasonable as long as energy of the electron is below the threshold of the electronic excitation of the molecule.

The results of calculation of the cross section of the electron molecule processes are compared with the available experimental data and with other calculations [2,4].

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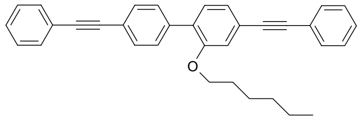
Tu1-34

INTERACTION OF LOW-ENERGY ELECTRONS WITH ORGANIC MOLECULES CONTAINING TRIPLE BONDS

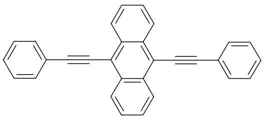
A.V. Kukhta[a], I.N.Kukhta[a], S.M. Kazakov[b], O.V.Khristophorov[b], V.A. Andreev[b],
O.L.Neyra[c], E.Meza[c]

[a] Institute of Molecular and Atomic Physics of the National Academy of Sciences of Belarus, Nezalezhnastsi Ave. 70, 220072 Minsk, Belarus, kukhta@imaph.bas-net.by
[b] Chuvash State University, Moskovski Ave. 15, 428015 Cheboxary, Russia
[c] Popular University of Cesar, Barrio Sabana, Campus Universitario, Valledupar, Colombia

There is poor information about electron-molecule interaction for organic compounds as compared to atoms and small molecules though they find manifold applications in molecular electronics, radiation chemistry, biology, and medicine. At least, the study of low-energy electron scattering with organic molecules gives the possibility to find the structure of vibrational and electronic levels including direct population of optically forbidden states. In this report the relative efficiency of excitation into singlet and triplet states in the region between 1.5 and 18 eV, their dependence on projectile electron energies for the scattering of monoenergetic electrons with tunable energies from 0 to 50 eV at an angle of 90°, for two organic electroactive molecules such as biphenylethenylbiphenyl derivative (DPDE) and biphenylethenylanthracene (DEA) in the gas phase are presented. The chemical structure of these molecules are presented below. Also such molecules are often used to study electrical conductivity through molecules and molecular wires. The spectrum of singlet and the positions of triplet transitions are studied using density functional theory techniques.



DPDE



DEA

A special electron spectrometer containing an electron gun and 127° electrostatic analyzer with channel electron multiplier were used for the energy loss spectra measurements. A monokinetic electron beam 1.5 mm in diameter is formed in 10^{-6} Torr vacuum; the electron beam current did not exceed 1 μA ; the full--energy resolution determined using elastic scattering peak was 0.3 eV. The organic vapor density in the collision cell was less than 10^{-3} Torr to avoid multiple collisions and secondary processes.

In electron energy loss spectra of DPDE intensive 1.3 and 1.7 eV peaks are observed. They decrease strongly with incident electron energy, confirming singlet-triplet nature of these transitions. In the optical absorption and the calculated spectra there are no any peaks in this region. It can be noted that high intensity of these peaks is comparable with singlet-singlet transitions as opposite to many π-conjugated organic compounds. The intensity of these transitions in DEA is essentially less than in DPDE. Moreover there are a number of intensive transitions in the range higher than 10 eV. The calculated spectra are in rather good accordance with experimental. The reasons of strong singlet-triplet transition in DPDE and contribution of triple bonds and other parts of the molecule are analyzed. The behaviour of singlet transitions at different projectile energies is usual as for other molecules.

Tu1-35

Ground state correlation and dynamical processes in fast ion-helium-collisions

M. S. Schöffler[1*], J. Titze[1], L. Ph. H. Schmidt[1], O. Jagutzki[1], T. Jahnke[1], R. Dörner[1],
H. Schmidt-Böcking[1], J. Walters[2], A. Godunov[3] and C. Whelan[3]

[1] Institut für Kernphysik, Universität Frankfurt, 60486 Frankfurt, Germany
[2] The Queens University of Belfast, Belfast, UK
[3] Old Dominion University, Norfolk, USA

Correlated many-particle dynamics in coulombic systems is one of the unsolved fundamental problems in AMO-physics. The recent development of the COLTRIMS technique (COLd Target Recoil Ion Momentum Spectroscopy) provides a coincident multi-fragment imaging technique for quasi snapshots of the correlated dynamics between electrons and nuclei. With a new experimental approach, using transfer ionization (P^{q+} + He -> $P^{(q-1)+}$ + He^{2+} + e), we accessed the question of ground state correlation effects with so far unprecedented completeness and precision. These transfer ionization studies in H^+, He^+ and He^{2+}-He collisions (40 – 630 keV/u) will be presented and the direct observation of bound correlated electron pairs will be discussed. We could distinguish between different ionization mechanisms and reveal the tiny non-s^2 contributions from helium groundstate [1,2].

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[*] electronic address: schoeffler@atom.uni-frankfurt.de

Tu1-36

ELECTRON-ION RECOMBINATION MEASUREMENTS OF IRON M-SHELL IONS MOTIVATED BY ACTIVE GALACTIC NUCLEI X-RAY ABSORPTION FEATURES

E. W. Schmidt, S. Schippers^{+}, C. Brandau§, D. Bernhardt, D. Yu*, A. Müller,
M. Lestinsky†, F. Sprenger†, J. Hoffmann†, D. A. Orlov†, M. Grieser†, R. Repnow†,
A. Wolf †, D. Lukić‡, M. Schnell‡, D. W. Savin‡

Institut für Atom- und Molekülphysik, Justus-Liebig-Universität Giessen, Germany
($^{+}$) email: Stefan.E.Schippers@iamp.physik.uni-giessen.de
(§) Gesellschaft für Schwerionenforschung (GSI), Darmstadt, Germany
(*) Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, P. R. China
(†) Max-Planck-Institut für Kernphysik, Heidelberg, Germany
(‡) Columbia Astrophysics Laboratory, Columbia University, New York, USA

Recent observations of active galactic nuclei (AGN) have shown a prominent absorption feature in the 15–17 Å bandpass [1]. This has been identified as an unresolved transition array (UTA) of $2p \rightarrow 3d$ inner shell absorption by iron ions with an open M-shell (Fe I–Fe XVI). This UTA can be be used as a powerful diagnostic tool for the absorbing material surrounding the AGNs' super massive black hole [2]. However, recent model calculations of the X-ray absorbing gas have failed to reproduce the shape of the UTA [3]. This has been attributed [4,5] to the fact that the available dielectronic recombination (DR) rate coefficients of iron M-shell ions, which are so far only known from theoretical calculations, are too low at the temperatures where these ions are formed in photoionized plasmas.

In a series of studies, aiming at providing reliable DR data for astrophysical modeling, we have measured DR rate coefficients of several iron M-shell ions ranging from Fe VIII to Fe XV using the ion storage ring TSR at the Max Planck Institute for Nuclear Physics in Heidelberg, Germany. Already in our first measurement for Fe XIV [6], we found unusually strong DR resonances at low electron-ion collision energies. The corresponding low-temperature plasma DR rate coefficient is orders of magnitude larger than the presently available theoretical results. This very recent finding has already stimulated new theoretical calculations [7]. Further results and their implications for astrophysics will be discussed.

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Tu1-37

COMPREHENSIVE CALCULATIONS OF ELASTIC, IONIZATION AND TOTAL CROSS SECTIONS FOR INERT GASES ON ELECTRON IMPACT

Minaxi Vinodkumar[1], Chetan Limbachiya[2], K. N. Joshipura[3], Nigel Mason[4]

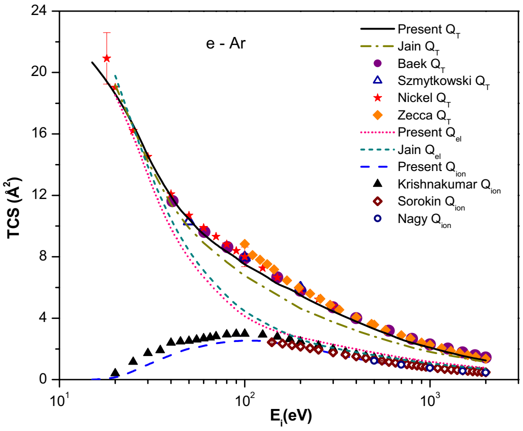
[1]V P & R P T P Science College, Vallabh Vidyanagar – 388 120, Gujarat, India
[2]P S Science College, Kadi - 382 715, Gujarat, India
[3]Department of Physics, Sardar Patel University, Vallabh Vidyanagar – 388 120, Gujarat, India
[4]Department of Physics & Astronomy, Open University, Milton Keynes, MK7 6AA, United Kingdom

Here we report comprehensive calculations covering total elastic Q_{el}, total ionization Q_{ion} and total (complete) cross sections Q_T for the impact of electrons on inert gases (He, Ne, Ar, Kr and Xe) at energies from circa threshold to 2000 eV. Theoretical and experimental studies on ionizing collisions of electrons have remained an important subject of interest in view of the applications of relevant cross-section data in various pure and applied sciences [1].

We have employed the well-known spherical complex optical potential (SCOP) formalism, through which the total elastic cross sections Q_{el} and its inelastic counterpart, Q_{inel} are obtained [2,3]. Q_{ion} may be estimated by defining a dynamic ratio of cross sections,

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)}, \text{ with a form, } R(E_i) = 1 - C_1\left(\frac{C_2}{U+a} + \frac{\ln(U)}{U}\right), \text{ where, } U = \frac{E_i}{I}$$

The parameters C_1, C_2, and a, reflect the properties of the target. This method is called our Complex Scattering Potential –ionization contribution, (CSP-ic) [2-4].



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Tu1-38

ELECTRON TRANSFER INTO FIXED-IN-SPACE HYDROGEN MOLECULES IN SLOW COLLISIONS

Sven Schössler, Lothar Ph. H. Schmidt, Lutz Foucar,
Horst Schmidt-Böcking, Reinhard Dörner

Institut für Kernphysik, J.W.Goethe Universität,
Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

The dissociative electron transfer $H_2^+ + He \rightarrow H_2^* + He^+ \rightarrow H + H + He^+$ has been studied at impact velocities below 1 a.u. The He^+ recoil ion has been measured using the COLTRIMS technique, while the two neutral hydrogen atoms of the projectile have been detected coincidentally on a position sensitive, multi-hit capable MCP detector with delay-line readout.

The cinematically complete measurement allows for the selection of the reaction channel where the fragments of the molecule as well as the He^+ target are in the electronic ground state. Inverse kinematics is used to present the data of this channel: a He atom then scatters at a H_2^+ molecule and transfers an electron. The orientation of the molecule at the time of the impact can be determined from the direction of the molecular breakup. For events where the molecular axis was orientated perpendicular to the beam axis, the measured diffraction pattern of the He^+ can be described as an interference of two spherical waves originated at the two nuclei of the molecule.

Tu1-39

LONG RANGE DISPERSION FORCES BETWEEN ATOMS AND DIATOMIC MOLECULES

M. Lysebo and L. Veseth

Department of Physics, University of Oslo, Norway

Accurate knowledge of long range (van der Waals) forces are very important for the study of cold collisions between atomic systems. For non-polar systems the interaction arises from induced dipole moments (dispersion). Hence, they may be derived from the polarizabilities of the individual systems. For two neutral atoms A and B with polarizabilities α_A and α_B the long range dispersion energy may be expressed as [1,2]

$$V(R) = -\frac{C_6}{R^6} \ ,$$

$$C_6 = \frac{3e^4}{\pi}\int_0^\infty \alpha_A(i\eta)\alpha_B(i\eta)d\eta \ ,$$

where the polarizabilities are given for imaginary frequencies $i\eta$ (real quantities). In a similar way the long range dispersion energy between a linear molecule and an atom takes the form

$$V(R,\theta) = -\left(C_6^{(0)} + C_6^{(2)}P_2(\cos\theta)\right)/R^6 \ ,$$

$$C_6^{(0)} = \frac{3\hbar}{\pi}\int_0^\infty \alpha_A(i\eta)\bar{\alpha}(i\eta)d\eta \ ,$$

$$C_6^{(2)} = \frac{\hbar}{\pi}\int_0^\infty \alpha_A(i\eta)\Delta\alpha(i\eta)d\eta \ .$$

The polarizabilities $\bar{\alpha}$ and $\Delta\alpha$ are given in terms of the parallel and perpendicular polarizabilities as

$$\bar{\alpha} = \frac{1}{3}(\alpha_\parallel + 2\alpha_\perp) \ ,$$

$$\Delta\alpha = \alpha_\parallel - \alpha_\perp \ .$$

The long range dispersion energy between two linear molecules may also be expressed in terms of their polarizabilities in a similar way [1,2].

The present work reports polarizabilities for atoms and diatomic molecules computed at imaginary frequencies by use of many-body perturbation theory. The many-body expansion is complete through fourth order, and is expected to yield polarizabilities of high accuracy. In the next step long range potentials are obtained by computing the van der Waals coefficients, as outlined above. Emphasis is put on atom-diatomic molecule interactions, which are of particular relevance for buffer gas cooling of molecules, and on diatomic-diatomic interactions. The present long range potentials are compared with results from direct calculations of potential surfaces by use of quantum chemistry program packages.

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Tu1-40

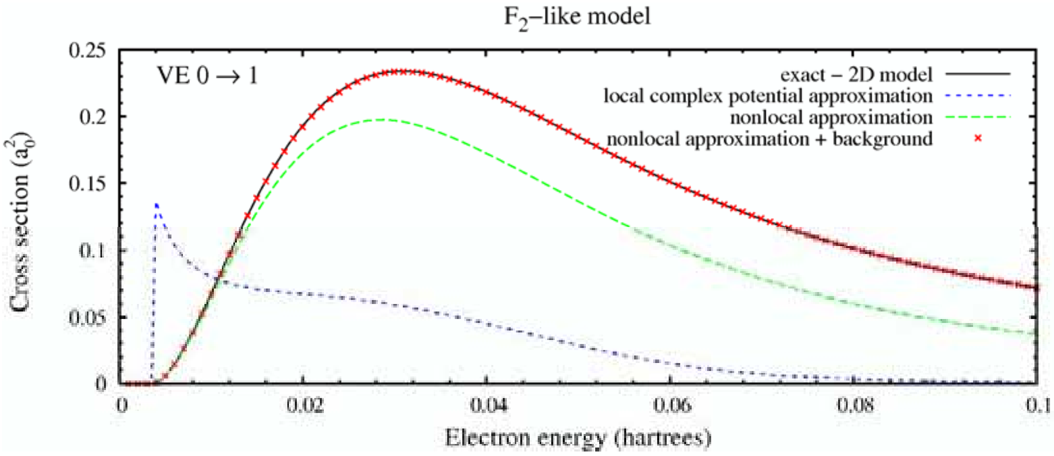
PROBING THE NONLOCAL APPROXIMATION TO NUCLEAR DYNAMICS OF RESONANT COLLISIONS OF ELECTRONS WITH DIATOMIC MOLECULES USING NUMERICALLY SOLVABLE MODEL

Karel Houfek[1], T.N. Rescigno[2], and C.W. McCurdy[2,3]

[1]Institute of Theoretical Physics, Faculty of Mathematics and Physics,
Charles University in Prague, Prague, Czech Republic
e-mail: houfek@mbox.troja.mff.cuni.cz
[2]Chemical Sciences, Lawrence Berkeley National Laboratory, Berkeley, USA
[3]Department of Applied Science and Department of Chemistry,
University of California, Davis, USA

The nonlocal approximation [1] to nuclear dynamics of low-energy resonant collisions of electrons with molecules was successfully applied to many diatomics, e.g. to hydrogen and nitrogen molecules, hydrogen halides etc (see for example [2] and [3]). The applicability of this approach to these processes was usually supported by a good agreement with experimental data but the underlying assumptions of the theory were never investigated in greater details because of the obvious difficulty of obtaining an exact solution of this many-body problem.

We show how some of these underlying assumptions can be tested using a simple model of the electron-molecule collisions with one electronic and one nuclear degree of freedom, which was introduced by the authors in [4]. The basic result of our investigation is that the "background" contribution to the cross sections can be significant not only in elastic scattering (as is usually assumed) but even in the inelastic collision such as vibrational excitation of the molecule F_2 (see figure).



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Tu1-41

Low-Energy electron scattering from Lithium and Potassium

S.Y. Yousif Al-Mulla
University of Borås, College of Engineering, Physics and Mathematics Group,
50190 Borås, Sweden.
E-mail : samir.al-mulla@hb.se

Abstract / Poster

Differential cross sections for the elastic scattering of electrons from the ground states of lithium and potassium have been calculated. Local density approximations to the exchange and correlation potentials have been used in these calculations, and it is confirmed that Hara exchange coupled with a Hedin-Lundqvist electron-gas-type correlation potential joined to an adiabatic polarization potential gives good predictions for differential cross sections.

A comparison of the calculated results with other experimental and theoretical data are presented and discussed.

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Tu1-42

ELECTRON-IMPACT IONIZATION TOTAL CROSS SECTIONS FOR H-, Li- AND Na-LIKE POSITIVE IONS

L. U. Ancarani [1] and P.-A. Hervieux [2]

[1] Laboratoire de Physique Moléculaire et des Collisions,
Université Paul Verlaine - Metz, 57078 Metz, France
[2] Institut de Physique et Chimie des Matériaux de Strasbourg,
GONLO, 23 rue du Loess, 67034 Strasbourg, France

In this contribution, we report on calculations of total cross sections for electron-impact direct ionization of the valence electron of several H-, Li- and Na-like positive ions. The frozen-core Hartree-Fock approximation is used to describe the target. It is also employed to extract two constant effective charges which are used in the collision model described in [1,2] : the non-relativistic Coulomb Born with exchange approximation (the choice of maximum interference is made [3]).
Comparison with theoretical and experimental data is made. Except for singly charged ions, for which we do not except a Coulomb Born model to work, our results are in very good agreement with other more sophisticated models (*e.g.* Distorted Wave [3] and Convergent Close-Coupling [4,5]). The overall agreement with experimental data is rather good.
For H-like ions, Thomson's [6] classical approach predicts that total cross sections scale as the square of the ionization potentials. This has been experimentally confirmed by Aichele *et al.* [7]. For alkali-like ions, this scaling law is seen to break down [2]. Within our simple Coulomb Born model, we have identified an approximate scaling law (with no fitting parameters) for total cross sections [1,2]. The latter is well verified by the best experimental data for Li-like, and to a lesser extent Na-like, ions of moderate ionic charge. A simple Lotz-type [8] fit.is then able to reproduce most of the experimental data.

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Tu1-43

RESONANCES IN LASER-ASSISTED ELECTRON-HYDROGEN SCATTERING

K.M. Dunseath, M. Terao-Dunseath

Equipe SIMPA, Laboratoire PALMS,
UMR 6627 CNRS-Université de Rennes1,
Campus de Beaulieu, F-35042 Rennes Cedex, France

The *R*-matrix Floquet theory [1] provides a rigorous, *ab initio* and non perturbative approach to laser-assisted electron scattering by a general atomic target. The method has already been applied to free-free processes during low-energy electron-helium scattering in CO_2 and Nd:YAG laser fields [2-4], and to the excitation of helium by simultaneous impact of an electron and several photons [5]. In this latter case, the excitation cross section is dominated by the He^- ($1s2s^2\ ^2S$) resonance situated just below the He ($1s2s\ ^3S$) threshold, which cannot be reproduced with for example the Kroll-Watson low-frequency approximation [6].

The description of electronic correlations in laser-assisted electron-hydrogen scattering is even more demanding. At low energies, the incoming electron can be captured temporarily by the target through emission of one or more photons, thus forming the ion H^-. This transitory state, which is completely absent in field-free scattering, gives rise to a sequence of resonances at low scattering energies, separated by integer multiples of the photon energy. We will present results concerning the evolution of these resonances with intensity as well as the frequency of the laser field.

At higher collision energies, the field-free scattering cross sections show series of Feshbach resonances converging on the n=2 excitation thresholds. In the presence of a laser field, each of these 'principal' resonances gives rise to a sequence of secondary resonances, again separated by integer multiples of the photon energy. We have studied the evolution of these resonances with increasing field intensity, and have shown in particular that there is an intensity at which a given resonance can be completely suppressed.

We also intend to present results for the simultaneous electron-photon excitation of the n=2 states at collision energies near threshold.

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THE PLANNED HITRAP FACILITY FOR EXPERIMENTS ON HEAVY HIGHLY CHARGED IONS

T. Beier[a], L. Dahl[a], S. Eliseev[a], F. Herfurth[a], B. Hofmann[b], O. Kester[a], H.-J. Kluge[a],
S. Koszudowski[a], C. Kozhuharov[a], G. Maero[a], W. Nörtershäuser[a], J. Pfister[a],
W. Quint[a], U. Ratzinger[b], A. Schempp[b], M. Vogel[a], G. Vorobyev[a], D. Winters[a],
and the HITRAP Collaboration

[a] *Gesellschaft für Schwerionenforschung (GSI), Planckstr. 1, 64291 Darmstadt*
[b] *University of Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt a.M., Germany*

Single particles in traps allow for clean investigations of basic interactions and also for the determination of fundamental constants. This has been demonstrated by investigations of Quantum Electrodynamics (QED) with respect to the g-factor of the free electron [1, 2] and of hydrogen-like carbon and oxygen [3, 4] which form the most precise determinations of the fine-structure constant and of the mass of the electron, respectively.

The trapping of hydrogen-like heavy ions up to uranium has not been performed so far because the production of U^{91+} requires either an EBIT with an operating voltage of about 350 kV or a heavy-ion accelerator with stripping and post-deceleration. At the HITRAP facility [5] at GSI, the final stage for deceleration and trapping of bare and hydrogen-like heavy ions up to uranium is currently under construction. After stripping, the ions will be decelerated down to 4 MeV/u in the Experimental Storage Ring (ESR) and further down to 6 keV/u by a combination of new IH and RFQ structures operating as decelerators. Finally, the ions will be captured and cooled down to cryogenic temperatures in a Penning trap by means of electron cooling and resistive cooling. From this trap, they can be extracted and used for experiments.

With this novel technique of deceleration, trapping and cooling of highly charged ions, atomic physics studies on slow highly charged ions up to uranium U^{92+} interacting with photons, atoms, molecules, clusters, and surfaces will be performed. In addition to collision studies, high-accuracy atomic physics experiments on trapped HCI will be a significant part of the atomic physics program of the HITRAP facility. At the GSI Future Facility FAIR, the HITRAP facility will serve as a low-energy source of antiprotons and radioactive ions. HITRAP will form an integral component of both the SPARC as well as the FLAIR Collaborations for low-energy experiments with antiprotons and heavy ions [6, 7]. This work was supported by the European Union within the RTD programme (HPRI-CT-2001-50036 HITRAP).

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Tu1-45

ENERGY APPROACH TO QED THEORY OF CALCULATING THE ELECTRON-COLLISION STRENGTHS AND RATE COEFFICIENTS

A.V.Glushkov, A.V. Loboda, D.A.Sukharev and T.A.Florko

Odessa University, P.O.Box 24a, Odessa-9, 65009, Ukraine-Russia

The X-ray laser problem has stimulated a great interest to development of theoretical methods for modelling the elementary processes in a collisionally pumped plasma. The shocking example is a scheme for accomplishing tabletop x-ray lasing in Li-like ion of Ne at 98 Å in an optically ionized plasma during recombination in the transient regime (Lawrence Livermore Nat. Lab.; Univ. of California). Saturation effects and parametric heating processes by stimulated Raman scattering are analyzed and found to allow energy efficiencies in excess of 10^{-5} for a 100-fsec duration, 0.25-μm laser driver of intensity 10^{17} W/cm^2. Two key theoretical problems must be solved in order to develop a special code and to predict necessary plasma parameters needed for X-ray lasing: i). Highly accurate definition of the rate coefficients for plasma elementary processes that are responsible for the forming emission lines spectra; ii).Developing new exact kinetics calculation schemes for defining the level populations, inversions, line intensities, gain coefficients at definite plasma parameters. The most consistent approach to problem is based on QED. Here the generalized energy approach in gauge invariant scheme [1] is used for consistent QED describing elementary processes in collisionally pumped laser plasma. We develop an optimal scheme for calculation of the electron-collision strength and rate coefficients for the de-excitation (excitation) processes in the Ne-like multi charged ions plasma with estimating optimal plasma parameters for X-ray lasing. We applied our approach to estimate of the electron collisional excitation cross-sections and strengths for Ne-and Ar-like ions. In table 1 we present calculated and measured electron-collisional excitation cross-sections σ for Ne-like barium for two values of incident electron energy 5.69keV and 8.20 keV. For comparison we present also the measured values σ and calculated ones within other schemes [1,2].

Level J	Measured Marrs etal [2]	Calculated Ivanov etal [1]
Sum (J=0)	2,50±0,35	2,48
2p$_{3/2}$3d$_{5/2}$ 1	3,98±0,56	3,20
2p$_{1/2}$3d$_{3/2}$ 1	2,12±0,30	1,78
Level J	Calculated Reed [2]	Calculated Present Paper
Sum (J=0)	2,60	2,51
2p$_{3/2}$3d$_{5/2}$ 1	3,56	3,42
2p$_{1/2}$3d$_{3/2}$ 1	2,00	1,88

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Tu1-46

RESONANT CHARGE EXCHANGE CROSS-SECTIONS OF IONS IN HELIUM, NEON, ARGON, KRIPTON, XENON, RUBIDIUM, CESIUM, MERCURY

S.A. Maiorov

A.M. Prokhorov General Physics Institute of RAS, Moscow, 119991, Russia

The motivation for the work reported is to improve the resonant charge transfer cross-sections to precision of experimental data of ion mobility in parent cases at weak electric field □ 1%. We are particularly interested here with ions **He, Ne, Ar, Kr, Xe, Rb, Cs, Hg** [1].

A model of ion collisions with gas atoms is constructed with allowance for the ion resonant charge exchange, the polarization interaction, and the elastic (gas-kinetic) interaction. On the basis of experimental data on ion mobility and the results of simulation of ion collisions with parent gas atoms in a homogeneous electric field, the approximations of the ion resonant charge exchange cross sections for noble gases were fitted which are applicable for the description of the ion drift in any fields. The model of molecular ion mobility in a gas was constructed which provides the discharge characteristics in moderate fields at low temperatures.

The proposed algorithm allows obtaining the ion drift velocity for a given charge exchange cross section. The obtained approximation is based on the choice of the physically grounded dependence $\sigma_{res}(\varepsilon) = \sigma_{res}(\varepsilon_1)[1 + a\ln(\varepsilon_1/\varepsilon)]^2$ for which two fitting constants, $\sigma_{res}(\varepsilon_1)$ and a, are necessary. To determine them, one can use some two known values of the resonant charge exchange cross section. One of them was the value of $\sigma_{res}(\varepsilon_2)$ for $\varepsilon_2 = 10000$ eV, becouse the accuracy of the data on cross sections is high for high energies. The second value of the resonant charge exchange cross section was chosen from the condition that this algorithm should reproduce the mobility and diffusion coefficients known to high accuracy for low fields.

The approximation dependences of charge exchange cross sections are tabulated: $\sigma_{res}(\varepsilon) = \sigma_{res}(\varepsilon_1)[1 + a\ln(\varepsilon_1/\varepsilon)]^2$, in table are presented approximation parameters. Cross sections in unit 10^{-16} cm^2, $\varepsilon-$kinetic energy at eV, $\varepsilon_1 = 1$ eV.

System	$\sigma_{res}(\varepsilon_1)$	a
He^+- He	*27.9*	*0.0557*
Ne^+- Ne	*29.0*	*0.060*
Ar^+ - Ar	*55.3*	*0.0543*
Kr^+-Kr	*61.2*	*0.0497*
Xe^+-Xe	*84.2*	*0.046*
Rb^+- Rb	*247*	*0.024*
Cs^+- Cs	*295*	*0.025*
Hg^+ - Hg	*164*	*0.052*

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Tu1-47

ATTOSECOND TIME-SCALE MULTI-ELECTON COLLISIONS IN THE COULOMB FOUR-BODY PROBLEM: IMPRINTS ON DOUBLE AND SINGLE ENERGY DIFFERENTIAL CROSS SECTIONS

Agapi Emmanouilidou[1]
[1] *ITS, University of Oregon, Eugene, Oregon 97403-5203*
agapi@uoregon.edu

Using a quasiclassical formulation we have recently treated theoretically the triple proto-ionization from the ground state of Lithium, for a wide range of energies [1]. Our results for the total photoionization cross section were found to be in very good agreement with experimental results [2] as well as theoretical ab-initio ones. An important finding of our work is a classification scheme which organizes the triply photo-ionizing trajectories in groups according to the respective sequence of electron-electron collisions [3].

The collision sequences in triple ionization of Li take place on an attosecond time scale. While the first collision, in each ionization path, occurs around a couple of attoseconds after photoabsorption the second collision takes place around 70 attoseconds. The advancement of ultra-short laser science and its so far success in exploring and controlling electronic motion renders a future direct experimental verification of our collision sequences possible. These electron-electron collision sequences manifest themselves not only on the level of single trajectories but most importantly on the level of ensemble averages. As we have very recently shown, the two main collision sequences the three electrons follow to ionize have unique traces in the classical probability densities [4].

Furthermore, our classification scheme can explain the electronic angular correlation probability in terms of the dominant “T-shaped” pattern of the three escaping electrons [3] for excess energies close to threshold. The angular correlation probability is not yet know experimentally but should be measurable with state of the art experimental techniques. Besides, the above single differential cross sections, we have very recently formulated quasiclassically the double energy differential cross sections [5]. For large energies (the only energies currently treated by ab-initio calculations) we have very good agreement with ab-initio results. For small energies we discuss the structure of the double and single energy differential cross sections and show how this structure bares the imprint of the “T-shaped” pattern of the three escaping electrons and thus of the electron-electron collision sequences.

Finally, applying our collision scheme for the five-body Coulomb problem we discuss the collision pathways the four electrons follow to escape in the quadruple photoionization of Beryllium. We also discuss the dominant angular patterns of the four escaping electrons for energies close to threshold.

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Tu1-48

MONTE-CARLO SIMULATIONS OF THE RELAXATION OF EXCITED ELECTRONS IN SWITH HEAVY ION TRACKS

A.E. Volkov*, N.A. Medvedev

Russian Research Centre 'Kurchatov Institute', Kurchatov Sq.1, Moscow, 123182,
Russia, (*) volkov@dni.polyn.kiae.su

Swift heavy ions (SHI) with energies more than 1 MeV/amu, and masses more than 20 proton masses lose the most part of their energy by the excitation of the electronic subsystem of irradiated targets. The density of the energy deposited during 10^{-17} s in the vicinity of one nanometer from the trajectory of such projectiles can achieve extremely high values up to 50-70 keV/nm. Subsequent energy transfer to the lattice stimulates nanometric structure and phase transformations along the trajectory. Elastic recoils produce orders of magnitude lower damage to provide the observed structure modifications [1].

Having the energy up to 50 keV, δ-electrons generated due to ionization of target atoms by a projectile can produce ionization cascades resulting in non-equilibrium ionization states of deep atomic shells in the nanometric vicinity of the ion trajectory. Peculiarities of the kinetics of spatial expansion and relaxation of the electronic excitations determine the energy transfer to the lattice.

We made MC simulations for gold and quartz in order to investigate this kinetics. We observed ballistic expansion of excited electrons in the perpendicular direction from the projectile trajectory up to one tenth of picosecond from the projectile pass when the front position moves away up to two hundred nanometers. Such expansion can not be described in the framework of usually used thermodiffusion model. It was discovered that more than 30 percents of the energy deposited by the ion are converted to long living ionization states which life times are much larger than the cooling down time (10^{-14} s) of the delocalized electrons. The most part of this conserved energy is concentrated in the nearest ten nanometers from the projectile trajectory. It was observed that considerable energy is transferred to the lattice during times which are much shorter than that of the electron-phonon coupling. At time scales shorter than a picosecond the solid dynamics can not be described by collective atomic oscillations because no phonons can appear. This results in deviation of the energy relaxation mechanism from that predicted by the electron-phonon coupling [2].

Our simulation obviously indicated that models based on the conceptions of the local equilibrium, temperature and thermo-diffusion (ionization equilibrium, two-temperature thermal spike [3]) can be hardly applied to the subpicosecodn temporal scale of relaxation of the electronic subsystem in nanometric SHI tracks.

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Electron impact single ionization of Na, Mg, K and Ca atoms- A Comparative Study

G. Purohit[1], U. Hitawala and K. K. Sud

[1]Department of Physics, Faculty of Engineering & Technology
Mody Institute of Technology and Science
Lakshmangarh-332311, Dist- Sikar, Rajasthan, India

Department of Physics, University College of Science
M L S University, Udaipur-313002, India

e-mail: g_vpurohit@yahoo.com

Abstract. The ionization of atoms, ions and molecules by electron impact are the basic processes of atomic and molecular physics, with fundamental applications in different areas as fusion physics, plasma physics, advanced fusion technologies, condensed matter physics, surface science etc. Electron coincidence experiments in which an incoming electron knocks out a bound electron in a collision with target and the two outgoing electrons are then detected in coincidence with defined kinematics are known as (e, 2e) experiments. Extensive studies of (e, 2e) processes have been reported on various targets including hydrogen, helium and rare gases [1-2]. Recently, Purohit et al [3-4] have calculated triple differential cross sections (TDCS) and spin asymmetry in (e, 2e) processes for lithium like ions and helium like ions using distorted wave Born approximation (DWBA) formalisms. We present in this communication the results of our calculation of TDCS in (e, 2e) processes for alkali targets Na and K and alkaline earth targets Mg and Ca atoms in coplanar symmetric geometry. We have performed the calculation in DWBA formalism using spin averaged static exchange potential. We compare the results of our calculation of TDCS for the above-mentioned targets with the available experimental data [5-6]. We will discuss silent features of the electron impact ionization of alkali and alkaline earth targets. The effects of incident electron energy, distortion, polarization will also be discussed for the alkali and alkaline atoms investigated by us

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Tu1-50

DISSOCIATIVE RECOMBINATION OF POLYATOMIC IONS AND FREE ELECTRONS

J. Öjekull[1], P.U. Andersson[1], H. Danared[3], A.M. Derkatch[4], M.B. Någård[2],
J.B.C. Pettersson[1],. A. Neau[4], S. Rosén[4], R.D. Thomas[4], M. Larsson[4], J. Semaniak[5],
A. Källberg[3], N. Markovic´[6], M. af. Ugglas[3] and F. Österdahl[4]

[1]Department of Chemistry, Atmospheric Science, Göteborg University, Sweden
[2]Physical and Computational Chemistry, DMPK and Bio-analytical Chemistry, AstraZeneca R&D Mölndal, Sweden
[3]Manne Siegbahn Laboratory, Stockholm University, Sweden
[4]Department of Physics, Stockholm University, AlbaNova University Center, Sweden
[5]Institute of Physics, Pedagogical University, Poland
[6]Department of Chemistry and Bioscience, Chalmers University of Technology, Sweden

Dissociative recombination (DR) is a binary process involving a molecular ion and an electron. The electron energy has to be lower than a few eV in order for the reaction to take place. In the D-region of the terrestrial atmosphere (60 – 85 km) cluster ions exist in a weak plasma with free electrons and electron–ion recombination is expected to be the principal mechanism for removal of the ions [1]. Hydrated ions are present in large abundance and they have been suggested to act as condensation nuclei in the formation of *nuctilucent clouds* via ion-induced nucleation [2]. We will present DR studies of ammonium cluster ions $H^+(NH_3)_n$ and $D^+(ND_3)_n$, n = 1-3, and water cluster ions $H^+(H_2O)_n$ and $D^+(D_2O)_n$, n=1 - 3. The experiments have been performed at the heavy-ion storage ring CRYRING at the Manne Siegbahn Laboratory, Stockholm University, Sweden. Long storage times due to very low pressure (~ 10^{-11} Torr) ensures for vibrationally cooled ion beams with narrow momentum spread, low divergence and a small cross-sectional area. Multiple passages through the interaction region and an ability to smoothly vary the interaction energies between ions and electrons from a few meV to tens of eV made it possible to determine DR cross sections, as well as thermal rate coefficients, in the corresponding range. Branching ratios between energetically allowed fragmentation channels have also been determined. The results will be compared with earlier work and the effect of cluster size on the DR rate will be discussed.

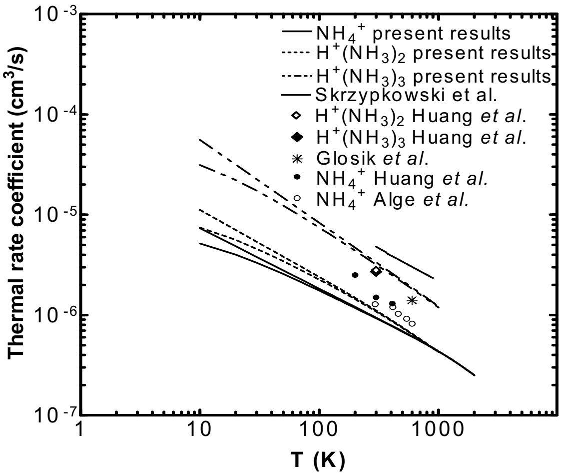

Fig. 1. Comparison between experimental and literature thermal rate data for ammonium cluster ions. Thermal rate coefficients for storage ring experiments for NH_4^+, $H^+(NH_3)_2$ and $H^+(NH_3)_3$ as a function of electron temperature.

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Tu1-51

THE CAPTURE OF NEGATIVE MUONS BY ATOMS: ENERGY APPROACH

Khetselius O.Yu. and Dubrovskaya Yu.V.

Odessa University, P.O.Box 24a, Odessa-9, 65009, Ukraine

Relativistic ab initio method [1] is used for calculating the cross-sections of the negative muon capture by atoms within a consistent energy approach in the QED theory. The Auger capture part of energy shift *Im ΔE* appears first in the second order of the atomic perturbation theory (fourth order of the QED perturbation theory) in the form: $Im\Delta E=\pi G(\varepsilon_{iv},\varepsilon_{ie},\varepsilon^{\mu}_{in},\varepsilon^{\mu}_{fk})$. Indices *e,v* are coresponding to atomic electrons. Here *G* is a definite squired combination of the two-particle matrix elements. The value $\sigma=-2\ Im\Delta E$ represents the capture cross-section if the incident muon eigenfunction is normalized by the unit flow condition. Results of calculating the cross-section of the μ^- capture by He are obtained (fig.1.).

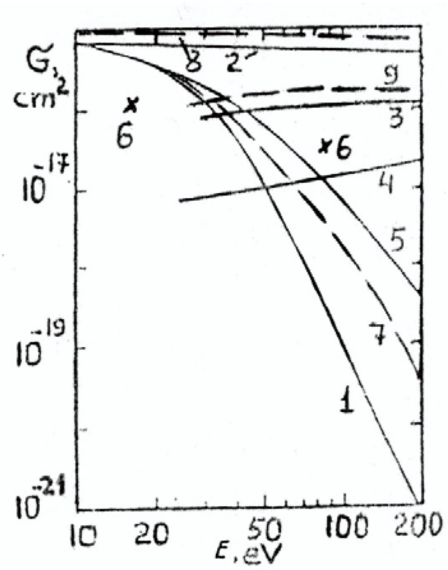

Fig1. The cross-section of the Auger capture, elastic and inelastic scattering, obtained within the Hartree-Fock method (curves 1,2,3), cross-section of the inelastic scattering by Rosenberg (curve 4), cross-section of the Auger capture by Copenman and Rogova (curve 5), the transport cross-section (cross symbol) [1] and the muon capture, elastic and inelastic scattering (present paper; dotted line curves 7,8,9 respectively).

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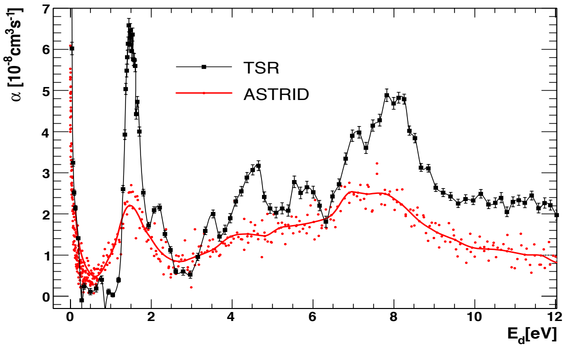
Tu1-52

FRAGMENTATION STUDIES OF CF^+ IN COLLISIONS WITH ELECTRONS

O. Novotny, S. Novotny, J. Hoffmann, M. Mendes, H. Buhr, B. Jordon-Thaden,
M. Lange, A. Petrignani, D. Bing, M. Berg, C. Krantz, A.S. Jaroshevich*,
M. Lestinsky, D.A. Orlov, H. Fadil, A. Wolf

Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany
*Institute of Semiconductor Physics, 630090 Novosibirsk, Russia



Collisions of molecular ions with low-energy electrons imply several types of reactions important in a variety of plasma environments. Dissociative recombination (DR) in particular is usually the main neutralization channel controlling ionization states and chemical composition. This also holds for the DR of CF^+ in CF_4 plasmas, commonly used in microelectronics processing to dry-etch features into silicon wafers [1]. Also, it was shown recently [2] that DR rate of CF^+ is a key parameter for fluorine chemistry in cold interstellar medium. Absolute rate coefficients and their temperature dependencies are therefore needed for meaningful modeling of such plasma environments. Energy dependent DR rates and kinetic energy releases of neutral products indicate the coupling of excited ion states to states of the neutral molecule. The knowledge of further details, such as angular dependency of the DR rate, the branching ratios between dissociative channels, and their energy dependency, contributes to comprehensive theoretical insight into molecular structure and reaction dynamics.

The DR of CF^+ has been investigated at the heavy-ion Test Storage Ring (TSR) in Heidelberg. The twin electron beam configuration with an electron cooler and a separate electron target for collision measurements, allows efficient phase-space cooling of the heavy (mass 31) molecular ions at 3 MeV and, correspondingly, unprecedented high collision energy resolution at the electron target with electron beam temperatures of $T_{\parallel} = 0.4$ meV and $T_{\perp} = 5.4$ meV in longitudinal and transverse direction, respectively. The DR measurements were performed by mass selective counting of neutral products at distance ~12 m from the reaction zone. The figure displays the obtained DR rate coefficient (absolute rate coefficient scale preliminary) in range of relative energies of 0-12 eV in comparison to the previous measurement [3] at the ASTRID storage ring. The DR rate coefficient displays highly resolved structure at ~1.5 eV and above 3 eV which is expected to rise due to indirect DR process through neutral Rydberg states lying below excited states of CF^+. Further improvement of the energy resolution is expected by using a photocathode providing electrons at $T_{\parallel} = 25$ μeV and $T_{\perp} = 0.5$ meV. Neutral fragments have been also investigated by upgraded 3D-imaging system providing branching ratios of particular dissociation channels and their angular dependence. Strong anisotropy has been observed at non-zero relative energies.

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Tu1-53

Asymptotic Green function Approximation to e^--He Scattering

S. N. Tiwary
University Department of Physics
BRA Bihar University, Muzaffarpur, Bihar, India
e-mail: sntiwaryin@yahoo.com

A number of different theoretical approaches to electron-atom or electron-molecule scattering problems have been introduced which have the interesting feature of including a large number of channels. In contrast to a method like the close-coupling approximation, an R-matrix method which treats a small number of channels exactly, methods such as the Glauber approximation, the eikonal-Born series methods, and the second-order potential method include all channels, but in an approximate way.

The close-coupling method is successfully applied to the scattering of electrons or positrons by atoms, molecules, and ions. The total wave function for an (N +1)-electron system consists of an N-electron system consists of an N-electron target's eigenfunctions and a set of unknown functions representing the integro-differentials (ID) equations which are derived from the vibrational principle. If it were possible to retain an infinite number of terms in the expansion (including the open channel) the close-coupling method would yield the exact solutions to the physical problems. In practice, a finite number of terms are retained. In many cases the convergence is very slow and many equations have to be solved which makes the close-coupling (CC) method complicated from the computational point of view. In the light of the convergence as well as the cumbersome computational problem we[1] have proposed a new linear-algebraic approach to electron-atom scattering which allows the incorporation of any number of target states in order to achieve regular and systematic improvement of results. Our method is based on an asymptotic Green's-function approximation (AGFA).

We have performed calculation for the excitation of the $2p_m$ states of the helium atom by electron impact for λ, χ, and $d\sigma/d\Omega$ within our asymptotic Green function approximation, and the results are compared with the experimental observations and other theoretical predictions. Agreement between our calculated results and experimental data is reasonably good. Results will be presented in the conference.

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ANGULAR DEPENDENCE IN THE DISSOCIATIVE RECOMBINATION PROCESS OF HD^+

S. Novotny, H. Rubinstein[1], H. Buhr, J. Hoffmann, M. Mendes, O. Novotny,
D.A. Orlov, M. Berg, B. Jordan-Thaden, A.S. Jaroshevich[*], C. Krantz, M. Lestinsky,
A. Petrignani, I.F. Schneider[#], D. Shafir[1], M. Lange, D. Zajfman[1],
D. Schwalm, A. Wolf

Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany
[1] Department of Particle Physics, Weizmann Institute of Science,
Rehovot, 76100, Israel
[*] permanent address: Institute of Semiconductor Physics, 630090 Novosibirsk, Russia
[#] permanent address: University of Le Havre, 25, rue Philippe Lebon, P.O.B. 540,
76058, Le Havre, France

In low density ionized media molecular cations are exposed to one of the most effective neutralization reactions, the process of dissociative recombination (DR). Caused by the capture of an electron the molecular cation forms a highly excited neutral state before it dissociates into neutral fragments with certain final states and possible kinetic energy. Because of the importance of the DR process in interstellar media, the higher atmosphere, and various laboratory plasma, interest in its studies both theoretically and experimentally has risen in the past decades (see for example [1]). While the DR rate and the branching ratios of the escaping fragments have been studied intensively, the dependence of this process on the angle between the incoming electron and the molecular axis found less attention so far.

At the heavy-ion test storage ring (TSR) in Heidelberg, Germany, the DR process is studied in a new twin-merged-beam configuration where the ion beam is phase-space cooled continuously by one electron cooler device, while a second device, equipped with a GaAs-photocathode [2], provides electrons with low transversal and longitudinal electron temperatures for the DR process at precisely tuneable collision energies. The fragment distances are then recorded downstream of the interaction region by a new high resolution fragment-imaging detector.

The infrared active molecular ion HD^+, serving as a benchmark system in theoretical calculations, was chosen to investigate the angular distribution on a dense grid of energies between 10 and 80 meV. With only one final state being accessed at these energies, the observed fragment distance distribution can be analysed precisely with regard to angular distribution and to contributions from individual rotational levels of HD^+.

The results show a strong energy dependence of the angular distribution. The anisotropic character described by Legendre polynomials changes rapidly even over small energy steps and partly varies on a likewise narrow energy scale as the DR rate coefficient. Also the relative DR contributions from the HD^+ rotational levels show distinct energetic structures. The ensemble of these data reveals new aspects of the DR process of HD^+ at low energies.

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Tu1-55

Cross-section and rate coefficient calculation for electron impact excitation, ionisation and dissociation of H_2 and OH molecules

R. Riahi[1], Ph. Teulet[2], Z. Ben Lakhdar[1], and A. Gleizes[2]

[1] Laboratoire de Spectroscopie Atomique, Moléculaire et Applications, Département de Physique, Faculté des Sciences de Tunis,
Université de Tunis El Manar, 1060 Tunis, Tunisia
[2] Centre de Physique des Plasmas et Applications de Toulouse, UMR CNRS 5002,
Université Paul Sabatier Toulouse 3,
118 route de Narbonne, 31062 Toulouse Cedex 09, France

Abstract

The weighted total cross-section (WTCS) theory [1] is used to calculate electron impact excitation, ionisation and dissociation cross-sections and rate coefficients of OH, H_2, OH^+, H^+_2, OH^- and H^-_2 diatomic molecules in the temperature range 1500–15000 K. Calculations are performed for H_2(X, B, C), OH(X, A,B), H^+_2 (X), OH^+(X, a, A, b, c), H^-_2 (X) and OH^-(X) electronic states for which Dunham coefficients are available. Rate coefficients are calculated from WTCS assuming Maxwellian energy distribution functions for electrons and heavy particles. One and two temperature (θ_e and θ_g respectively for electron and heavy particles kinetic temperatures) results are presented and fitting parameters (a, b and c) are given for each reaction rate coefficient: $k(\theta) = a(\theta^b) \exp(-c/\theta)$.

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Tu1-56

Ab initio treatment of H^++N_2 collisions

L. F. Errea, L. Méndez, I. Rabadán and A. Riera

Laboratorio asociado al Ciemat de Física atómica y molecular en plasmas de fusión.
Departamento de Química, Universidad Autónoma de Madrid, 28049-Madrid, Spain

The H^++N_2 collisional system is of particular relevance to model the proton auroral precipitation into the Earth's upper atmosphere [1,2]. While this system has been studied in a number of experimental works (see references in [2]), it has received very limited attention from the theoretical side.

Using a multi-reference configuration interaction method, we have calculated the potential energy curves of the first ten electronic states of $(HN_2)^+$ (see figure 1), and the non-adiabatic couplings between them. The cross sections for the charge transfer, electronic and vibrational excitation processes are obtained by employing the eikonal [3] approximation to describe the projectile motion, while the vibrational degree of freedom of the target molecule is treated using the sudden approximation [4]. Dynamical calculations will be presented at the conference.

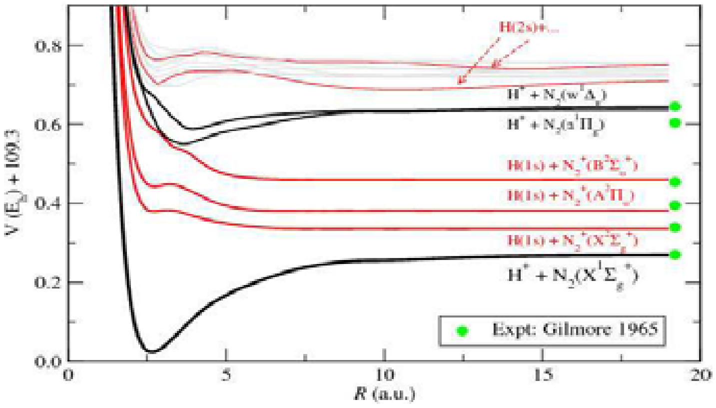

Figure 1: Electronic energies as functions of the projectile-target distance. The N-N distance is 2.08 bohr, and the angle between the projectile position and the N-N internuclear vectors is 45°.

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Tu1-57

QUANTUM HYDRODYNAMICS CALCULATIONS OF THE STOPPING CROSS SECTION OF H^0 FOR 1 keV - 2 MeV PROTON AND ANTIPROTON IMPACTS.

Mario M. Jakas

Departamento de Física Fundamental y Experimental, Electrónica y Sistemas.
Universidad de La Laguna, 38205 La Laguna. Canary Islands. Spain.

The so-called quantum hydrodynamics method (QHDM) [1], or quantum fluid dynamics approach (QFD) [2], is used to calculate the electronic stopping cross section (S_e) of atomic hydrogen for energetic protons and antiprotons projectiles. The results in this paper show that the S_e's so obtained, appear to be in good agreement with previous calculations and experimental data as well. Since the utilisation of quantum trajectories is a key feature of the QHMD, the "motion" of the electron during the collision can be readily analysed. In this way, one can observe several aspects of the electron dynamics during scattering which may help to improve our understanding of the stopping process.

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Tu1-58

Theory of electron collisions with polar molecules

Roman Čurík[1] and David Field[2]

[1]J.Heyrovský Institute of Physical Chemistry, Dolejškova 3, Prague 8, Czech Republic
[2]Institute for Physics and Astronomy, Aarhus University, DK-8000 Aarhus, Denmark

The phenomenon of low energy rotationally inelastic scattering by electrons was first observed in Randell *et al* 1993 and data on a variety of molecules may be found for example in Field *et al* 2001. These results are of fundamental theoretical interest and also have numerous potential applications in atmospheric, interstellar and man-made plasmas. We developed a theory for the interaction of electrons with polar species, extending methods in Mittleman *et al* 1965 and Greene *et al* 1985. In our work we show how state-to-state rotationally inelastic cross-sections may be derived from experimental cold electron scattering data for polar molecules, using H_2O as an example. Fig. 1 shows state-to-state inelastic cross sections extracted from the experimental data.

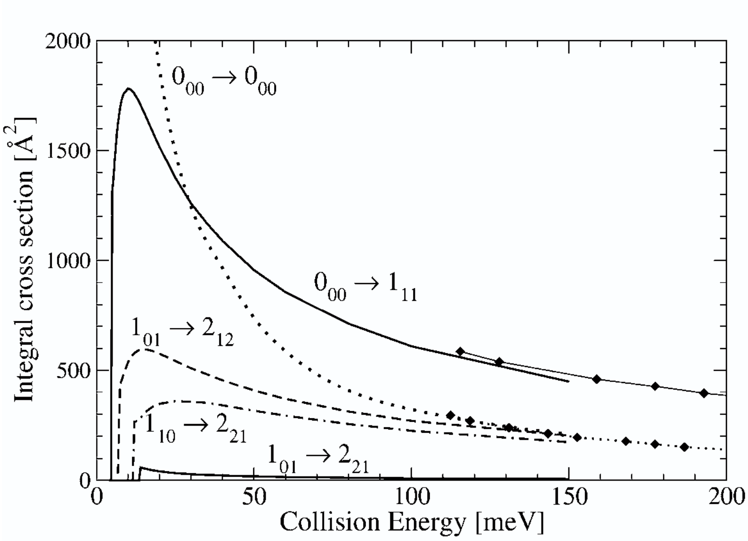

Figure 1: Selected state-to-state integral cross-sections for rotational excitation of the H_2O molecule determined from experimental data. Full curves represent results for para-H_2O and dashed for ortho-H_2O.The dotted curve represents elastic scattering for para-H_2O in its lowest rotational state. Curves with diamonds show the results of R-matrix calculations in Faure *et al* 2004.

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Tu1-59

Partially integrated differential cross sections of e+Ca scattering

Sergey Gedeon, Viktor Gedeon, Vladimir Lazur† and Ludmila Bandurina‡

†Department of Theoretical Physics, Uzhgorod National University, 88000, Ukraine
‡Institute of Electron Physics, Uzhgorod, 88017, Ukraine

The *B*-spline *R*-matrix method [1] is used to investigate differential cross sections (DCS) of elastic electron scattering from neutral calcium in the low-energy range from threshold to 3 eV. The close-coupling expansion includes 39 bound states of neutral calcium, covering all states from the ground state to $4s8s\ ^1S$ (see also [2]).

In Fig. 1a the calculated function $S(E)$, upper solid curve,

$$S(E)=\int_{\theta_1(E)}^{\theta_2(E)}\frac{d\sigma}{d\Omega}d\Omega\ , \quad (1) \qquad \begin{aligned}\theta_1(E)&=\sin^{-1}[(k_1/E)^{1/2}],\\ \theta_2(E)&=\sin^{-1}[(k_2/E)^{1/2}]\end{aligned} \quad (2)$$

is compared with the measured data [3] (square scatter) and theoretical results [4] (dot-dashed curve) obtained at k_1=0.482, k_2=0.508. The relative experimental data were normalized to the theoretical value of $S(E)$ at E = 1.8 eV. The calculations of $S(E)$ were carried out also at other sets values k_1 and k_2, among other things at k_1=1.260, k_2=1.274 (Fig. 1a, lover solid curve). Figure 2 exhibits the elastic DCS used to calculate the function $S(E)$. The significant structure DCS suggests that the elastic DCS might serve as a sensitive test when comparing theory and experiment.

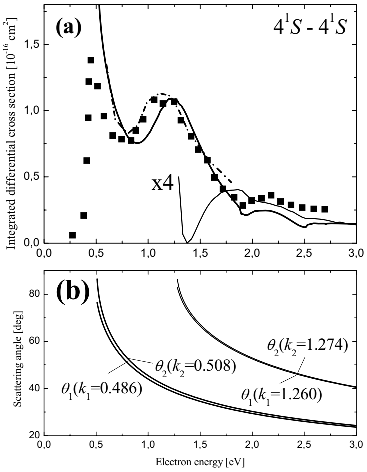

Fig. 1. (a) Partially integrated DCS for elastic e+Ca scattering; (b) the energy dependence of angles θ_1 and θ_2 at difference values k_1 and k_2.

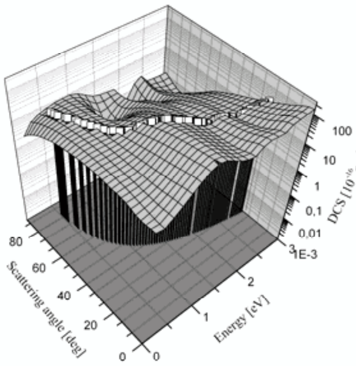

Fig. 2. Angle-differential cross sections for elastic electron scattering from Ca atoms.

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Tu1-60

REDISTRIBUTION OF THE SPIN-POLARIZATION AT THE INTERACTION BETWEEN GROUND STATE ALKALI AND NITROGEN ATOMS.

Victor A .Kartoshkin

A.F.Ioffe Psysico-Technical Institute, Russian Academy of Sciences, Polytechnical
str.26,194021 St.-Petersburg, RUSSIA. e-mail: victor.kart@mail.ioffe.ru

In gas discharge an effective spin-exchange process is proceeding between spin-polarized ground state alkali atoms and ground state nitrogen atoms, that demonstrates a conservation of total electron spin and, consequently, a transfer of angular momentum from an ensemble of the previously spin-polarized alkali atoms to the electronic part of the N atoms in $^4S_{3/2}$ state.

Consider the behaviour of a quasi-molecular system consists of the nitrogen atom with electron spin angular momentum $\mathbf{S_A = 3/2}$, and alkali atom with electron spin angular momentum $\mathbf{S_B = 1/2}$**.** If the spins of the two interacting particles be $\mathbf{S_A}$ and $\mathbf{S_B}$**,** there are two molecular states V_i, which correspond to different values of the total spin (**S**) of the quasi-molecule. In our case there are two molecular terms V_q ($\mathbf{S = 2}$) and V_t ($\mathbf{S = 1}$). Therefore the spin-exchange process can be described by two cross sections σ_1 and σ_2 corresponding to the change in the magnetic quantum numbers of the interacting particles, respectively, 3/2,1/2↔3/2,-1/2; -3/2,1/2↔-1/2,-1/2, 3/2,-1/2↔1/2,1/2, -1/2,-1/2↔-3/2,1/2 and -1/2,-1/2↔1/2,-1/2, 1/2,-1/2↔-1/2,1/2

$$\sigma_1 = \frac{3}{16}\left|f_q - f_t\right|^2 \quad \text{and} \quad \sigma_1 = \frac{1}{4}\left|f_q - f_t\right|^2,$$

where f_q and f_t are the scattering amplitudes on the quintet (V_q) and triplet (V_t) terms.

At the recombination of the spin-polarized N atoms the polarization can be transmitted to the N_2 molecules. The mechanism of the N atoms recombination involves nitrogen atom recombination into the $N_2(A^5\Sigma)$ state. At the conservation of angular momentum during the interaction the transfer of angular momentum from atoms to molecule takes place leading to the spin-polarization of the N_2 molecule. The redistribution of angular momentum between electron spin system and rotational system in the N_2 molecule results in rotational polarization of the molecule too.

In this work the kinetics of optical orientation and spin-exchange collisions between alkali and nitrogen atoms have been investigated and equations, describing the evolutions of the polarized moments have been received. The equations describing the redistribution of the polarization in the N_2 have been received too.

Tu1-61

POLARIZATION OF MOLECULAR PARTICLES DURING ATOM-MOLECULAR INTERACTIONS.

Victor A. Kartoshkin and George V. Klementiev

A.F.Ioffe Psysico-Technical Institute, Russian Academy of Sciences, Polytechnical str.26,
194021 St.-Petersburg, RUSSIA. e-mail:victor.kart@mail.ioffe.ru

At the interaction between spin-polarized excited helium atom $He(2^3S_1)^*$ and dia- and paramagnetic molecules (BC) in the optical orientation experiment the spin-polarization can be transmitted to the molecular particles. Because molecular particles have a rotational angular momentum of **j** during the time of spin-rotational interaction ($\tau \sim 10^{-6}$ sec) the electron spin **S** of a molecule particle is coupled to the rotational angular momentum **j** to give the total angular momentum **K=S+j**. The result of such a process is a rotational polarization of molecular particles.

1. The $O_2(^3\Sigma_g^-)$ molecules. In the O_2 molecules a coupling is possible of the electron spin **S** = **1** with the rotational momentum **J**, giving rise to the total angular momentum **K** = **S** + **J**.

The first question is, how the initially obtained polarization will be redistributed between the electron and rotational systems of the molecule. When solving the problem, we may make use of the theory of spin-exchange between two atomic particles, the one, being polarized, with the angular momentum $\mathbf{J_1} = \mathbf{S} = \mathbf{1}$, and the other, unpolarized, with the momentum $\mathbf{J_2} = \mathbf{J}$. The initial angular momentum **S** is found to be redistributed, after coupling **S + J = K** and decoupling **K = S'+ J'** (where <**J'**>+ <**S'**> = <**S**>), according to the relation

$$e = \langle \mathbf{J'} \rangle / \langle \mathbf{S'} \rangle = J(J+1)/2 \,. \qquad (1).$$

For Hund's case "b" within the level K = J + 1 the amplitude of resonance signal, for the transition $\Delta m = 1$ in a weak magnetic field of order of 1 Oe, will be proportional to

$$h = 2(J+1)/(2J+1)[J(J+1)+2] \qquad (2).$$

2. The H_2^+-molecular ions. We have considered a redistribution of the polarization between three systems of angular momenta, one, being initially polarized, with the electron spin **S**=**1/2**, and two others, initially unpolarized, with the rotational momentum **j**, and the nuclear spin **I**. A more simple situation is realized for even **j** when **I**=0. Then, in supposing the polarization degree not to be great, the initial angular momentum <$\mathbf{S_0}$>, transferred from the helium metastable atom, would be redistributed according to the formula:

$$\langle J \rangle / \langle S \rangle = {}^4\!/_3\, J(J+1), \qquad (3)$$

in which <**S**>+<**j**>=<$\mathbf{S_0}$>. Calculations have been also made for some odd N (N=1,3,5).

Hence, in chemi-ionizing the H_2 molecules by the metastable helium atoms are forming the H_2^+ molecular ions which are rotationally and spin-polarized. No doubt, these ions may be directly observed. The spin and rotational polarization of the H_2^+-molecular ions has been determined from the optical orientation experiment.

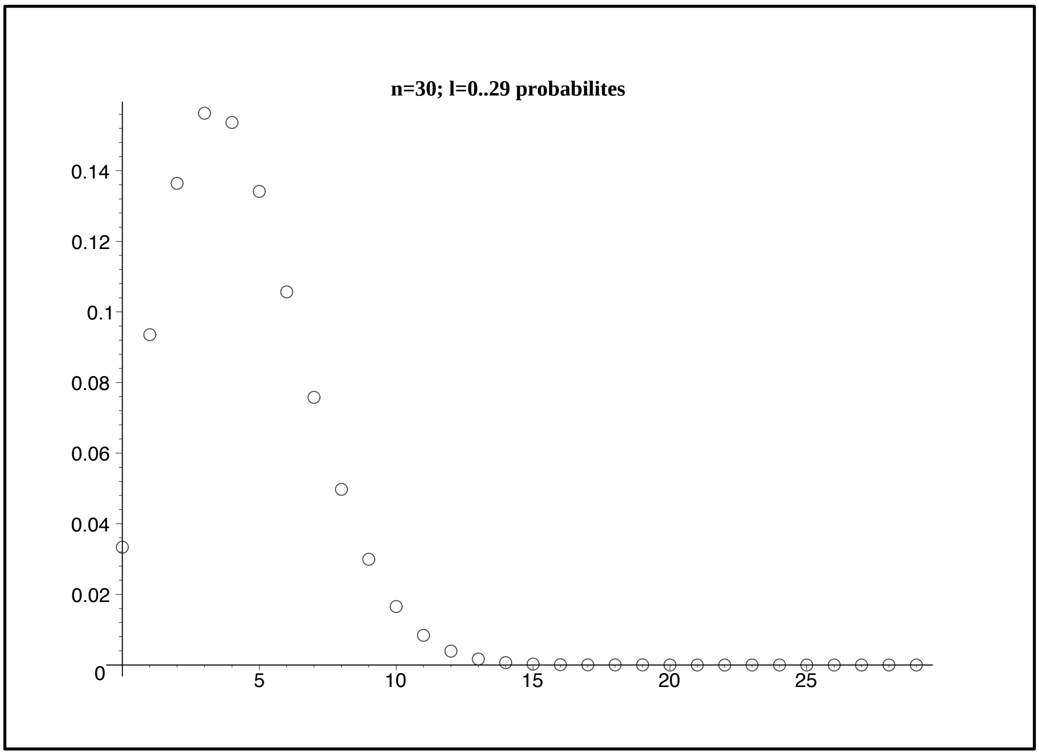
Tu1-62

PROTONIUM ATOM Pn(n=30, l) FORMATION IN $\bar{p} + H(1s)$ COLLISIONS AT VERY LOW ENERGIES

A. V. Matveenko , E. O. Alt and Hiroshi Fukuda

Bogoliubov Laboratory, JINR 141980 Dubna, Russia
Institut für Physik, Universität Mainz, D-55099, Mainz, Germany
University of Shizuoka, Shizuoka 422-8526, Japan

Recently, Esry and Sadeghpour (2003) have published calculations of protonium formation in $\bar{p} + H$ collisions at very low energies, using hyperspherical coordinates in a hyperradial adiabatic approach, where for the representation of the adiabatic eigenfunctions they used a Jacobi-channel direct product of basic splines [1]. Here, in a similar approach, we utilize a natural generalization of the spheroidal coordinates, namely the hyperspheroidal coordinates [2, 3]. We also have found that variational primitives that have the proper nodal structure both simplify the numerical calculation of the adiabatic eigenvalue problem and and make the results more easily amenable to physical interpretation [4]. From the Figure we can conclude that the $l = 0 - 9$ angular momemtum states, where l equals the $\bar{p} - H(1s)$ relative orbital momentum, are expected to be pretty intensely populated. The details of the calculations will be presented.



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Tu1-63

Nuclear Finite-Size Effects in Bound-Free Pair Production at Relativistic Heavy Ion Collisions

Kh.Yu. Rakhimov and D.U. Matrasulov

Heat Physics Department of the Uzbek Academy of Sciences
28 Katartal St., Tashkent 700135, Uzbekistan

In Recent years extremely high energy heavy ion collisions has become one of the hot topics in high energy physics and related fields. The studies in this area are mostly intended to the creation hot and dense state of matter, so-called quark-gluon plasma by colliding nuclei at very high energy [1].

However, besides being interesting from the viewpoint of high energy physics, such collisions represent ideal testing ground for the study of few-body effects at relativistic energies. In particular, the processes preceding to the formation of hadronic and quark-gluon matter are of considerable interest of relativistic atomic collisions and few-body system dynamics [2]. Such processes as excitation, ionization and electron-positron pair production can be explored in relativistic and ultrarelativistic collisions of partially stripped heavy ions.

In these high energy collisions finite-size effects of the nuclei of colliding ions become considerable and transition cross sections should be estimated with account of these effects. In this work we treat how to take into account these effects within the frameworks of perturbation theory and nonperturbative [3] approach. The obtained corrections to the total cross section are rather considerable (up to 15%) and even more higher for differential cross sections.

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Singly differential cross section for Ps-fragmentation with exchange

Hasi Ray
Institute of Plasma Research, Bhat, Gandhinagar, Gujrat, India
E-mail: *hasi_ray@yahoo.com*

Projectile ionization in Ps-atom scattering is of fundamental importance [1-7]. We study Ps-H and Ps-He systems. We evaluate singly differential cross sections for Ps-ionization in Ps-He scattering to compare them with the recently available experimental data. These provide more accurate test of a theory than integrated or total ionization cross sections due to the fact that the energy averaging is relaxed in the former case. The agreement of our integrated ionization cross sections with experiment in Ps-He scattering and the available data using a coupled-pseudostate R-matrix theory for Ps-H scattering impose the success of our theory and importance of exchange at lower incident energies which are incorporated in the comparison of singly differential cross sections with experimental data.

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Tu1-65

SUPERELASTIC ELECTRON SCATTERING BY METASTABLE THALLIUM ATOMS

Fedorko R.O., Marushka V.I., Snegurskaya T.A., Margitich M.O., Shafranyosh I.I.

Department of Physics, Uzhgorod State University, Voloshyn st. 54, Uzhgorod 88000, Ukraine
E-mail:shafivan@rambler.ru

This report deals with the results of the studies of superelastic electron scattering by the metastable $6s^2 6p\ ^2P_{3/2}$ states of thallium atom at the incident electron energies of 0.2–3.0 eV. The investigations were carried out using the electron and atomic beams crossed at the right angle [1].

The experimental conditions were as follows: the concentration of the thallium atoms in the metastable $6s^2 6p\ ^2P_{3/2}$ state was $4 \cdot 10^9$ cm^{-3}, that of the ground $6s^2 6p\ ^2P_{1/2}$ thallium atoms was $5 \cdot 10^{10}$ cm^{-3}, the atomic beam divergence angle was ~$8.7 \cdot 10^{-2}$ rad. The experiments were carried out at the ~10^{-5} Pa pressure. The electron beam was produced by the five-electrode electron gun. The electron beam current was $5 \cdot 10^{-8}$ at the ~0.3 eV energy spread. Superelastically scattered electrons were detected at the angles close to zero.

The scattered electron deceleration energy analyzer contained a system of three plane electrodes with round diaphragms [2]. The potentials at the electrode edges were set equal to the accelerating potential. The energy resolution of the analyzer was about $5 \cdot 10^{-2}$ eV at 2 eV.

The energy dependence of the cross-section is determined by the following expression: $Q^S(E)=I_S,/I_0$, where I_S is the superelastically scattered electron current, I_0 is the primary electron beam current. Note that the I_S current was measured while keeping the central analyzer electrode at the –0.4 V potential with respect to the cathode.

In these experiments, the energy dependence of the effective cross-section of superelastic electron scattering by the metastable $6s^2 6p\ ^2P_{3/2}$-state thallium atoms was measured for the first time. The result of the experiments is shown in Fig. 1, where the *x*-axis stands for the incident electron energy (in eV), and the *y*-axis represents the cross-section in arbitrary units.

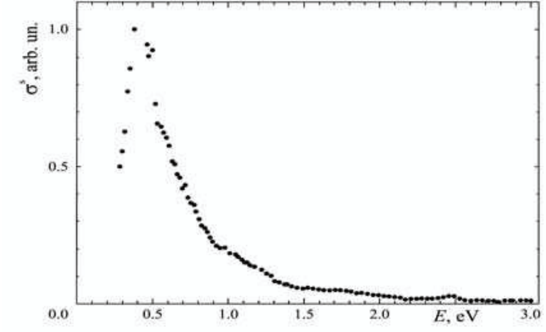

Fig. 1. Energy dependence of superelastic electron scattering cross-section for metastable thallium atoms.

The analysis of Fig. 1 shows a distinct structure in the cross-section at the electron energies of 0.4 eV, 0.55 eV, 1 eV and 2.5 eV. This structure has a form of narrow resonances interfering with each another. The presence of the structure testifies clearly to the complicated character of superelastic electron scattering process.

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Tu1-66

ELECTRON-PHOTON COINCIDENCE EXPERIMENTS AT VERY LARGE SCATTERING ANGLES WITH APPLICATION OF MAGNETIC ANGLE CHANGER

Ł. Kłosowski, M. Piwiński, D. Dziczek, K. Wiśniewska, S. Chwirot

Nicolaus Copernicus University, Institute of Physics, Grudziądzka 5/7, 87-100 Toruń, Poland

Electron-photon coincidence technique [1,2] has been for many years successfully employed in studies of inelastic electron-atom collisions and on many occasions allowed for quantum-mechanically complete experimental determination of excitation amplitudes. However, because of purely geometrical reasons such measurements were not possible in a region of large scattering angles especially interesting from a point of view of testing theoretical models of scattering processes. A possible way of overcoming the problem is to apply a technique of local magnetic field [3,4] successfully employed in recent years in variety of measurements, for instance differential cross-section for electron scattering.

A novel system for electron – photon coincidence experiments on electron inelastic scattering with magnetic angle changer was set up. Some new ideas in MAC's designing are proposed – the magnetic field is effective for 100 eV electrons and does not affect the angular resolution of the system. The first tests are performed with helium atoms used as target in angular correlation configuration [1]. Results of first measurements will be presented. It is expected that data obtained using this technique will help to sort out some discrepanciens among theoretical predictions of backscattering processes [2,5].

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Tu1-67

EXCITATION OF He ATOMS INTO 2^3P STATE IN BINARY LOW-ENERGY He-He COLLISIONS

S.Yu. Kurskov, A.S. Kashuba

Department of Physics and Engineering, Petrozavodsk State University
185910 Petrozavodsk, Russia

In this work we report the results of the experimental research of excitation cross section of He I 2^3P level and polarization degree of radiation emitted from this level in He-He system from a spectroscopic threshold up to 500 eV collision energy.

The measurements of the excitation cross section at interaction of an atomic beam with a gas target were carried out by optical methods on experimental setup, controlled by computer [1]. The neutral atoms beam was produced by means of charge exchange of He ions in own gas in extending electrode channels of ion source. The fraction of $3^{1,3}$S state metastable atoms in the beam was measured by the photoionization method, and it was equal to 0.6 % of the total number of atoms. The target gas pressure in the collision chamber was equal to $4.5 \cdot 10^{-1}$ Pa. The radiation of exited particles was observed at right angle respectively to the atomic beam, therefore, radiating particles of the beam and the target were not distinguished. The systematic error could reach ±60 %.

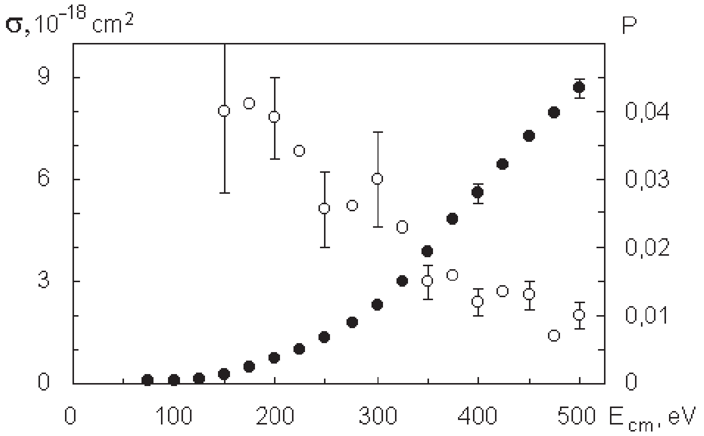

Figure 1. He I 2^3P level excitation cross section (●) and degree of polarization for 2^3S-2^3P transition (○) versus collision energy of He atoms

Relative partial cross sections of excitation of magnetic sublevels from $M_l = 0, \pm 1$ were determined. These data reveals that magnetic sublevel from $M_l = 0$ are populated mainly, what can be reasoned by radial coupling of Σ_g-Σ'_g states of He_2 quasimolecule. Taking into account simultaneous excitation of both particles probable excitation mechanism of 2^3P level may include, for example, following transition sequence:

$$(1s\sigma_g)^2(2p\sigma_u)^2 X\,{}^1\Sigma_g^+ \rightarrow (1s\sigma_g)^2 2s\sigma_g 3s\sigma_g\,{}^1\Sigma_g^+ \rightarrow (1s\sigma_g)^2 2s\sigma_g 3d\sigma_g\,{}^1\Sigma_g^+ .$$

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POSTERS

Tuesday 8/5

2. Strong field – Ultrafast phenomena – Non linear propagation

Tu2-1

Time-dependent theory of double ionization of helium under xuv radiation

L. A. A. Nikolopoulos[∗] and P. Lambropoulos[†]

[∗]*Dep. of Physics and Astronomy, Univ. of Aarhus, 8000 Aarhus C, Denmark.*
[†]*IESL-FORTH and Phys. Dep. Univ. of Crete, Heraklion, Greece*

Abstract. We present non-perturbative time-dependent calculations of single and double ionization of helium, under XUV radiation of photon energy ranging from 40 to 45 eV, through the direct propagation of the time dependent Schrödinger equation.

Motivated mainly by the problem of direct versus sequential two-electron double ionization under strong lasers of short duration, much attention has focused in the last few years or so on two-photon double ionization (TPDI) in two-valence electron atoms. Helium has received much of the attention, as it is the most amenable to ab initio and hopefully accurate calculations [1, 2] The first experimental results by radiation of photon energy □42 eV, obtained through high-order harmonic generation (HOHG) have been published [3], while further experimental studies with radiation from the free-electron laser source (FEL/FLASH) in Hamburg appear to be under preparation. On the theoretical front, the results of new calculations based on a variety of approaches and computational techniques have appeared in the literature, adding insight as well as highlighting the complexity of the problem [2, 4, 5, 6].

The time dependent wavefunction of the atom under the field is expanded in terms of correlated multichannel states normalized with incoming-wave boundary conditions. In addition to presenting a new non-perturbative approach to the three-body problem, in a fully correlated scheme, capable of providing in the same calculation photoelectron energy and angularly resolved spectra, as well as cross sections through the lowest non-vanishing order transition amplitude, we also present a detailed comparison of the values of certain key quantities that have been obtained through a variety of other methods. The degree of agreement we find, while lending credence to the approach and its versatility, does also highlight the remaining open questions in this novel context of double ionization.

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Tu2-2

FORMATION OF DOUBLY CHARGED IONS UPON MULTIPHOTON IONIZATION OF BARIUM ATOMS BY DIFFERENT POLARIZED RADIATION

V. V. Suran and I. I. Bondar'

Uzhgorod National University, Voloshina str. 54, Uzhgorod, 88000, Ukraine
suran@uzh.ukrtel.net; bondar.ivan@gmail.com

Multiphoton doubly ionization of atoms was discovered in mid-seventies [1]. Up to now mechanism of doubly charge ion formation for different atoms, spectral range, (intensities) and pulse duration don't studied. Recently in the frequency range of the laser radiation ω=14800–16900 cm^{-1} we investigate dependences of the yields of singly charged (N^+) and doubly charged (N^{2+}) barium ions on the laser radiation frequency at linear and circular (only for Ba^{2+} ions) polarizations of laser radiation. This dependences for this polarizations of the radiation were studied at a fixed strength $\varepsilon=2\times10^6$ V/cm of the laser radiation field. Depending on the laser radiation frequency (linearly polarized) the ratio between the yields of Ba^{2+} and Ba^+ ions changed from $N^{2+}/N^+\approx10^{-6}$ to $N^{2+}/N^+\approx10^{-1}$.

The experiments were performed by the method of crossing atomic and laser beams. The line width of the dye laser radiation $\Delta\omega \approx 3$ cm^{-1} and the pulse duration was $\tau \approx 50$ ns. The dependences $N^+(\omega)$ and $N^{2+}(\omega)$ allow us to make the following conclusions: in the majority of cases, the resonance maxima in the yields of the Ba^+ and Ba^{2+} ions appear at different frequencies of the laser radiation; the resonance maxima in the yield of Ba^{2+} ions have widths from 5 to 40 cm^{-1} and amplitudes from one to four orders of magnitude; some resonance maxima in the dependences $N^{2+}(\omega)$ are manifestation for both linear and circular polarizations of the radiation, while other maxima exist only in the case of linear or ***circular*** polarization.

Comparing the transitions in the spectrum of Ba atoms and Ba^+ ions that correspond to the frequencies ω_t and the maxima appearing at different polarizations of radiation, we can divide the maxima into the following four types. (**A**) The resonance maxima appear for linear and circular polarizations of radiation and the resonance transitions in the spectrum of Ba^+ ions at the corresponding frequencies ω_t are allowed for these two polarizations. This fact unambiguously proves the realization of the cascade mechanism of formation of Ba^{2+} ions ($Ba+k_1\hbar\omega\rightarrow Ba^++e$; $Ba^++k_2\hbar\omega\rightarrow Ba^{2+}+e$). (**B**) The resonance maxima appear only for linear polarization of radiation and the resonance transitions in the spectrum of Ba^+ ions at the corresponding frequencies ω_t are allowed only for this polarization. (**C**) The resonance maxima appear only for linear polarization of radiation, but the resonance transitions in the spectrum of Ba^+ ions at the corresponding frequencies ω_t are allowed for both linear and circular polarizations of radiation. The maxima of **B** and **C** type can also indicate the realization of the cascade mechanism of formation of Ba^{2+} ions. The greatest part maxima of the **D** type are observed both for linear and circular and only linear or ***circular*** polarizations of radiation and cannot be identified with the resonance transitions in the spectrum of Ba atoms and Ba^+ ions. This fact proves the realization of the noncascade mechanism of Ba^{2+} ions formation.

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Tu2-3

TWO-PHOTON DIRECT DOUBLE IONIZATION: A NON-LINEAR MEDIUM FOR XUV METROLOGY

E.P. Benis[1], P. Tzallas[1], G.D.Tsakiris[4] and D. Charalambidis[1, 2]

[1]Foundation for Research and Technology – Hellas, Institute of Electronic Structure and Laser, P.O. Box 1527, GR-71110 Heraklion, Greece
[2]Dept. of Physics, Univ. of Crete, PO Box 2208, GR71003 Heraklion, Greece
[3]Dept. of Chemistry, Univ. of Crete, PO Box 2208, GR71003 Heraklion, Greece
[4]Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany

In recent years, higher order harmonic generation has reached intensities high enough as to induce few-photon ionization processes, the backbone of XUV non-linear optics as also of XUV and attosecond pulses metrology. The first observation of a two-XUV-photon ionization of He by a superposition of harmonics [1] was a decisive step towards the temporal characterization of an attosecond pulse train through 2nd order autocorrelation (AC) [2-4]. In these types of experiments, the ionization threshold of He sets an upper limit for the harmonic order of the superposition to be characterized. This limitation may be overcome through alternative two-XUV-photon processes such as above threshold ionization [4], ionic ionization or atomic direct double ionization (DDI). Towards this goal, we reported on the observation of two-XUV-photon DDI of Ar and Kr by superpositions of the 11th, 13th and 15th harmonics of the 800 nm central wavelength Ti:Sapph laser [5].

The maximum number of harmonics combinations that participate in the DDI is limited by the energy gap between the first and the second ionization thresholds of the target. Thus, in Kr DDI is restricted in a bandwidth of harmonics ranging from 11th to 15th while in Ar it covers a range from 11th to 17th. In He, DDI covers a range of 17th to 35th indicating its usefullness in higher order harmonics. The appropriateness of DDI, as also other candidate processes, as non-linear media for attosecond metrology lies on the requirements of the flatness of the spectral response and of the "instantaneous" temporal response [3]. However, there are no available theoretical calculations as in the case of He [6], leaving this problem open to future investigation. Experimentally, 2nd order AC measurements using Ar or Kr could be crossed examined against the available He measurements.

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Tu2-4

PULSE FRONT DISTORTION CAUSED BY ABERRATIONS

Z. L. Horváth and A. P. Kovács

Department of Optics and Quantum Electronics, University of Szeged, Hungary.
H-6720 Dóm tér 9, Szeged, Hungary. *E-mail*: Z.Horvath@physx.u-szeged.hu

Ultrashort laser pulses are widely used in several fields of physics, chemistry and biology. All of the applications require the knowledge of the spatial and temporal properties of the pulses. The wave aberrations caused by the optical elements can alter the spatial and temporal behaviour of a pulse and result in disadvantageous temporal and spatial distortions.

This investigation is concerned with a theoretical treatment of the effect of the primary aberrations on the temporal and spatial shape of an ultrashort pulse. The effect of the aberrations is described by the Nijboer-Zernike theory [1]. The aberrations are represented by the Seidel form of the aberration function $\Phi_{nm} = \mu_{nm} \cdot \lambda_0 \cdot \rho^n \cdot \cos^m \theta$, where λ_0 is the central wavelength of the pulse, μ_{nm} is a dimensionless constant characterizing the amount of the aberration, $n = 4$ and $m = 0$ for spherical aberration, $n = m = 2$ for astigmatism, $n = 3$ and $m = 1$ for coma. The results of the geometrical and the wave optical treatments are compared. Some of the results are illustrated in Fig. 1.

Our results show that a few amount of aberration does not introduce a significant pulse broadening but it causes considerable distortions of the pulse front which yields significant loss of the intensity. Within it's validity, the geometrical optics predicts well the pulse front. All of the three cases of the aberrations, in addition to the pulse front predicted by the geometrical optics an extra pulse appears which is purely wave optical phenomenon, and it can be interpreted as the superposition of boundary diffraction waves [2].

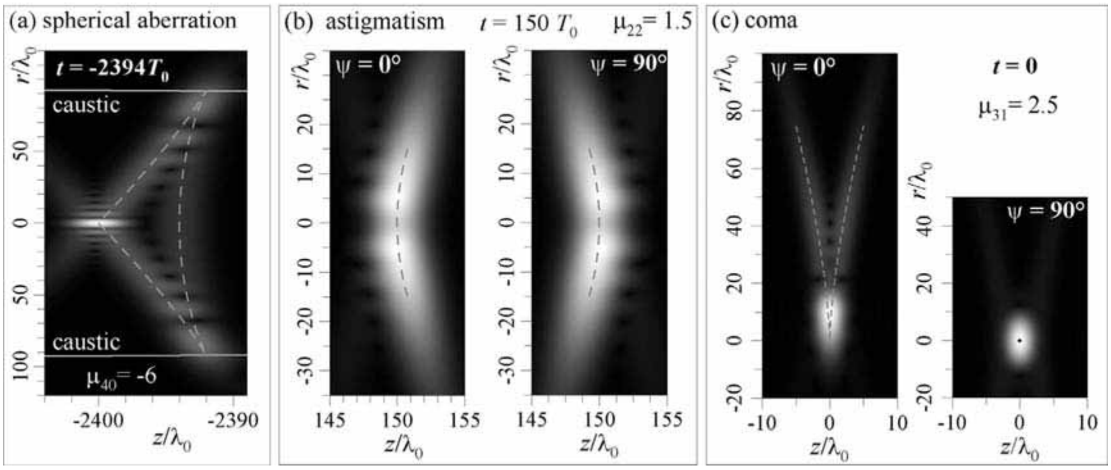

Fig. 1. Intensity distribution of a pulse with temporal duration $\tau = 2T_0$ at the moment t in the presence of aberrations, where T_0 is the period of the vibration at $\lambda_0 = cT_0$ (eg. $T_0 = 2.67$ fs and $\tau = 5.34$ fs at $\lambda_0 = 800$ nm). The amount of the aberrations are characterized by μ_{nm}. The angle $\psi = 0°$ and $\psi = 90°$ corresponds to the meridional and the sagital plane, respectively. The dashed line shows the pulse front predicted by the geometrical optics.

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Tu2-5

Numerical solution of the one-dimensional Dirac equation for an atom in external laser field: the role of the potential depth.

Madalina Boca and Viorica Florescu

Department of Physics, University of Bucharest
MG11, Bucharest Magurele 077125, Romania

For very high laser field intensity relativistic effects must be taken into account in tbe description of laser atom interaction. We numerically solve the Dirac equation using the split-operator technique in the case of an electron in a one dimensional Gaussian potential and in a laser field.

For the electron initially in a bound state we study the transfer of population between positive and negative energy states during the pulse. We also numerically calculate the one-dimensional Volkov solutions and study the influence of the laser pulse intensity and that of the atomic potential depth and width on the transfer of population on Volkov states originating from negative energy free solutions.

Our conclusion is that if the potential is not too deep (the ground state energy less than about 20 au) the Volkov states originating from negative energy solutions are not populated during the pulse, such that the expansion of the system wave spinor in a basis set consisting only in Volkov spinors originating from positive energy states should be possible. The validity of this conclusion for the three dimensional case is qualitatively discussed.

Tu2-6

MAPPING THE VIBRATION OF FAST MOLECULES WITH ULTRASHORT LASER PULSES

C R Calvert[*], J McKenna[*], D S Murphy[*], W A Bryan[†], E M L English[†], J Wood[†],
I C E Turcu[δ], J F McCann[*], W R Newell[†] and I D Williams[*].

[*] School of Mathematics and Physics, Queen's University Belfast, Belfast, UK
[†] Department of Physics and Astronomy, University College London, London, UK
[δ] Central Laser Facility, CCLRC Rutherford Appleton Laboratory, Chilton, UK

Dynamical studies of bound vibrational motion in the fastest moving molecular systems [1,2] have recently become possible due to state of the art advancements in laser pulse technology. Using ultrashort intense field laser pulses in a 'pump-probe' arrangement, we have initiated and probed coherent wavepacket motion of the deuterium molecular ion (D_2^+) on a sub-vibrational timescale. In our experiment the nuclear wavepacket is initiated in a coherent superposition of vibrational states and consequently we observe the dephasing of these vibrational components with subsequent re-phasing (the so-called 'Quantum Revival') occurring at later times.

At this meeting we will present unambiguous observations of vibrational wavepacket revivals in D_2^+ imaged via both the photo-dissociation and Coulomb explosion channels. We will also show how Fourier transform analysis provides a measure of vibrational population and how this population may be manipulated [3] in order to obtain state selective control of vibrational motion.

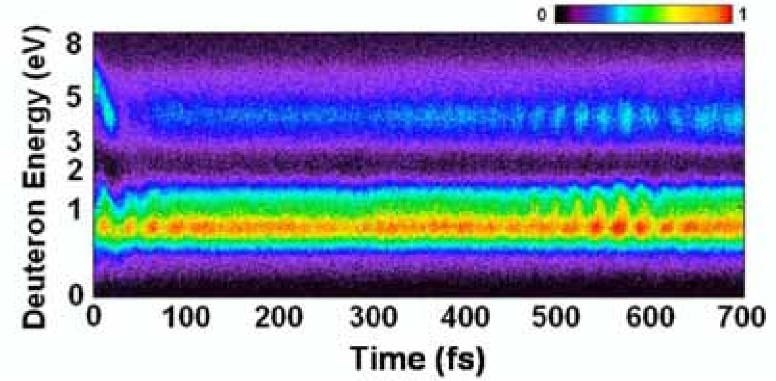

Figure 1:
Deuteron yield as a function of wavepacket evolution time. High energy fragments arise from Coulomb explosion events and low energy fragments are from photodissociation. Both of these imaging channels are enhanced at large internuclear separation for the D_2^+ molecule. Thus the notable modulation in the 500 – 600 fs region signifies a quantum revival wherein the individual vibrational components rephase and the vibrational wavepacket executes semi-classical motion.

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Email: c.calvert@qub.ac.uk

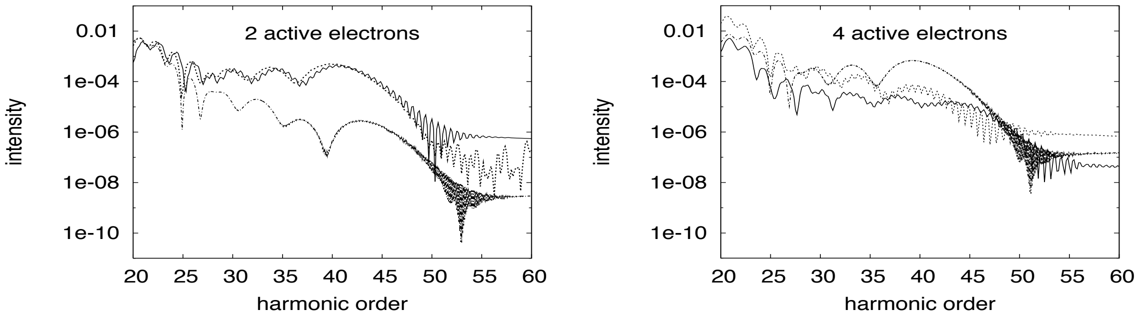
Tu2-7
HIGH-HARMONIC GENERATION WITH MULTI-ELECTRON MOLECULES

Gerald Jordan, and Armin Scrinzi
Photonics Institute, Vienna U. of Technology, Gusshausstrasse 27/387, 1040 Vienna, Austria
e-mail: gerald.jordan@tuwien.ac.at

We investigate multi-electron effects on high-harmonic (HH) generation, which may have implications for its application to orbital imaging [1]. A 3d diatomic model molecule with 2 and 4 active electrons in a strong laser pulse is simulated including correlation by the multi-configuration time-dependent Hartree-Fock (MCTDHF) method [2], where the multi-electron wave function is expanded as a linear combination of Slater determinants. The HH spectra obtained in the multi-electron approach are compared with spectra from the strong field approximation (SFA) and the time-dependent Schrödinger equation in single active electron (SAE) approximation.

The SFA is the basis for the Lewenstein model, which provides the common framework for the interpretation of HH generation. The model can be extended to the multi-particle case [3], which amounts to a modification of the dipole transition element. We calculated harmonic spectra in the Lewenstein model with three different dipole matrix elements: for the highest Hartree-Fock orbital, for the Dyson orbital, and for the Dyson orbital augmented with exchange-correlation corrections [3, 4]. However, the spectra for different choices of the matrix element differ only insignificantly, and neither of them can reproduce the multi-electron results.

To go one step beyond the SFA, but retain the SAE, we solve the TDSE with an effective 1-electron Hamiltonian, whose ground state is identical to the Dyson orbital ϕ_D: $H_{eff} = P_\perp H P_\perp - I_p |\phi_D\rangle\langle\phi_D|$, $P_\perp = \mathbb{1} - |\phi_D\rangle\langle\phi_D|$. While the agreement of the TDSE spectrum with MCTDHF is good in the 2-electron case, we observe qualitative differences in the 4-electron case. The two cases are distinct by even symmetry of the Dyson orbital for the 2-electron system and odd symmetry for 4 electrons. The remaining disagreement between multi- and single-electron calculations is tentatively ascribed to multi-electron effects.



Comparison of HH spectra near the cutoff: TDHF (solid) with 2 and 4 active electrons, 1e-TDSE (dashed), Lewenstein model (dashed-dotted)

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Tu2-8

Time-dependent theory of multiphoton single and double ionization of two-electron atomic systems exposed to XUV radiation.

Emmanuel Foumouo and **Bernard Piraux**

Laboratoire de Physique Atomique, Moléculaire et Optique (unité PAMO),
Université Catholique de Louvain, 2, chemin du Cyclotron,
B-1348 Louvain-la-Neuve, Belgium

We present non-perturbative time-dependent calculations of two- and three-photon single ionization (with or without excitation of the residual ion) as well as double ionization of He and H^- under XUV radiation. Our computational treatment of the corresponding time-dependent Schroedinger equation is based on a spectral method of configuration interaction type combined with Jacobi matrix calculations. It involves an accurate treatment of the electron-electron correlation in the initial and final states as well as during the time propagation. The atom eigenvalue problem is first solved by means of the spectral method that consists in expanding the atom wavefunction in a basis of products of complex Coulomb Sturmian functions of the electron radial coordinates and multipolar harmonics of the angular coordinates. This method allows a high-resolution study of many atomic states in particular high-lying singly and doubly excited states. The time-dependent Schroedinger equation is solved by means of an explicit scheme of Runge-Kutta type. The accurate calculation of the probability of single and double ionization is carried out by projecting the ionizing wavepacket on fully correlated multichannel scattering wave functions generated by means of the Jacobi-matrix method.

Results for the total cross section of two- and three-photon single and direct double ionization of He and H^- are presented and discussed in detail. The comparison of our results for two-photon single and double ionization total cross sections with those obtained through other methods raise important questions about the actual mechanism of two-photon single and direct double ionization. In particular, our results in Helium show that the direct double ionization is much higher than expected [1] and becomes more important than single ionization above a photon energy of 48 eV. This result turns out to be a consequence of the electron-electron correlation in the final state.

In order to gain more insight we performed a variational calculation. As a first step, we treated the final multichannel scattering wave function generated by the Jacobi matrix method as a trial function. The results clearly indicate that the correction to our previous time-dependent calculations is negligibly small thus validating our approach and confirming recent results obtained by Nikolopoulos et al. [2]. As a second step, we used a product of coulomb wave functions with effective charges (that are determined semiclassically in the asymptotic region) as a trial double continuum wave function. This gives access to differential cross sections (in angle and energy) thus providing valuable information regarding the two-photon double ionization mechanism.

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Tu2-9

PROBING COLLAPSES AND REVIVALS OF MOLECULAR VIBRATIONAL WAVE PACKET USING HIGH HARMONIC GENERATION

M. Yu. Emelin, M. Yu. Ryabikin, and A. M. Sergeev

Institute of Applied Physics, RAS, 46 Ulyanov Str., 603950 Nizhny Novgorod, Russia
E-mail: mike@ufp.appl.sci-nnov.ru

Among the promising methods for molecular ultrafast dynamic imaging are those based on the use of high-order harmonic generation (HHG). However, most of the methods demonstrated so far [1, 2] are either inapplicable to light molecules [3] or work in the time window restricted to only few fs [4]. In this work, we present an HHG-based approach which can be used to monitor long-term evolution of the nuclear vibrational wave packets in molecules, even in light-weight ones.

Previous study has shown that the overall harmonic yield in a molecular medium depends rather strongly on the molecular alignment with respect to the field as well as on the nuclear separation. Apparently, this fact is very useful, since it can be used to extract dynamic information on the molecular structure. Our approach uses transient enhancement of high harmonic generation in expanding molecules [5] for monitoring nuclear vibrational wave-packet evolution.

We present a 3D numerical simulation of HHG in a D_2 molecular sample illuminated with two ultrashort laser pulses. The first one serves as the pump pulse preparing a coherent superposition of the D_2^+ vibrational states via tunneling ionization of D_2, whereas the second time-delayed pulse is the driver for HHG, probing the nonlinear dipole response of the system at different times. The probe pulse with λ=800 nm was considered to have Gaussian shape with the peak intensity of 10^{14} W/cm^2 and FWHM of 8 fs, which are the parameters accessible at present. The bond-length dependence of an integrated harmonic signal in H19-H49 spectral range for various orientations of molecular axis with respect to the laser field was calculated. The harmonic yield is shown to be most strongly dependent on the internuclear distance in the case of parallel alignment of the molecular axis. However, for the randomly oriented ensemble this dependence is shown to be rather strong too. In both cases, the pump-probe signal calculated for the time window of few ps exhibits pronounced features which are due to the partial revivals [6] of the nuclear wave packet, as confirmed by the wavelet analysis. With the laser parameters used, the nuclear motion is shown to have a negligible effect on the resulting signal.

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Tu2-10

PUMP-PROBE EXPERIMENTS ON CH_4 FRAGMENTATION IN INTENSE LASER FIELDS

U. Wiedemann, A. Rudenko, Th. Ergler, B. Feuerstein, K. Zrost,
C.D. Schröter, R. Moshammer and J. Ullrich

Max-Planck-Institut für Kernphysik, 69117 Saupfercheckweg 1, Heidelberg, Germany
e-mail: Artem.Rudenko@mpi-hd.mpg.de

Three-dimensional coincident momentum spectroscopy combined with the pump-probe technique nowadays becomes a powerful tool to study molecular structure and dynamics. This approach has been recently used to perform complete time-resolved mapping of both dissociating and bound-state nuclear wave packets in the simplest molecules [1,2], and to visualize the photo-induced break-up of more complicated molecular systems [3].

Here we report on time-resolved 3D imaging of CH_4 fragmentation in intense (~ $3*10^{14}$ W/cm^2) short (9 fs) laser pulses, and demonstrate that this technique can be applied to study the dynamics of not only bond-breaking, but also bond-forming reactions. From earlier experiments on CH_4 break-up by ion impact [4] or VUV radiation [5] it is known that these processes can lead to a formation of H_2^+ ions. Since initially the CH_4 molecule has the tetrahedral geometry with the carbon atom in the center and four hydrogen atoms in the vertexes, this means that a new chemical bond is formed. As can be seen in the Fig. 1a, H_2^+ ions are also detected after the CH_4 fragmentation by a single 9 fs laser pulse, which means that the formation of an H-H bond in this process occurs on a time scale of a few femtoseconds.

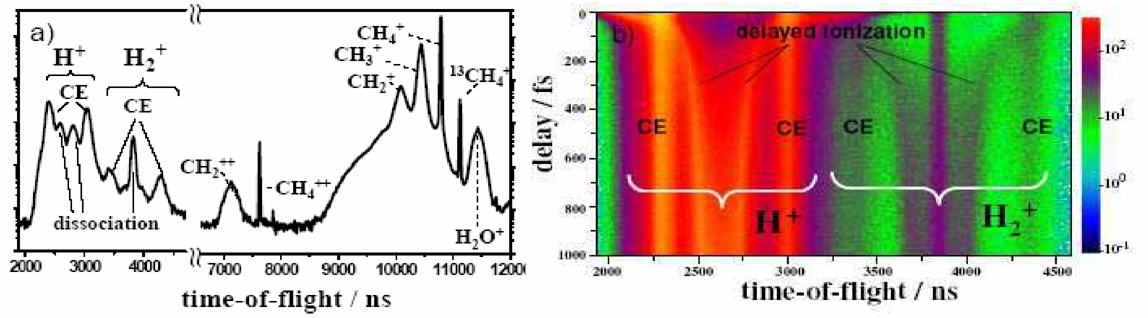

Figure 1. (a) Time-of-flight spectrum (ToF) of ions measured after the break-up of CH_4 by a single 9 fs laser. (b) ToF spectrum of light ionic fragments measured in a pump-probe experiment as a function of the delay between the pump- and the probe pulses.

As shown in Fig.1b, in the pump-probe experiment, besides the delay-independent contributions similar to those in the single-pulse data, clear delay-dependent structures can be observed for both H^+ and H_2^+ ions. These bands contain the events for which the dissociation reaction has been initiated by the pump pulse, and the dissociating complex has been further ionized by the probe ('delayed ionization'), resulting in the Coulomb explosion (CE). The CE energy decreases as the fragments fly apart, allowing for the reconstruction of the internuclear distance at the moment of explosion.

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Tu2-11

Dissociation of Vibrationally Cold HD^+ Molecules by an Intense Laser Field

J. Alexander, P.A. Orr, I.D. Williams, J.B. Greenwood
School of Maths and Physics, Queen's University Belfast, Belfast, UK

I.C.E. Turcu, W.A. Bryan
Central Laser Facility, Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK

J. Pedregosa-Gutierrez
School of Physical Sciences, Dublin City University, Dublin, Ireland

C.W. Walter
Department of Physics and Astronomy, Denison University, Granville, Ohio USA

The dissociation of HD^+ molecules in a 40 fs, 800nm laser field at interaction intensities up to 10^{15} Wcm^{-2} has been studied experimentally. Unlike previous experiments which have employed either a gaseous or ion beam target with a range of vibrational levels populated, dissociation has been studied from a pure ground state as well as a range of different populations starting from the initial Frank-Condon distribution. This was achieved by confining the ions in a linear electrostatic storage device and allowing the HD^+ to radiatively cool prior to interaction with the laser. Our results show that the dissociation rate and mechanisms are highly dependent on the population distribution. When high vibrational levels were populated, the kinetic energy release from the dissociation was low but with a pure ground state population dissociation via absorption of 4 or 5 photons was enhanced at the highest intensities. This represents conclusive evidence for an above threshold dissociation process. Unlike above threshold ionization where the probability of additional photon absorption tends to reduce with the order, in this case absorption of more photons than the minimum required for dissociation is the dominant process.

Tu2-12

HIGH EFFECTIVE THG OF HIGH INTENSIVE FEMTOSECOND LASER PULSE

Vyacheslav A. Trofimov , Vladislav V. Trofimov

Lomonosov Moscow State University, Department of Computational Mathematics &
Cybernetics, Leninskye Gory, Moscow 119992, Russia
vatro@cs.msu.su

The report is devoted to an analytical solution and computer simulation of the THG for femtosecond pulses taking into account self- and cross- modulation of interacting waves. As it is well-known, for the case under consideration because of pulses self-action the low efficiency of frequency conversion takes place for phase and group wave matching as rule. As a consequence, in physical experiment THG is realized on the base of SHG and then summary frequency wave generation for waves with basic and doubling frequencies. Using an original approach we obtained explicit solution of Schrödinger equations describing THG in the frame-work of longer duration of pulses. It should be stressed, that the main feature of our approach is an using of conservation lows for interaction waves. We found various regime of trebling frequency and shown that under some conditions the THG process has a bistable features on conversion efficiency.

On the base of our solution we show an existence of two regimes: one of them corresponds to low frequency conversion efficiency and other to high one. It is very important for practice realization that switching between two stable states can be realized due to changing of phase mismatching in short intervals of its values. It should be noticed that computer simulation results, which are obtained with taking into account second order dispersion and without it, has confirmed analytical results. For computer simulation we constructed conservative difference scheme, which gave a possibility to made simulation with high accuracy.

Tu2-13

Signature of the final state electron-electron correlation in two-photon double ionization of helium

Philippe Antoine, Emmanuel Foumouo and Bernard Piraux

Laboratoire de Physique Atomique, Moléculaire et Optique, UCL
chemin du cyclotron, 2, B-1348 Louvain-la-Neuve, Belgium

Hirokazu Hasegawa, Yasuo Nabekawa and Katsumi Midorikawa

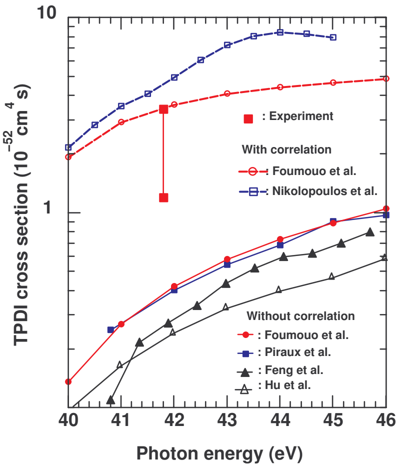
Laser Technology Laboratory, RIKEN
2-1 Hirosawa, Wako-shi, Saitama, 351-0198, Japan

We report a novel analysis of the two-photon double ionization (TPDI) cross section of helium by comparing the experimental observation and the theoretical predictions. This is important in view of understanding the TPDI mechanism taking into account the significant discrepancies between the existing theoretical models. Models, that revealed the important influence of the electron-electron correlation in the output channel, are in agreement with the observation.

We have already reported the production of He^{++} via TPDI process by applying the 27th harmonic, whose photon energy is 41.8eV, generated with a femtosecond pulse of a Ti:sapphire laser [1]. The harmonic intensity was estimated to be $6\text{x}10^{13}$W/cm^2. The ratio of the He^{++} yield over the He$^+$ yield was extracted from the observed time-of-flight mass spectrum, resulting in the ratio lying between $8\text{x}10^{-5}$ and $2\text{x}10^{-4}$. The measurement of the ratio between ion yields should be more reliable than that of the absolute ion yields for the determination of the TPDI cross section because it can be hardly affected with the absolute efficiency of the detection system or the gas density and it is less sensitive to the laser intensity. The experimental cross section actually is a lower bound as the estimated laser intensity is an upper bound.

Because it's not possible to experimentally disentangle the contribution of the direct and sequential yields, raw experimental data have to be interpreted by means of a rate equation model that describes the competition between the possible channels. Assuming that all the cross sections characterizing the sequential channels are accurately known the only unknown parameter is the TPDI cross section. In practice the TPDI cross section is tuned in order to reproduce the experimental result. The model includes spatial and temporal averages over the laser beam and pulse profile respectively to mimic the experimental conditions.

The figure compares the experimental estimation with various theoretical predictions [2-3]. The good agreement with the models including the final state electron-electron correlation [2] (dashed curves) highly suggests that this effect plays a significant role.



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Tu2-14

PHOTOELECTRON SPECTROSCOPY OF RARE GAS ATOMS AFTER MULTI-PHOTON IONIZATION BY FEL RADIATION

M.Braune[1], A. Reinköster[1], J. Viefhaus[2], B. Lohmann[3], and U.Becker[1]

[1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin
corresponding author: braune@fhi-berlin.mpg.de
[2]DESY, Notkestr. 85, 22607 Hamburg
[3]Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster

Angle resolving photoelectron spectroscopy of neutral atoms and molecules in the gas phase is widely used for investigation of the electronic structure of matter [1]. However, for ionised targets only very few studies with this method have been reported due to the low achievable target density so far [2, 3]. Since operation of the VUV free electron laser FLASH at DESY in Hamburg multi-photon ionization experiments became possible for the first time. It turned out that ionization by several photons of the intense FEL radiation can occur both simultaneously and sequentially. In our recent experiments on rare gas atoms the intensity of simultaneous multi-photon ionization was lower than the intensity of single photon ionization of neutral atoms by two orders of magnitude. On the other hand, the photoelectron intensity of sequential twofold ionization was in the same order of magnitude as single photo-ionization (Fig.1). Apparently, ionic targets of considerable densities can be created and further ionized within the duration of a single FEL light pulse of about 50fs, before dilution due to their Coulomb repulsion. Hence this opportunity opens up the possibility to study the various subsequent ionization stages of gaseous matter by means of angle-resolving and spin-sensitive photoelectron spectroscopy, investigating in particular the interplay between sequential and simultaneous ionization in multi-photon processes.

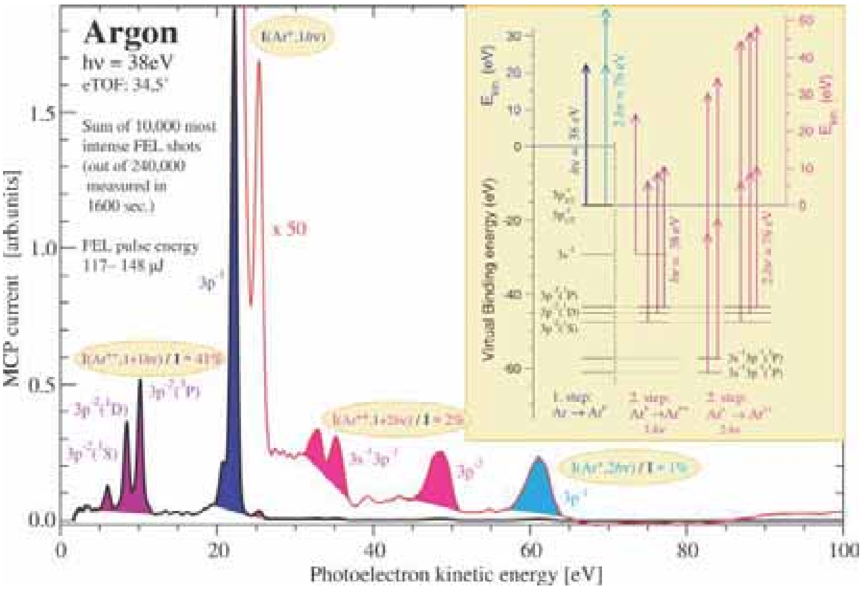

Fig. 1 Photoelectron spectrum of free Ar atoms irradiated by photons of hν=38 eV of the free electron laser FLASH, Hamburg

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Tu2-15

Three-photon-excited stimulated hyper-Raman scattering in sodium from two laser beams

Hrvoje Skenderovic*

Institute of Physics, Bijenicka cesta 46, HR-10001 Zagreb, Croatia

Three-photon excitation of the Na 6p level by 100 fs laser pulse and associated parametric four wave mixing was studied. The near-infrared (NIR) laser light produces several ultraviolet (UV) lines after passing through the dense Na vapour. A huge enhancement of the UV coherent radiation is observed in a crossed-beam geometry with two beams compared to the single-beam case. The two generated UV rays are placed between the original beams, Fig. 1 according to angular phase-matching. A change in NIR wavelength results in tunability of the UV lines.

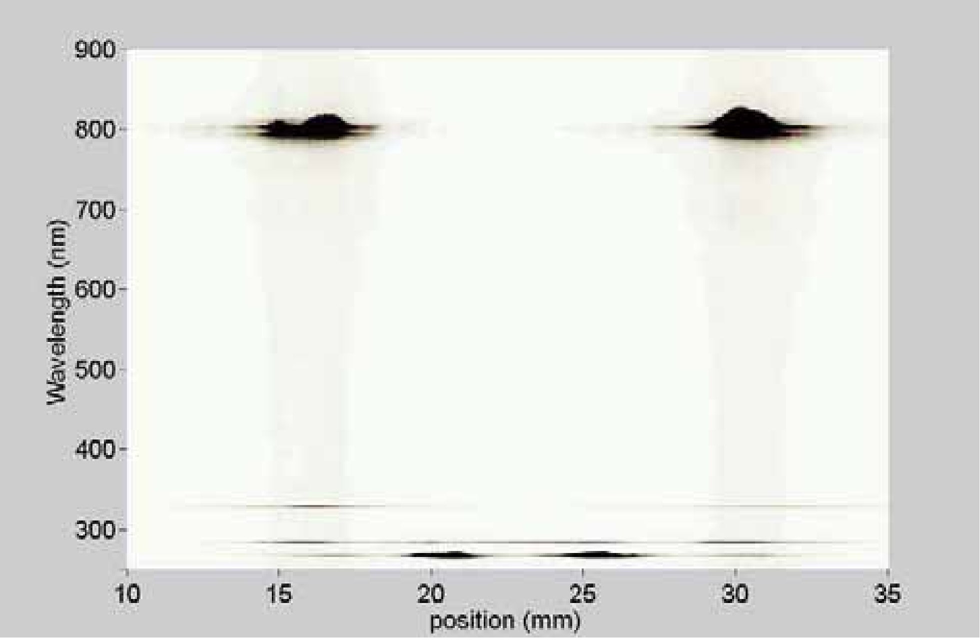

Fig.1 Wavelength landscape of the hyper-Raman scattering in sodium

By introducing a third NIR beam the UV radiation from the other two can be diminished by wave-mixing interference. In this way, a fast optical switch on fs timescale is formed because all three beams must overlap in time.

*email: hrvoje@ifs.hr

Tu2-16

TUNNEL IONIZATION AS A HIGH-DYNAMIC RANGE AT-FOCUS ULTRAFAST PULSE MEASUREMENT

W A Bryan*, E M L English*, J McKenna†, J Wood*, C R Calvert†, I C E Turcu$, I D Williams† and W R Newell*

* Department of Physics and Astronomy, University College London, London. UK.
† School of Mathematics and Physics, Queen's University Belfast, Belfast. UK.
$ Central Laser Facility, Rutherford Appleton Laboratory, Oxon. UK.

We propose a novel technique to recover the temporal intensity profile of a few-cycle pulse (FCP) by measuring the ionization yield from two co-propagating replicas derived from the same initial FCP. The FCP is split into two pulse replicas in a Mach-Zehnder interferometer [1]. The pump-probe pulses are reflection focused in an ion time-of-flight mass spectrometer, individually generating an intensity in excess of 10^{14} Wcm^{-2}. Ionization yield depends nonlinearly on laser intensity and pulse duration, thus by measuring the ionization yield as a function of pump-probe delay, the pulses can be cross-correlated, and compared to a modified (allowing for recollision) ADK model [2], as illustrated in Fig. 1. The measured ionization yield of Xe^{+} to Xe^{5+} is presented, and compared to the simulated yield produced by the same 12 femtosecond pulse split 40:60 in intensity.

The probability of atomic ionization changes by multiple orders for a single order of magnitude intensity change, therefore a broad dynamic range is possible. Unlike standard autocorrelation techniques, using an ionized gas as the optically-active medium, this technique allows an straightforward yet accurate measure of the laser intensity at focus, and is only limited by the spatial resolution of the interferometer. As a consequence, it can potentially be used to diagnose attosecond-scale pulses: in the present work, a temporal resolution of 300 attoseconds is achieved.

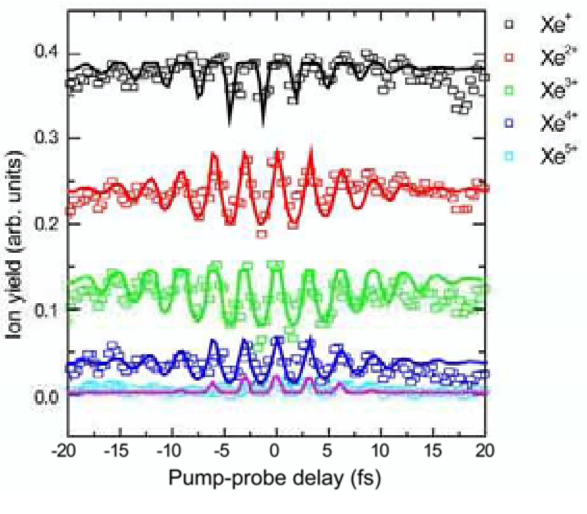

Fig.1. Xe^{+} to Xe^{5+} ion yield as a function of delay between pump and probe FCPs. The solid line is the ionization rate integrated over two interfering 12 fs FCPs, including a quantification of the laser focal volume.

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Tu2-17

ATOMS IN LASER FIELDS: THE FLOQUET ANALYSIS OF WAVE FUNCTIONS

Mihai Dondera

Department of Physics, University of Bucharest, Bucharest-Magurele, MG11, R-76900 Romania

For an atom exposed to a laser field of constant intensity, a current working hypothesis is that the wave function can be represented as a linear superposition of Floquet states corresponding to that intensity. We investigate this hypothesis, through numerical means and in a systematic way, for an electron under the combined action of a laser pulse and an 1D short range potential, and we observe the conditions for which the single state Floquet approximation is valid.

From the results obtained through direct numerical integration of time dependent Schrodinger equation we infer an *orthogonality property* of the Floquet states. We explore possible applications of this property.

Tu2-18

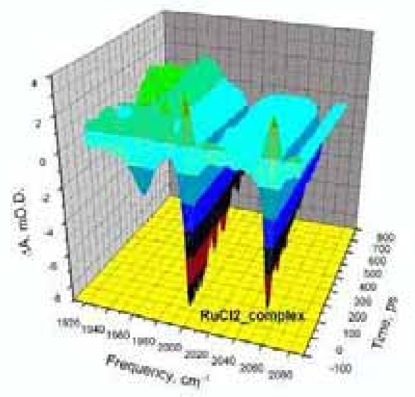
ULTRAFAST CARBONYL DISSOCIATION REACTION IN TETRAHEDRAL RUTHENIUM AND OSMIUM COMPLEXES

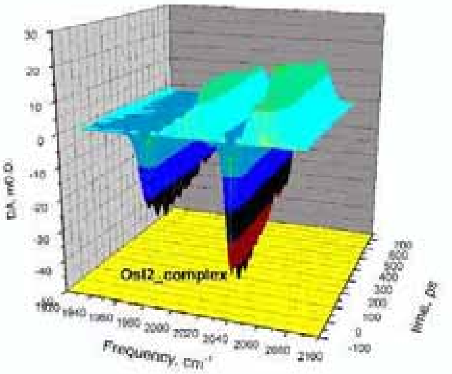
Robertas Kananavicius, Viivi Lehtovuori, Pasi Myllyperkiö, Juha Linnanto, Cristian Manzoni[†]*, Dario Polli*[†]*, Giulio Cerullo*[†]*, Matteo Rini*[#]*, Erik Nibbering*[#]*, Matti Haukka*[‡] *and*
Jouko Korppi-Tommola

Department of Chemistry, P.O. Box 35, FIN-40014 University of Jyvaskyla, Finland
[†]National Laboratory for Ultrafast and Ultraintense Optical Science –INFM Dipartimento di Fisica, Politecnico di Milano P.za Leonardo da Vinci 32, I-20133 Milano, Italy
[#]Max-Born Institute fur Nichtlineare Optik und Kurzzeitspktroskopie, Max-Born Strasse 2A, D-12489 Berlin, Germany
[‡]University of Joensuu, Department of Chemistry, P.O. Box 111, FIN-80101 Joensuu, Finland

Abstract

Light induced carbonyl dissociation reaction in (*trans*-I)Ru(dcbpy)$(CO)_2I_2$ (dcbpy=4,4'-dicarboxylic acid-2,2'-bipyridine), (*trans*-I)Ru(bpy)$(CO)_2Cl_2$ (bpy=2,2'-bipyridine), and (*trans*-I)Os(dcbpy)$(CO)_2I_2$ in solution has been studied by IR and UV-visible transient absorption spectroscopy down to 20 fs time resolution. It was observed that after UV femtosecond excitation both ruthenium complexes lost one carbonyl group in about 60 to 80 fs. Dissociation was followed by *trans – cis* re-organization of the halogens and solvent addition reaction to the vacant ligand site left open after dissociation in about one picosecond. Exponential damping of the low frequency oscillation at 90 cm^{-1} in (*trans*-I)Ru(dcbpy)$(CO)_2I_2$ (typical of Ru-halogen stretching and bending vibration) in 500 fs was considered indicative of *trans-cis* reorganization of halogens of the five-coordinated transition state complex. Quite contrary, no carbonyl dissociation reaction was observed in the osmium complex, instead a long lived excited state species, with a more tightly bound ligand sphere than in the ground state, was created. For the reactive species appearance of a broad transient IR absorption in the product absorption region indicated formation of the photoproducts within the time resolution of the experiment of about 150 fs. Cooling of the hot reactants was seen decays of red shifted absorption bands of highly excited vibronic states and as narrowing of the initially broad absorption of the photoproduct in time. Time constants for cooling processes ranged from 5 to 300ps.





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Tu2-19

Ionization of helium by 5.9fs elliptical laser pulses

Mathias Smolarski[1], André Staudte[2], Markus Schöffler[1], Ottmar Jagutzki[1], Reinhard Dörner[1], Petrissa Eckle[3], Philip Schlup[3], Jens Biegert[4], and Ursula Keller[3]

1) Institut f¨ur Kernphysik, Johann Wolfgang Goethe Universität, Max-Von-Laue-Str. 1, 60438 Frankurt am Main, Germany
2) Steacie Institute for Molecular Sciences, National Research Council of Canada, 100 Sussex Drive, Ottawa, ON K1A 0R6 Canada
3) Department Physik, ETH Zurich, Wolfgang-Pauli-Str. 16, 8093-Zurich, Switzerland
4) ICFO – Institut de Ci`encies Fot`oniques, Parc Mediterrani de la Tecnologia, Av. de l Canal Ol´ımpic s/n, 08860 Castelldefels, (Barcelona), Spain

The present work presents the momentum distribution of helium ions, created in the single ionization of helium by a 5.9 fs, CEO phase stabilized laser pulse with a small ellipticity. The difference from the expected momentum distribution created by circular light is explained using the ADK theory and classical propagation of the particles in the electric field of the laser.

Tu2-20

PHOTOELECTRON RESCATTERING SIGNATURE IN ABOVE THRESHOLD IONIZATION OF ATOMS BY INTENSE LASER RADIATION OF LINEAR POLARIZATION

H. K. Avetissian and A. G. Markossian

Department of Quantum Electronics, Yerevan State University,
1 A. Manukian, 375025 Yerevan, Armenia
E-mail: avetissian@ysu.am

The theoretical investigation of multiphoton ATI of the atoms in strong laser fields requires a relativistic consideration taking also into account the photoelectron rescattering process on the electrostatic field of the residual ion. The solution of this problem analytically is more complicated in case of the linear polarization of electromagnetic wave (EMW). At the circular polarization of EMW the relativistic consideration with the secondary rescattering process in the Coulomb field of an ion has been succeeded analytically [1]. In the present work the final results for the photoelectron energy/angular distributions and total rate of ATI at the linear polarization of EMW are obtained via numerical simulations. While for a circularly polarized EMW the contribution of the rescattering effect to the total ATI rate is only four time larger than the ATI rate of the direct process [2], and to the angular distribution of the photoelectrons is nonessential [1], in case of a linearly polarized EMW these contributions are essential, especially to the angular distribution of the photoelectrons. The analysis of obtained results shows that the ATI rate has a tendency to fall off more slowly with the increase of the wave intensity when the new side-lobs in the photoelectron high-energy spectra arise already due to the rescattering process. These new side-lobs in the field of a linearly polarized EMW result to so-called rings in the angular distribution of the photoelectrons with higher energies in accordance with the recent experimental observations [3]. The developed relativistic approach allows to explain the mentioned experimental results and predict the position of these rings.

This work was supported by International Science and Technology Center (ISTC) Project No. A-1307.

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Tu2-21

SPATIO-SPECTRAL SHAPING AND COMPRESSION OF FS-LASER PULSES IN SELF-INDUCED WHITE-LIGHT FILAMENT

Nickolai Zhavoronkov[1],Gero Stibenz[1],Günter Steinmeyer[1],Stefan Skupin[2] and Luc Bergé[2]

[1]Max-Born-Institut, Max-Born-Str. 2a, 12489 Berlin, Germany,e-mail: zhavoron@mbi-berlin.de

[2]Département de Physique Théorique et Appliquée, CEA-DAM/Ile de France, B.P. 12, 91680
Bruyères-le-Châtel, France

Experimental investigation of the phenomena of physical or chemical nature have frequently to recourse to powerful femtosecond laser pulses. Intensities in a range far above 10^{12} W/cm^2 are nowadays commonplace for application to ionization and dissociation dynamics. The variety of the nonlinear effects accompanying pulse propagation can drastically change the pulse properties at the point of the experimental interest and even self-trap the beam into a light filament by the combined action of self-focusing and multi-photon ionization. Recently, it was shown that filaments in noble gases are applicable for femtosecond pulse compression utilizing the nonlinear pulse shaping effects in self-guided geometries [1,2].

We conducted our experiments with Ti:sapphire laser system, delivering 45-fs, 5 mJ pulses at a 1 kHz repetition rate, and a gas cell filled with argon or krypton at 0.3 to 0.5 atmospheres. The filament formed inside the gas cell can extend up to 50 cm or more. Pulses as short as 7.4 fs have been measured at pulse energies of 2 mJ (Fig. 1(a)), yielding 6-fold compression. The spectrum (Fig. 1(b)) displays significant broadening into the blue, whereas only little broadening is observed in the red. The spectral phase of this pulse is remarkably flat in two isolated spectral regions, but displays a phase kink in between. XFROG analysis of the measured data reveals that the observed self-compressed pulses generated inside the filament are composed of a short pulse generated in the blue wing of the spectrum and a second pedestal-like structure encompassing the spectral region of the original pulse, see Fig.1(c).

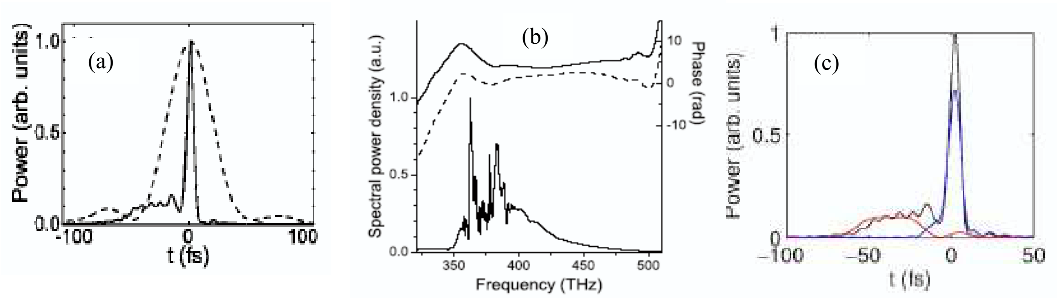

Fig.1. (a) the original (dashed line) and filament-compressed (solid line) pulses, (b) spectrum and measured spectral phase of the compressed pulses, (c) output pulse (solid line) in comparison to the temporal shape of the blue and red part of the spectrum (red and blue lines respectively).

Our numerical simulation [3] indicates the major shaping effect that compresses the pulses. The leading and trailing time-slices diffract faster, than the high intensity center, forming of on-axis temporally compressed structure, while radial averaging indicates little to no compression at the spatial profile edge. The trailing edge of the pulse is shortened additionally by self-steepening, that leads to asymmetric broadening into the blue.

In contrast to hollow-fiber compressors, filament technology eliminates coupling losses and limitations on the pulse energy due to potential destruction of the guiding structure, and appears to be the most promising technique for advanced radiation sources with sub-10-fs temporal signature.

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THE DYNAMICS OF META-STABLE STATES DESCRIBED WITH A COMPLEX SCALED HAMILTONIAN

J. Bengtsson, E. Lindroth, and S. Selstø

Atomic Physics, Fysikum, Stockholm University, S-106 91 Stockholm, Sweden

The laser development has given access to light pulses in the femto- and subfemtosecond regime and thereby opened the possibility to follow electron dynamics directly in the time domain. Of special interest is the dynamics of *resonant states*, and pioneering experimental studies were made a few years ago on the Auger decay of inner-shell vacancies[1].

Here we present a new method for time-dependent calculations of the whole sequence of events when an atom is exposed to a short light pulse followed by the population of a meta-stable state, and with the possibility to follow its subsequent decay by electron ejection. We use a complex scaled Hamiltonian, a method proven successful in describing resonant states, and show how this method can be used to solve also the time-dependent Schrödinger equation (TDSE). There are two major advantages with this approach. First, the meta-stable states are obtained as unique eigenstates to the field-free complex scaled Hamiltonian, simplifying their description significantly. Second, the continuum is adequately represented by a very modest number of eigenstates. A similar accuracy cannot be achieved using a conventional pseudo continuum. The complex scaled Hamiltonian is non-Hermitian and the extension to dynamical calculations is not straight forward. We have tested our approach against conventional methods for the case of hydrogen and established the connection to Floquet theory for monochromatic radiation.

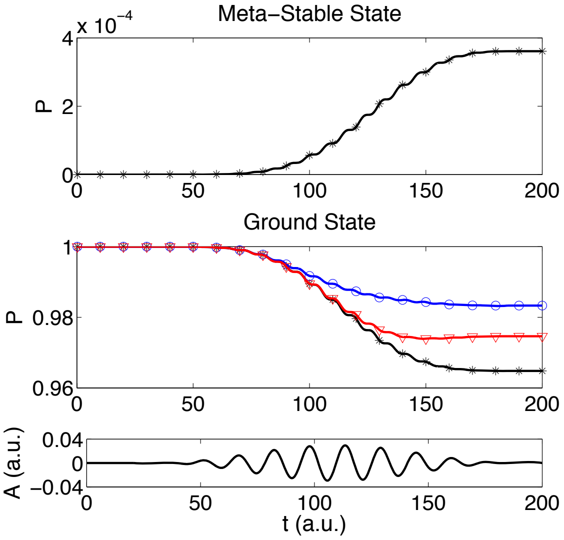

Figure 1: Upper panel: The population of the lowest energy ^1P meta-stable state of H^- when exposed to a $\cos^2$ - shaped laser pulse (bottom panel) with $\omega = 0.4014$ a.u. and peak intensity 10^{13} W/cm^2. Middle panel: Corresponding population of the ground state. The black curves (stars) show the complex rotated calculation and the red (triangles) and blue(circles) curves show how a non-complex rotated pseudo continuum approaches this results when the basis set is increased.

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Tu2-23

RELATIVISTIC DYNAMICS OF HIGHLY CHARGED HYDROGEN LIKE SYSTEMS EXPOSED TO INTENSE HIGH-FREQUENCY ELECTROMAGNETIC FIELDS

S. Selstø, J. Bengtsson, and E. Lindroth

Atomic Physics, Fysikum, Stockholm University, S-106 91 Stockholm, Sweden

We solve the time dependent Dirac equation in a basis consisting of the eigenstates of the field free Hamiltonian $H_0 = c\boldsymbol{\alpha}\cdot\mathbf{p} + V(r) + mc^2\beta$. This basis is obtained through a method of Salomonsen and Öster [1]. The dynamics induced by the time dependent perturbation, $H'_v = c\boldsymbol{\alpha}\cdot\mathbf{A}(\mathbf{r},t)$ in the velocity gauge, or equivalently $H'_l = \mathbf{r}\cdot\mathbf{E}(\mathbf{r},t)(1-\boldsymbol{\alpha}\cdot\hat{\mathbf{k}})$ in the length gauge, is resolved by solving the first order ordinary differential equation arising from the expansion.

The number of continuum states needed in order to get converged results is reduced by complex scaling on the coordinates, $r \to re^{i\theta}$ [2]. We investigate the importance of relativistic effects for various field strengths E_0 and nuclear charges Z, including negative energy states, by comparing the solutions of the Dirac equation with the corresponding prediction of the Schrödinger equation. It is to be expected that a high E_0 or high Z alone would necessitate the use of a relativistic treatment of the system. However, the combined effect of a strong external field and a strong Coulomb field should increase the significance of relativistic corrections further.

The dynamics is described both within and without the dipole approximation ($\mathbf{A}(\mathbf{r},t) \approx \mathbf{A}(t)$). For high E_0 and high photon energy, $\hbar\omega$, it is clear that this approximation breaks down [3]. However, for increasing Z, the electron is increasingly tightly bound, which to some extent reduces the importance of non-dipole effects.

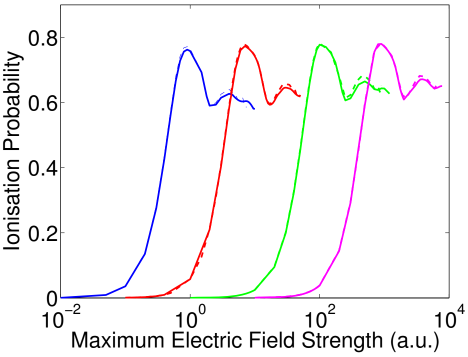

Figure 1: The ionisation probability for (from left to right) H (blue), He^{+} (red), B^{4+} (green) and Ne^{9+} (magenta) obtained from the Dirac equation (full curve) and the Schrödinger equation (dashed curve). In all cases the laser pulse duration corresponds to three optical cycles and the central frequency of the pulse is $\omega = 0.8\,Z^2$ a.u.. In these preliminary calculations, the dipole approximation has been used and negative energy states have been omitted.

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Tu2-24

QED THEORY OF LASER-ATOM AND LASER-NUCLEUS INTERACTION AND ATOMIC DYNAMICS WITH NON-RECTANGULAR LASER PULSES

Alexander V. Glushkov

Odessa University, P.O.Box 24a, Odessa-9, 65009, Ukraine-Russia
E-mail: glushkov@paco.net

QED theory is developed for studying interaction of atoms and nuclei with an intense and superintense laser field. Method bases on a description of system in the field by the k- photon emission and absorption lines [1,2]. The lines are described by their QED moments of different orders, which are calculated within Gell-Mann & Low adiabatic formalism. The analogous S-matrix approach is developed for consistent description of the laser-nucleus interaction. We have studied the cases of single-, multi-mode, coherent, stochastic laser pulse shape. An account for stochastic fluctuations in a field effect is of a great importance. Results of the calculation for the multi-photon resonance and ionization profile in Na,Cs, Yb, Gd atoms are presented. Our method is compared with other (DFT et al) approaches [3]. It is also studied the phenomenon of the above threshold ionization. Efficiency of method is demonstrated by QED perturbation theory calculations for the two-photon ionization cross-sections for extended photon energy range (including above-threshold ionization) in Mg. Comparison with the R-matrix calculation of Luc-Koenig et al [3] is given. There is considered a phenomenon of the Rydberg stabilization of the H atom in a strong laser field and estimated the rate of transition between the stabilized Rydberg state (n=40,m=2; E~10(8)V/cm) and ground state, when it's possible the radiation of photons with very high energy (short-wave laser amplification).

Atomic dynamics with non-rectangular laser pulses is studied and the results of numerical calculation of population kinetics of the resonant levels for atoms in the non-rectangular pulse field on the basis of the modified Bloch equations are presented. The equations describe an interaction between two-level atoms ensemble and resonant radiation with an account of the atomic dipole-dipole interaction. A new idea of this work is discovery of strengthen possibility of manifestation for the internal optical bi-stability effect special features in the temporary dynamics of populations for the atomic resonant levels under adiabatic slow changing the acting field intensity. A discovery and observation and adequate explanation of the optical bi-stability effect is discussed.

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Tu2-25

SPECTRAL FEATURES OF HHG IN DIATOMIC MOLECULES DRIVEN BY FEMTOSECOND LASER PULSE

I. A. Gonoskov, M. Yu. Ryabikin, and A. M. Sergeev

Institute of Applied Physics, RAS, 46 Ulyanov Str., 603950 Nizhny Novgorod, Russia
E-mail: gonoskov@ufp.appl.sci-nnov.ru

The spectral features of HHG in molecules can be used in attosecond physics for diagnostic purposes (such as the molecular dynamic imaging). In this work we consider the problem of extracting information on the molecular structure from the positions of two-centre interference minima [1] in HHG spectra. The visibility and shape of the spectral interference patterns is examined in frame of different theoretical approaches to HHG in a diatomic molecule (with fixed and moving nuclei) [2].

In particular, we show that the interference minima located in the low-energy region of the frozen-nuclei spectra are described more satisfactorily as $\hbar\omega=\hbar^2k^2/2$ while the higher-energy minima are shifted closer to the positions given by $\hbar\omega=\hbar^2k^2/2+I_p$ (here k satisfies the destructive interference condition $k=(2n+1)\pi/(D\cos\theta)$). In moving-nuclei case the interference structure is much less pronounced and the correspondence between the positions of the minima and the molecular structure is less direct.

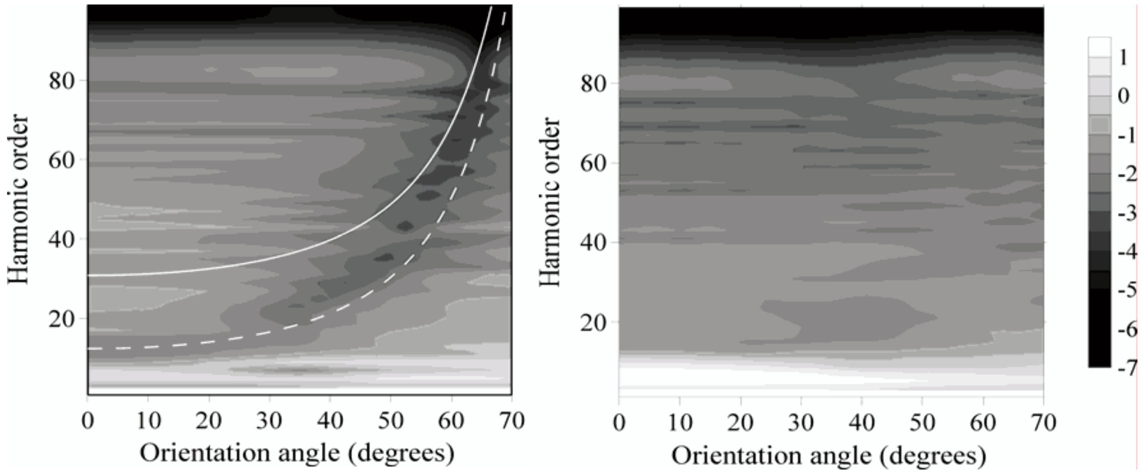

Fig. 1. HHG spectra for H_2^+ in a 27 fs, 800 nm pulse with $I = 5\times10^{14}$ W cm^{-2} calculated in the frozen-nuclei (left panel) and moving-nuclei (right panel) approximation for different values of the molecular orientation angle

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Tu2-26

CONTROL OF THIRD-ORDER DISPERSION USING A BIREFRINGENT CRYSTAL

A. P. Kovács, M. Erdélyi, K. Mecseki, G. Szabó

Department of Optics and Quantum Electronics, University of Szeged, H-6701
Szeged, P.O. Box 406, Hungary; e-mail: a.p.kovacs@physx.u-szeged.hu

Independent control of the group-delay dispersion (*GDD*) and the third-order dispersion (*TOD*) of the laser pulses are important in the generation of ultrashort laser pulses by chirped pulse amplification and in the pulse shaping used for molecular control.

In this work a new device is proposed for dispersion control. The *GDD* and the *TOD* of the pulses is controlled by the position of a birefringent, semi-cylinder crystal placed around the focal point of an achromatic lens (Fig. 1). The spectral components of the pulse propagate as extraordinary rays in the crystal. For the evaluation of the phase shift introduced by the proposed device, a ray tracing program was written, which allows optimization of the parameters of the device. Calcite was applied because it is a strong birefringent material. Calculations showed that there is a trajectory, and the *TOD* can be tuned independently of the *GDD* (Fig. 2) by shifting the crystal along that trajectory. Although the defocus also affects the angular dispersion of the pulse leaving the compressor, it does not exceed the 40 μrad/nm value.

For experimental verification, the proposed device was placed in one arm of a Michelson-type interferometer illuminated by a Ti:sapphire oscillator. The dispersion coefficients of the device were determined from the spectrally resolved interferograms (SRI). The difference between the measured and calculated GDD and TOD was about 25 %, which is acceptable if we take into consideration that the simulation is based on paraxial approximation. The simulation results can be used as rough estimation, and SRI can be applied for real-time fine tuning.

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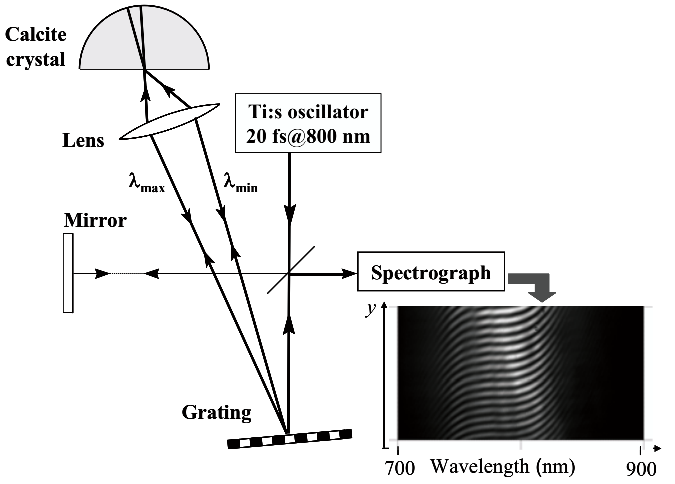

Fig. 1

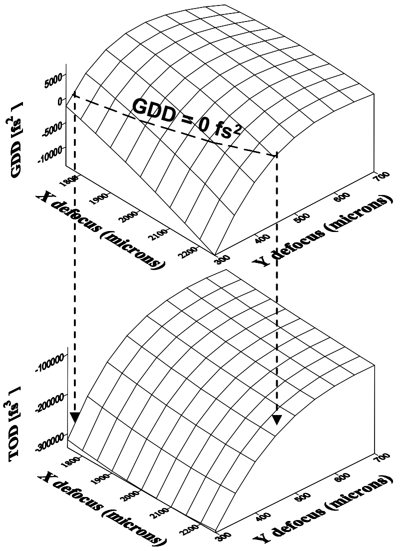

Fig. 2

Tu2-27

All-in-one Pulse Shaping and Measurement of Ultrashort UV Pulses

N. Forget, S. Coudreau, F. Lepetit*, O. Albert and T. Oksenhendler**

FASTLITE, Bat 403, Ecole Polytechnique, 91128 Palaiseau, France
**DSM/DRECAM/SPAM CEA Saclay, France*
***LOA, ENSTA, Ecole Polytechnique, CNRS UMR 7639, 91761 Palaiseau Cedex, France*

Ultrashort pulse characterization techniques based on second harmonic generation (SHG), such as frequency resolved optical gating (SH-FROG), were developed for the near infrared and cannot be easily transposed to the UV and the visible because of the lack of suited and efficient non linear crystals for broadband SHG. Such difficulties can be overcome by the use of a third order non linear effect such as induced birefringence which is achromatic and frequency conserving. However, third order non linear effects usually require non collinear geometry in order to be able to extract the useful signal, which greatly increases the complexity of the system. Conversely, a single-beam geometry would greatly simplify the optical setup but comes at the expense of an interferometric control of the delay between pulses replicas and signal discrimination.

In this talk we demonstrate a single beam, achromatic, programmable and self-compensated spectrally resolved interferometric autocorrelation technique which overcomes such drawbacks. This technique is based on the conjugate use of cross-polarized wave generation (XPW), an exotic third order non linear effect [2], and of an UV acousto-optic programmable dispersive filter (UV-AOPDF) [1] which is used to produce pulse replicas with interferometric control within the acousto-optic crystal.

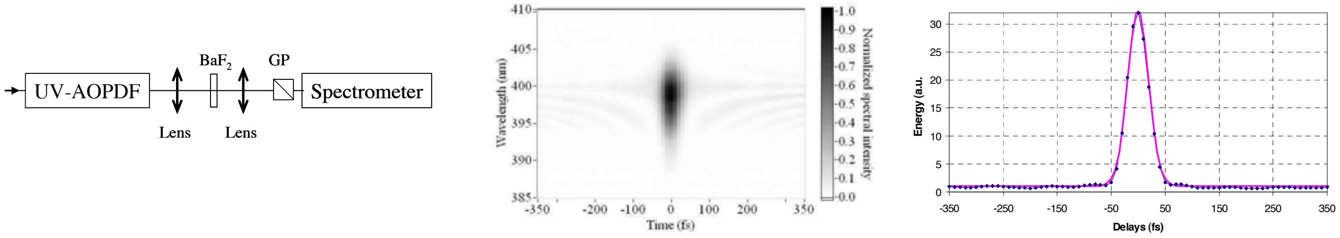

Fig. 1. Left: experimental setup (GP: Glan polarizer). Center and right: experimental baseband interferometric FROG trace and autocorrelation of the 40fs UV pulses.

As depicted in Fig. 1, the pulses diffracted by the UV-AOPDF are focused down into a 3mm thick BaF_2 crystal by a first lens and recollimated by a second lens. A Glan polarizer is used to isolate the XPW wave and a spectrometer records the XPW spectrum. The AOPDF (75mm-long KDP crystal) is also used to precompensate the optical dispersion of all optical elements: lenses and AOPDF and BaF_2 crystals. First experiments were performed on the SHG output of an amplified Ti:Sapphire system delivering Fourier-transform limited pulses of 40fs at 397nm. The baseband interferometric FROG and autocorrelation traces show a good agreement with the expected pulse width. The XPW conversion efficiency was not measured exactly but was estimated to be of the order of □1%. Given the extinction ratio of the polarizer (10^4), the signal to background ratio is estimated to □100. The talk will also address the numerical methods to retrieve the spectral phase and the extension of such a characterization technique for UV pulses in the 250-350nm range.

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MULTIPHOTON ABSORPTION IN LASER PRODUCED PLASMAS

Caroline Banahan, John T Costello, Paul van Kampen

National Centre for Plasma Science and Technology (NCPST)
& School of Physical Sciences
Dublin City University, Glasnevin, D9, Ireland

There has been a growing interest in recent years to study the photoionization of excited atoms, particularly the alkaline earths, owing to the rich structure they exhibit in the near threshold region due to discrete states embedded in the ionisation continuum (autoionizing states). Resonant laser driven ionisation (RLDI) [1] has been successfully applied to study such ionized atoms in dense atomic vapours [2-4] and determine the collective effects involved in the rapid ionization process. Super-elastic collisions have been deemed the dominant energy transfer mechanism between 'seed' electrons and the excited atoms, with associative ionization and collisions between excited atoms also included. Studying RLDI in laser-produced plasmas however is more complicated [5]; it requires sophisticated theoretical modelling to discern the underlying dynamics due to collective effects and effects inherent to the plasma.

In this work, the dual-laser plasma (DLP) [6] technique is used to generate a calcium plasma and the photoionization of calcium atoms excited to the 4s4p ^{1}P state (422.7nm) using an optical parametric oscillator (OPO) is studied. A laser-generated XUV plasma source probes the excited calcium plasma at various time delays to study the dynamics of the system. Ionisation from the 4p^2 two-photon transition and from the two-photon Rydberg series 4s*n*d (*n*=5-8) is also studied to determine how the ionization process varies for the different excitations. By varying the intensity of the OPO and detuning from resonance we aim to provide insight into the so-called 'space-charge' effects introduced to account for anomalies observed in the laser power dependence of charge yields. We intend to extend this work to barium also.

Work supported by the Irish Governments National Development Plan under the Basic Research Grants Scheme administered by the Irish Research Council for Science Engineering and Technology.

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Tu2-29

ON MECHANISM UNDERLYING NO SUPPRESSION IN STRONG-FIELD IONIZATION OF LASER-IRRADIATED F_2

Vladimir I. Usachenko and Vyacheslav V. Kim

Institute of Applied Laser Physics UzAS, Tashkent, 100185, Uzbekistan.

The puzzling phenomenon of strong-field ionization in F_2 molecule (which, according to experiment [1], does not show a suppression predicted in [2, 3] for ionization rate as compared to its atomic counterpart *Ar* of nearly equal ionization potential) is addressed within the *velocity-gauge* (VG) formulation of molecular *strong field approximation* (SFA) [2]. Unlike earlier alternative consideration [2], the currently applied VG-SFA approach is essentially based on a special *cc-pVDZ* Gaussian basis set extended by applying the model LB_α intramolecular binding potential (which incorporates both the *exchange* and *correlation LSDA*-potentials, see, e.g., [4], for details) under composition of initial (laser-free) molecular state using the GAUSSIAN code. The resulting calculated ionization rates demonstrate no suppression in ionization of F_2 (versus atomic *Ar*) and suggest that predominant contribution to F_2 ionization is to be always from the *highest-occupied molecular orbital* (HOMO) corresponding to $1\pi_g$ outermost molecular shell. The latter is in a contradiction to earlier consideration [4] based on *time-dependent density functional theory* (TD-DFT), which attributed the phenomenon of no suppression to ionization of $3\sigma_g$ inner molecular shell predominantly contributing compared to $1\pi_g$ HOMO (at least, within the high-intensity domain $\geq 3\times10^{14}$ W/cm^2). However, the interpretation given in [4] seems to be at least insufficient leaving unexplained the reason, for which the relative contribution from $3\sigma_g$ inner shell in O_2 is to be negligible compared to $1\pi_g$ HOMO predominantly contributing and showing a high suppression [1] in ionization rates for O_2 (versus its atomic counterpart *Xe*). Meantime, the phenomenon of no suppression in F_2 ionization allows for quite a transparent physical interpretation according to our present VG-SFA consideration assuming that $1\pi_g$ HOMO is always predominantly contributing. Namely, the phenomenon is just explained by the *closed-shell* nature of $1\pi_g$ HOMO in F_2 that leads to a domination of the *correlation LSDA*-potential used under composition of respective initial (laser-free) molecular state, in contrast to the *open-shell* $1\pi_g$ HOMO in O_2, for which the *exchange LSDA*-potential proved to contribute predominantly. Since the closed-shell and/or open-shell molecular orbitals are not distinguishable within any one-electron ADK-based theory, our latter alternative interpretation also helps in realizing the reason, for which the MO-ADK model [3] failed in correct description of strong-field ionization in laser-irradiated F_2.

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Tu2-30

Ionization of an atom in a strong laser pulse: numerical integration versus strong field theories

Yulian V. Vanne and Alejandro Saenz

AG Moderne Optik, Institut für Physik, Humboldt-Universität zu Berlin,
Hausvogteiplatz 5-7, D 10117 Berlin, Germany

Strong field ionization of atoms and molecules received much attention in the past years. Various nonperturbative approaches have been proposed to describe such highly non-linear processes as multiphoton ionization, above threshold ionization or high harmonic generation. Among them, different variations of the Keldysh-Faisal-Reiss (KFR) theory (also referred to as strong-field approximation) are often used nowadays, since they allow an analytical treatment of the problem. Although the general formulation of KFR is known for decades, there are still controversial issues, e. g., the strong gauge dependence, the possible choices for a Coulomb correction, and technical problems in the calculation of the ionization transition amplitude.

We discuss two aspects related to analytical study of KFR. First is related to the method of calculating the ionization transition amplitude in length gauge KFR. Recently, it has been proposed to substitute the widely used saddle-point approximation by an "exact" formula based on the residue theorem. Comparing the results of both approaches for atomic hydrogen a difference by a factor of 4 was found for the ionization rate of 1s, and an even more drastic deviation for the 2s state. We have proven [1] that this claim is incorrect, since the proposed "exact" Keldysh theory erroneously neglects an important term. Further, we have performed a careful analytical and numerical analysis of the quasistatic limit of the velocity-gauge KFR [2]. A simple analytical dependence on the laser frequency is found for long-range interaction potentials. The fact that the ionization rate is proportional to the laser frequency shows a break-down of velocity-gauge KFR in the quasistatic limit. The Coulomb correction proposed by A. Becker *et al.* [3] does not remove this problem. Based on the Perelomov-Popov-Terent'ev tunneling formula [4] we derive a Coulomb correction factor for velocity-gauge KFR in the weak field limit.

Based on a full numerical integration of the time-dependent Schrödinger equation we have performed a systematic test of different variants of KFR theory in a wide range of laser parameters like peak intensities, pulse lengths and frequencies.

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Tu2-31

DIRECT INTERACTION OF LASER FIELDS WITH DIPOLE-FORBIDDEN TRANSITIONS IN NUCLEI

Adriana Pálffy, Thomas J. Bürvenich*, Jörg Evers, Christoph H. Keitel

Max-Planck-Institut für Kernphysik, Heidelberg, Germany
(*) Frankfurt Institute for Advanced Studies, Frankfurt am Main, Germany

With present and upcoming light sources, the direct interaction between nuclei and super-intense laser fields has become feasible, opening the new field of nuclear quantum optics. Due to the large transition frequencies in nuclei, the resonant interaction of coherent light with nuclear transitions requires x-ray laser fields, potentially together with an acceleration of the target nuclei [1]. This approach is the most promising for potential applications similar to quantum optics in atomic systems, but demanding in terms of the light source, in particular due to the required photon frequency [1,2]. In view of atomic quantum optics [3], the most direct choices of suitable nuclear systems would be those with low-lying excited states connected by a E1 transition to a stable or metastable ground state.

While for atomic systems the dipole transition is playing the most important role, in the case of nuclei, which present rich structural properties like collective and single-particle excitations [4], mostly dipole-forbidden transitions occur. The spectrum of E1 transitions is limited to few low-lying nuclear excited states with small reduced transition probabilities, and giant resonances, at energies of several MeV, which are not directly accessible nowadays with the laser. We therefore investigate dipole-forbidden transitions of nuclei interacting with super-intense laser fields, considering several stable nuclei with suitable first excited states. The strong reduced transition probabilities and the suitable energy values make E2 and M1 nuclear transitions good candidates for the resonant interaction between nuclei and laser fields. This conclusion encourages the study and triggering of excited nuclear states via coherent laser fields. As an ultimate goal, one may hope that direct laser-nucleus interactions could become a versatile tool to enhance preparation, control and detection in nuclear physics.

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Tu2-32

POLARIZATION CONTROL OF DIRECT TWO-PHOTON DOUBLE-IONIZATION OF He BY VUV LIGHT

E. A. Pronin[1], A. Y. Istomin[2], N. L. Manakov[3], S. I. Marmo[3], A. F. Starace[1]

[1] Department of Physics, The University of Nebraska, Lincoln NE 68588, USA
[2] Dept. of Physics and Optical Science, Univ. of North Carolina, Charlotte, USA
[3] Department of Physics, Voronezh State University, Voronezh 394006, Russia

Advances in generating intense coherent vacuum ultraviolet (vuv) and soft-x-ray light have increased interest in fundamental multiphoton processes involving more than one electron, such as two-photon double-ionization of ground state helium: $2\gamma + \mathrm{He} \rightarrow \mathrm{He}^{++} + 2e^-$ (see [1] and references therein). This direct ('d') two-electron process occurs simultaneously with the sequential ('s'), third-order (in the light intensity, I) process involving 2 steps: $\gamma + \mathrm{He} \rightarrow \mathrm{He}^+ + e^-$ ('s1') and $2\gamma + \mathrm{He}^+ \rightarrow \mathrm{He}^{++} + e^-$ ('s2'). While the 'd' channel is of second-order in I, the 's' channel amplitude is usually of comparable or greater magnitude for intensities that produce a measurable ionization yield, i.e., I of order (10^{14}-10^{15}) W/cm^2 [1]. However, one can enhance the relative contribution of the 'd' channel by using an appropriate photon energy E_γ (e.g., $E_\gamma = 45$ eV for He), thereby suppressing the 's2' step of the 's' channel [1].

We analyze here how to control and distinguish between the 'd' and 's' channels (even when they have comparable electron yields) by measuring the electron angular distributions for different light polarizations. For the case of circularly polarized light, for example, the triply-differential cross section, $\sigma^{(3)} \equiv d^3\sigma/(dE_1 d\Omega_1 d\Omega_2)$, exhibits circular dichroism (CD) in the case of the 'd' channel (for both equal and non-equal energy sharing between the photoelectrons) [2], while CD in the 's' channel is absent. From our *ab initio* (dynamical model-independent) parametrization of $\sigma^{(3)}$ for the 'd'-channel [2], one may obtain the experimentally more feasible doubly-differential cross section (by integration of $\sigma^{(3)}$ over the ejection angle of the second electron),

$$\sigma^{(2)} \equiv d^2\sigma/(dE_1 d\Omega_1) = \sigma_0 + \xi l \sigma_{ed}, \qquad (1)$$

where l and ξ are the degrees of linear and circular polarization of the incident light ($l^2 + \xi^2 = 1$) [2]. The parameter σ_0 in (1) is invariant under a change in sign of ξ, while σ_{ed} describes the elliptic dichroism (ED) effect, i.e. the dependence of $\sigma^{(2)}$ on the handedness of elliptically polarized light. (Note that the ED effect vanishes for the case of circular polarization, $\xi = \pm 1$.) While the 's1'-step of the 's' channel is insensitive to the sign of ξ, the angular distribution for the two-photon step 's2' has the same form (1) as for 'd' channel [3]. However, the differences in ejected electron energies as well in physical electron-ejection mechanisms between the 's' and 'd' channels ensure pronounced differences in the magnitudes of ED effects in these channels, thus providing a means to control the 'd'-channel contribution. Using methods of Ref. [2], we discuss optimal conditions for experimental observation of the 'd' channel contribution to double ionization of He using elliptically polarized light with $E_\gamma = 45$ eV.

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Tu2-33

Quantitative investigation of non-linear effects on atomic and molecular photoionization

A.A. Sorokin[1,2], S.V. Bobashev[2], K. Tiedtke[3], and M. Richter[1]

[1]*Physikalisch-Technische Bundesanstalt, PTB, Abbestrasse 2-12, D-10587 Berlin, Germany*

[2]*Ioffe Physico-Technical Institute, Polytekhnicheskaya 26, 194021 St. Petersburg, Russia*

[3]*Deutsches Elektronensynchrotron, DESY, Notkestrasse 85, D-22603 Hamburg, Germany*

Photoionization of neon atoms and molecular nitrogen with pulsed and intense radiation of Free-electron LASser in Hamburg (FLASH) in the vacuum ultraviolet spectral range has been studied by ion time-of-flight spectroscopy. Emphasis was laid on the determination of absolute numbers for photons and generated ions per pulse with the help of a calibrated experimental setup. Non-linear effects, due to vanishing targets, space-charge, Coulomb explosion, and multi-photon excitation which are of general importance when high-intensity radiation interacts with matter could therefore be investigated by quantitative measurements.

Tu2-34

Visualizing and Controling Ultrafast Wave-Packet Interference in Diatomic Molecules

Hiroyuki Katsuki[1,2], Hisashi Chiba[1,2], Kenji Ohmori[1,2], Christoph Meier[3], and
Bertrand Girard[3]

[1]Institute for Molecular Science, Myodaiji, Okazaki 444-8585 Japan
[2] CREST, Japan Science and Technology Agency, Kawaguchi, Saitama 332-0012,
Japan
[3] LCAR –IRSAMC, CNRS, Université Paul Sabatier–Toulouse 3, France.

Inteference of matter waves has been a focus topic in the quantum world, playing important roles in the studies on the quantum-classical boundary, quantum computations, quantum cryptography and so on. Here we demonstrate unprecedently high-resolution measurements and control of the interference of vibrational wave packets created in diatomic molecules.

Recently we have observed transient interference of two counter-propagating vibrational wave-packets generated around the half-revival period on the *B*-state potential of the iodine molecule (I_2) [1]. ‘Quantum ripples’ appeared periodically only when the two wave packets cross each other, and their structures were measured successfully with a few picometers and ~100fs spatiotemporal resolutions (see Fig. 1).

In this talk, we also present ‘active’ control of these quantum ripples; the control has been carried out with a pair of fs laser pulses whose relative phase is locked with our highly-stable interferometer called an “attosecond phase modulator (APM)” [2, 3]. Two counter propagating wave packets are prepared by setting the delay τ between the phase-locked twin pulses to around $1.5T_{vib}$, where T_{vib} is a classical vibrational period of I_2. Depending on the relative phase between the twin pulses, the spatiotemporal pattern of the ripples, which we call “quantum fabric”, changes drastically. To the best of our knowledge, this is one of the finest manipulations within the molecules ever performed.

Moreover, we have utilized these experimental techniques to read and write amplitude and phase information of the vibrational eigenstates within the wave packets.

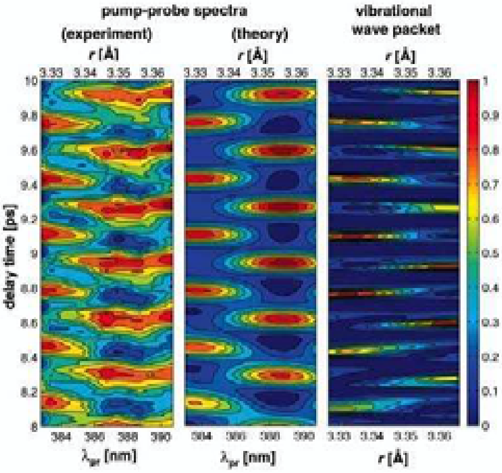

Fig. 1: (left) observed interferometric structure by pump-probe spectroscopy. (center) theoretical simulation.
Taken from reference [1].

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Tu2-35

THE ROLE OF NUCLEAR MOTION IN EXCITATION AND IONIZATION OF H_2 BY ULTRASHORT VUV LASER PULSES

Alicia Palacios*, Henri Bachau† and Fernando Martín*

*Departamento de Química, C-9, Universidad Autónoma de Madrid, 28049 Madrid, Spain
†CELIA (UMR 5107 du CNRS-CEA-Université de Bordeaux I), 33405 Talence Cedex, France

Free electron lasers and high-order harmonic generation are currently able to produce intense vuv pulses in the femtosecond (fs) and subfemtosecond (sub-fs) time domains. Vuv radiation can be used to induce ionization of simple atoms (He, Ne, ...) and molecules (H_2^+,H_2...)[1] by absorption of a few photons. In addition, fs and sub-fs durations are ideal to explore physical problems at the atomic and molecular time scales [2]. For example, the revolution time of an electron orbiting around a proton is □ 150 attoseconds. Molecular processes are even more interesting due to the presence of nuclear motion, which manifests through vibration, rotation and the possibility of dissociation (vibration and rotation typically occur in the fs time scale).

Our goal is to explore physical effects induced by the nuclear degrees of freedom and, therefore, not possible in atoms. We report *ab initio* calculations for excitation and ionization of the hydrogen molecule by using ultrashort vuv laser pulses.

Our theoretical method is based on solving the time-dependent Schrödinger equation in a basis of stationary molecular states which include correlation and all electronic and vibrational degrees of freedom [3]. We show that, by varying the pulse duration in the fs time domain, it is possible to control the radio of dissociative to non-dissociative ionization in H_2[4]. Furthermore, by using intense vuv/fs pulses it is possible to induce Rabi-type oscillations which proceed through a step-ladder mechanism involving the vibrational levels of the initial and intermediate electronic states [5]. This mechanism leads to an unexpected large population of excited electronic states, as well as to an effect reminiscent of the Autler-Townes splitting in the electron and vibrational energy distributions of the fragments in the ionization process.

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Tu2-36

THE EXPERIMENTAL INVESTIGATIONS OF MULTIPHOTON TRANSITIONS IN THE PRESENCE OF ADDITIONAL STRONG NONRESONANT RADIATION

I. I. Bondar' and V. V. Suran

Uzhgorod National University, Uzhgorod, 88000, Voloshina str.,54, Ukraine,
bondar.ivan@gmail.com

The experimental investigation of multiphoton transitions in barium atom in presence of additional nonresonant laser radiation was carried out. In particular we investigate the four-photon transition from ground $6s^2\ {}^1S_0$ in $6p^2\ {}^1S_0$ and $6p^2\ {}^3P_0$ states of Ba atom. The frequencies ω=8594 cm^{-1} and ω=8623 cm^{-1} are correspondent to these transitions between denoted unperturbed states. For realization of these transitions the radiation of laser on color centre (LCC) with tunable frequency (ω_1=8570-8650cm^{-1}) was used. The radiation of dye laser (DL) with fixed frequency ω_2=17345cm^{-1} was used as the additional nonresonant radiation. The polarization of both laser radiations was linear with parallel orientation of its electric vectors.

We measured the dependences of the yield of Ba^+ ions formed as a result of the ionization of *Ba* atoms on the LCC radiation frequency under the conditions when this radiation acted on *Ba* atoms both independently and in combination with the DL radiation. The results obtained in our experiment are shown in figure. When only LCC radiation acts on *Ba* atoms the yield of Ba^+ ions contains a one wide peak with asymmetry shape. This peak conditioned by four-photon excitation of strongly perturbed $6p^2\ {}^1S_0$ state by LCC radiation. When the LCC radiation acts on *Ba* atoms simultaneously with DL radiation besides mentioned wide peak the yield of Ba^+ ions contains two additional narrow peaks. These additional narrow peaks are conditioned by four-photon excitation of nonperturbed $6p^2\ {}^1S_0$ and $6p^2\ {}^3P_0$ states by LCC radiation.

The appearance of these two peaks indicates that in case of presence of DL radiation the excitation of $6p^2\ {}^1S_0$ and $6p^2\ {}^3P_0$ states by LCC radiation is realized at smaller intensities of this radiation then in case of DL radiation absence. These results show that addition of strong nonresonant laser radiation in process of multiphoton excitation of atomic states leads to increase of these process probability.

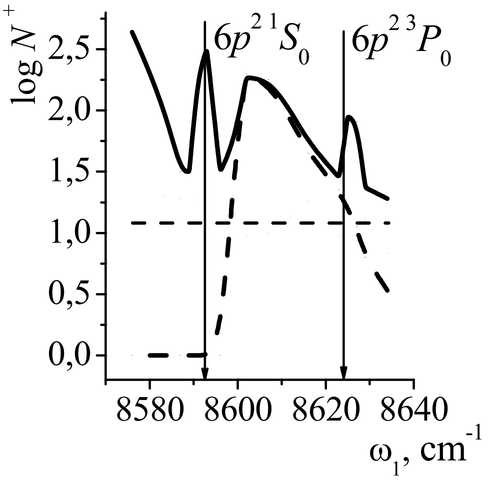

Fig. The dependences of the yield of Ba^+ ions (N^+) on the LCC radiation frequency (ω_1) measured under the conditions when the LCC radiation acted on *Ba* atoms independently (dashed curve) and simultaneously with the DL radiation (solid curve). The average yield of Ba^+ ions formed under the action of only LC radiation is shown by dashed horizontal line. By vertical arrows are denoted the frequencies of LCC radiation corresponding to four-photon excitation of nonperturbed of $6p^2\ {}^1S_0$ and $6p^2\ {}^3P_0$ states.

Tu2-37

IONIZATION-INDUCED CONVERSION OF FEW-CYCLE LASER PULSES INTO TERAHERTZ RADIATION

V.B. Gildenburg and N.V. Vvedenskii

Institute of Applied Physics RAS, Nizhny Novgorod 603950, Russia
e-mail: vved@appl.sci-nnov.ru

We suggest a new method of THz wave generation based on the ionization-induced excitation of the natural plasma oscillations during the gas breakdown produced by an ultra-short (few-cycle) laser pulse. The initial push for the natural plasma oscillations is driven, in this case, directly by the optical electric field imparting a large constant velocity component (depending on the field phase) to the newly born electrons. The ionization process apart, this excitation mechanism by itself is linear (or "linear-parametric") with respect to the pumping (exciting) optical field and, therefore, can ensure very efficient conversion of this field into the radiative plasma oscillations. The considered excitation mechanism is related to that studied theoretically and experimentally in Refs. [1-4], where the natural plasma oscillations were excited by extraneous (static or microwave) fields, and fs laser pulse served for the plasma creation only. The maximum permissible strengths of the external (pumping) field is determined in this case by the threshold of gas breakdown, that limits strongly the amplitude of oscillations and accessible value of THz radiation. The method of generation we suggest here is free from this limitation as both the gas ionization and excitation of plasma oscillations are produced by the same strong laser electric field (comparable in the order to the atomic one).

We have analyzed the processes of plasma creation, electron current excitation and THz wave emission induced by the axicon-focused Gaussian pulse. The efficiency of the conversion processes depends strongly on the duration, transverse scale, and carrier-envelope phase of the ionizing pulse. For a few-cycle (~ 5 fs) laser pulse of moderate intensity ($\sim 10^{14} - 10^{15}$ W/cm^2), the considered (ionization-induced) conversion mechanism is found to be much more effective than the alternative one based on the excitation of plasma oscillations in the laser wakefield by the ponderomotive force [5-7] and can provide THz radiation of the gigawatt power level. This work was supported by the Russian Foundation for Basic Research (project nos. 06-02-17496, 07-02-01265, and 07-02-01239) and the Russian Science Support Foundation.

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Tu2-38

Measurements by Evanescent Waves and Information

Yacob Ben-Aryeh
Department of Physics, Technion-Israel Institute of Technology ,Haifa,32000,Israel
e-mail: phr65yb@physics.techniom.ac.il

Usually the information included in evanescent waves is lost as the pictures of the objects are taken in the far field. However, by applying a 'tip detector' of a subwavelength dimension in an evanescent waves one can convert part of this field into propagating waves which include information on the smallest details of the object. It has been shown in a previous study [1] that the convolution between the spatial frequencies of the evanescent waves and those of the detectors leads to tunneling of evanescent waves into propagating waves. We show here that for imaging by evanescent waves the effective amplitude for this imaging will decrease inversely proportional to the amount of information obtained by this imaging. This conjecture is proved by analyzing a special example, e.g., for very narrow apertures in a plane screen. Then we explain why this conjecture will be valid also in the general case.

We assume a plane monochromatic light with a constant amplitude and wavevector $k_0 = 2\pi/\lambda$ incident on dielectric plane screen with narrow apertures (smaller than a wavelength) with a transmission T expanded into Fourier series:

$$T(x,y) = T(x)T(y) \quad , \quad T(x) = \sum_{m=-\infty}^{\infty} T_m \exp(imk_0x) \quad , \quad T(y) = \sum_{m=-\infty}^{\infty} T_n \exp(ink_0x) ,$$

where this expansion follows from the boundary conditions of the screen. For each component of the evanescent waves $(m \geq 1, n \geq 1)$ the imaginary component of the wavevector in the z direction is given by $\left[k_0{}^2 - (mk_0)^2 - (nk_0)^2\right]^{1/2}$. The multiplication of k_0 by m and/or n can be related to quantum mechanical correlations by which the effective wavelength is reduced by these factors, leading to higher resolution [2]. Since different components of the evanescent waves have different decay in the z direction the picture is distorted for finite z values. This problem can be avoided by using Pendrys' lens where the pictures can be taken in the focal plane [3].

We assume that the spatial frequency distribution of the detector is determined by $C\exp\left[-\left(k_x{}^2 + k_y{}^2\right)\sigma^2\right]$ where C is a normalization constant and $\sigma \ll \lambda$. Although the evanescent waves are composed of high spatial frequencies for which there is not any propagation of energy in the z direction the convolution with the high spatial frequencies of the detector leads to spreading of the spatial frequencies so that some of the convoluted spatial frequencies are in propagating modes. In other words tunneling of high spatial modes with wavevectors components mk_0 and nk_0 ($m \gg 1$, $n \gg 1$) in the x and y directions, respectively, to propagating modes (for which $k_x{}^2 + k_y{}^2 < k_0{}^2$) will occur if $\left[\left\{k_x - mk_0\right\}^2 + \left\{k_y - nk_0\right\}^2\right]\sigma^2 \leq 1$. In order to transform evanescent waves with larger values of k vectors (i.e, larger values of m and n) we need to use a tip detector with a narrower transfer function (i.e., with smaller value of σ). The transfer function will then include a broader band of wavevectors so that only a smaller part of this band of wavevectors will be obtained as propagating wavevectors.

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Tu2-39

RELATIVISTIC IONIZATION AND RESCATTERING

K. Z. Hatsagortsyan , M. Klaiber, R. Fischer, M. Lein, M. Verschl, and C. H. Keitel

Max-Planck-Institut für Kernphysik
Saupfercheckweg 1, D-69117 Heidelberg, Germany
e-mail:k.hatsagortsyan@mpi-hd.mpg.de

With modern laser technology it has become possible to investigate intense laser-matter interaction up to the relativistic regime. The relativistic effects have substantial impact on high-harmonic generation and other processes based on the recollision of the ionized electron with atomic core. The laser magnetic field induced drift of the ionized electron in the laser propagation direction severely suppresses the probability of the electron revisiting the ionic core and, consequently, the yield of harmonic photons or probabaility of other processes. We propose several methods to circumvent this effect and to increase the efficiency of rescattering in relativistic regime.

In the weakly relativistic regime, we demonstrate that the electron relativistic drift can be efficiently harnessed to enhance the recollisions of electrons from molecular orbitals with mirror antisymmetry [1]. We investigate this phenomenon by calculating high harmonic generation for the first excited electronic state of an H_2^+ subjected to an intense linearly polarized laser pulse beyond the dipole approximation. Depending on the orientation of the molecular axis, the harmonic signal can be considerably enhanced.

In the strong relativistic regime, we show how efficient recollisions are feasible by employing strong laser pulses specially tailored as an atosecond pulse train [2]. The temporal tailoring of the laser pulse is aimed to concentrate the ionizing and afterwards the accelerating laser forces in short time intervals within the laser period. Consequently, the time span during which the electron moves with relativistic velocity is much shorter than in the sinusoidal laser pulse which substantially reduces the relativistic drift. The high harmonic generation rate in in relativistically strong tailored laser pulse is calculated and shown to be increased by several orders of magnitude compared to the case of conventional laser pulses. For experimental realization it is more advantageous the employment of counter-propagating attosecond pulse trains of relativistic intensity. In this case the suppression of the relativistic drift is significantly higher, while restrictions on the pulse features of the train are much relaxed than in the previous case. By this way the energies of the revisiting electron at the atomic core can reach the MeV domain, thus rendering hard x-ray harmonics and nuclear reactions with single atoms feasible. Other recollision schemes proposed are based on two consecutive counterpropagating laser pulses [3] and magnetic field.

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Tu2-40

NEW FORMULATION TO CALCULATE HARMONIC GENERATION

M.V. Frolov[1)], A.V. Flegel[1)], N.L. Manakov[1)], and Anthony F. Starace[2)]

[1)]Department of Physics, Voronezh State University, Voronezh 394006, Russia
[2)]Department of Physics & Astronomy, The University of Nebraska, Lincoln NE 68588, USA

The high harmonic generation (HHG) process for a single atom driven by an intense monochromatic laser pulse is formulated in terms of the system's quasienergy [1]. This formulation makes use of the Hellmann-Feynman theorem for the quasistationary quasienergy (or Floquet) states (QQES) of the quantum system subjected to a periodic perturbation. In brief, we introduce the (complex) quasienergy, ε, of the atom in a bichromatic (strong laser and weak probe) field of frequencies ω and $N\omega$. The amplitude for generation of the Nth harmonic is then given by the derivative of ε with respect to the probe field amplitude. Because of its focus on the complex quasienergy, our formulation automatically includes both the Stark shift and the ionization width of the initial bound state subjected to a strong laser field. Our results thus permit a clear and unambiguous way to avoid the non-regularizable singularities that appear when using quantities that are only well-defined for a stable quantum system (e.g., the expectation value of the dipole operator) to describe HHG phenomena in the presence of multiphoton above-threshold ionization. Our formulation yields moreover a result for the HHG amplitude that is equivalent to that obtained using properly-normalized QQES wave functions, i.e. involving dual QQES wave functions to obtain so-called dual dipole moments, thereby justifying use of the concept of the dual dipole moment in accurate HHG calculations. Approximations to our exact results for the HHG amplitude allow connection to various commonly used approximate formulations for HHG and delineation of their differences. In addition to its utility for analyzing such formal aspects of HHG theory, another advantage of formulating the HHG amplitude in terms of the complex quasienergy is that one avoids having to know the explicit form of the QQES (as well as the initial bound state) wave function in calculations of HHG rates.

As an application of our new formulation for the HHG amplitude, we develop a self-consistent, essentially analytical theory of HHG within the framework of the time-dependent effective range (TDER) theory for describing intense laser processes [2]. This TDER HHG theory thus allows a quantitative description of harmonic generation by negative ions with outer (weakly bound) electrons in *s*- and *p*-states. As applications of this theory, we describe connections to (and the validity of) commonly used approximate theories for HHG, we elucidate the dependence of HHG rates on the spatial symmetry of the initial bound state, and we compare and contrast HHG rates for a number of negative ions.

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Tu2-41

AN IMPROVED QUSICLASSICAL APROACH FOR HIGH-ORDER HARMONIC GENERATION

M.V. Frolov[1], A.V. Flegel[1], N.L. Manakov[1], Anthony F. Starace[2]

[1]Department of Physics, Voronezh State University, Voronezh 394006, Russia
[2]Department of Physics & Astronomy, The University of Nebraska, Lincoln NE 68588, USA

Quasiclassical results for above-threshold ionization (ATI) [1] and high harmonic generation (HHG) [2] rates are very attractive in view of their dependence on only two atomic parameters, the binding energy of the initial state $|nlm>$, E_n, and the known asymptotic coefficient, C_{nl} , of the wave function for the state $|nlm>$. However, in contrast to ATI, the quasiclassical HHG rates [2] for bound states with nonzero angular momentum l have been found to be sensitive to the whole-space behavior of the wave function for the state $|nlm>$ [3]. The use of parametrized realistic wave functions for p-states in quasiclassical calculations [4] improves results for HHG rates but makes them quite sensitive to the parameters used.

We present here an improved quasiclassical approach for HHG calculations [5] within the framework of time-dependent effective range (TDER) theory for intense laser processes [6]. In contrast to standard quasiclassical methods [1,2], we do not employ steepest descent methods for spatial (or momentum) integrals involving the wave function for the state $|nlm>$ (which is typically approximated by its large-r asymptotic form). Instead, we present the HHG amplitude in terms of the complex quasienergy and use the steepest descent method only for the evaluation of temporal integrals over the laser period. As a result, we obtain analytic, two-parameter (E_n and C_{nl}) expressions for HHG rates that are correct for states with $l=0$ and $l=1$. For a weakly-bound s-state, our results coincide completely with those of the quasiclassical three-step model [2]; for halogen negative ions with an outer, weakly bound p-electron, our results for HHG rates agree with those in [4] using realistic wave functions. Comparisons of our quasiclassical HHG rates for s- and p-states with our exact TDER HHG rates show that quasiclassical results are in good quantitative agreement with exact results except in two cases: (a) for low-order harmonics just below the onset of the high-energy plateau, and (b) for high frequencies, when the laser photon energy is of order (0.3 – 0.5) $|E_n|$. Since TDER theory is applicable for a finite-range potential, we also introduce the quasiclassical scaling of our TDER results for negative ions to the case of neutral atom targets.

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Tu2-42

ULTRAFAST PHOTOPROCESSES IN CONTACT ION PAIRS OF INDOTRICARBOCYANINE DYES

[2]Tikhomirov S.A., [1]Samtsov M.P., [2]Dubovskii, V.L., [2]Buganov O.V.,
[1]Melnikov D.G., [1]Voropay E.S.

[1]A.N.Sevchenko Research Institute for Applied Physical Problems
of the Belarusian State University, Minsk, Belarus
[2]Institute of Molecular and Atomic Physics, National Academy of Sciences of
Belarus, Ave. Nezalezhnasti 70, 220072 Minsk, Belarus
E-mail: tikhomirov@imaph.bas-net.by

Cationic polymethine dyes have considerable promise as photosensitizers for photochemotherapy of cancer and as biological markers for various applications. As demonstrated in [1,2], indotricabocyanine dyes are localized in tumor cells within the region characterized by a low dielectric constant, mainly in the form of contact ion pairs. Proceeding from the fact that indotricarbocyanine dyes retain their photocytotoxicity in hypoxic conditions [2], the charge transfer in contact pairs with the formation of free radicals may be thought as a starting mechanism for the tumor cell damage. However, in literature one can find conflicting opinions concerning a possibility of the photochemical reactions proceeding with the electron phototransfer in contact ion pairs of polymethine dyes and simple "inert" ions (e.g., Br^-, ClO_4^-). This communication presents the recent experimental results obtained in studies into the spectroscopic properties of a series of indotricarbocyanine dyes in solvents of different nature. The principal objective of the work is to investigate fast relaxation processes taking place in the molecules under study just after their excitation and to analyze the possibility for the realization of fast direct and back charge transfer in ion pairs of indotricarbocyanine dyes with simple Br^-, I^- and ClO_4^- anions. A comparative analysis of the femtosecond transient absorption spectra recorded for these compounds in conditions enabling transition of the dye molecules into the excited state in a specific ionic form is performed.

The experiments and measurements of transient absorption spectra of the dyes conducted using a home-made femtosecond spectrometer [3], based on the original Ti: Sp generator with synchronous pumping by a Nd: YAG pulsed laser and a regenerative amplifier, are described.

Fast transformations (10 – 30 ps) of transient absorption spectra in a long wavelength absorption band of the compounds studied are interpreted within the framework of the concept of a hole burning at the profile of a vibronic band. The qualitative differences in registered absorption spectra from the excited electronic states of the molecules studied at different experimental conditions are explained assuming ultrafast charge transfer in contact ion pairs that results in the formation of free radicals.

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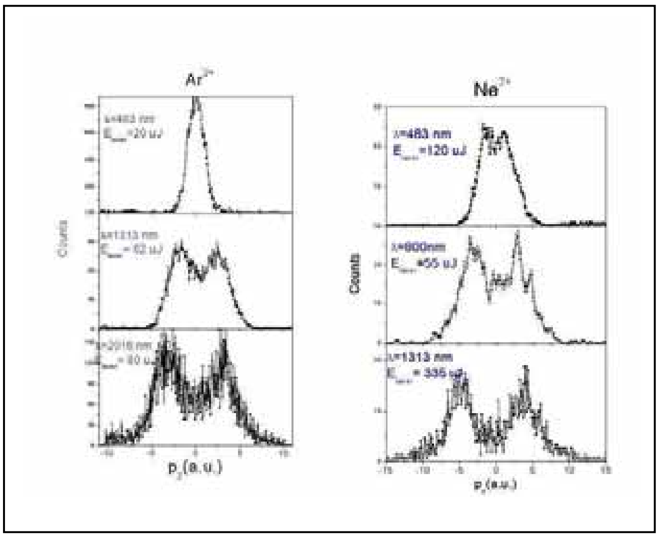
Tu2-43

Strong-Field Non-Sequential Double Ionization: Wavelength Scaling Similarity of Ion Momentum Distributions for Ne and Ar

A.S. Alnaser[1], D. Comtois[2], A.T. Hasan[1], D.M. Villeneuve[3], J.-C. Kieffer[2] and I.V. Litvinyuk[4]

[1]Physics Department, American University of Sharjah, Sharjah, UAE
[2]INRS-Énergie, Matériaux et Télécommunications, 1650, boul. Lionel-Boulet, Varennes, Québec, Canada J3X 1S2
[3]National Research Council of Canada, 100 Sussex Dr, Ottawa, Ontario, Canada K1A 0R6
[4] Presenting author - J.R. Macdonald Laboratory, Physics Department, Kansas State University, Manhattan, Kansas, USA 66506



Strong-field double ionization of atoms in non-sequential regime produces longitudinal ion momentum distributions with a characteristic double-peak structure. At 800 nm laser wavelength in Ne^{2+} the structure is very pronounced with a well resolved dip at zero momentum, while for Ar^{2+} the dip is very shallow, possibly indicating different mechanisms in the two atoms. We investigated the source of this difference by measuring longitudinal momentum distributions of Ne^{2+} and Ar^{2+} ions at different laser wavelengths (485, 800, 1313 and 2000 nm) and intensities. The shapes of experimental momentum distributions for the two atoms exhibit a simple wavelength scaling relationship: they are similar for the same value of a scaling parameter given by the ratio of maximum electron recollision energy ($3.17\ U_p$ at saturation intensity for single ionization) to ionization potential of a singly charged ion. This similarity indicates that the difference between Ne and Ar observed at 800 nm should not be attributed to differences in relative electron impact ionization and excitation cross-sections of the two atoms, stemming from their electronic structure, as was thought previously. It is rather due to interplay between values of maximum energy of recollision electrons at any given wavelength and ionization potential of a singly charged ion.

Tu2-44

TIME-DEPENDENT EFFECTIVE RANGE THEORY OF INTENSE LASER PROCESSES

M. V. Frolov (1), N.L. Manakov (1), Anthony F. Starace (2)

(1) Department of Physics, Voronezh State University, Voronezh 394006, Russia
(2) Department of Physics, The University of Nebraska, Lincoln NE 68588, USA

One of the most basic analytic theories in intense laser-atom physics is the Keldysh theory for above-threshold ionization (ATI) or detachment (ATD) of a bound electron in a strong, low-frequency laser field [1]. While it is nonperturbative in the laser field, the Keldysh theory neglects effects of the binding potential on continuum electron states. For this reason, although the Keldysh approximation provides reliable predictions for total decay rates, its results for photoelectron energy or momentum distributions are valid only in the low-energy, or "Keldysh", part of ATI/ATD spectra. The description of high-energy plateau structures in photoelectron spectra (which originate from rescattering effects) requires a proper account of the binding potential. The simplest exactly-solvable model providing an accurate quantum treatment of both laser and binding potential effects is the zero-range potential (ZRP) model, in which the potential modifies the three-dimensional continuum wave function of the ionized electron through the *S*-wave scattering phase [2]. The exact results for the quasistationary quasienergy state (QQES) or Floquet wave function of an initially bound electron in a ZRP allow one to reveal the underlying quantum origin of plateau features in laser-atom processes (in terms of the properties of the exact QQES wavefunction) [3].

We discuss here a more accurate, exactly-solvable quantum model of strong field processes than the ZRP model: the time-dependent effective range (TDER) theory [4]. This theory represents a generalization of the ZRP model in two main ways. First, in addition to the scattering length (or the binding energy), which is the only prescribed parameter of the problem within the ZRP model, TDER theory introduces a second parameter, the effective range (which is closely related to the coefficient of the known asymptotic form of the wave function for the initially bound electron in a finite-range potential $U(r)$). TDER theory thus provides a more precise, two-parameter description of atomic systems having a valence electron in a bound *S*-state. Second, TDER theory allows one to extend a ZRP-like analysis to weakly-bound valence electron states having non-zero angular momentum, thus allowing one to study the dependence of plateau features on the spatial symmetry of the initial bound state. To lowest order in $U(r)$, TDER results reduce to those of the Keldysh approximation (using the length gauge for the laser-atom interaction). TDER theory provides quantitatively accurate predictions for strong-field effects involving negative ions, while for atoms, Coulomb scaling factors should be introduced, similarly to those introduced in Keldysh theory.

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Tu2-45

CONVERGENT CLOSE COUPLING CALCULATIONS OF MULTIPHOTON IONIZATION OF HELIUM

I. A. Ivanov and A. S. Kheifets

Research School of Physical Sciences, The Australian National University
Canberra ACT 0200, Australia

Theoretical investigation of multiphoton ionization (MPI) of atomic and molecular species is one of the "hot" topics of contemporary atomic collision physics. Several time-dependent and Floquet-based techniques had been established in recent years to treat the MPI process. To broaden this theoretical arsenal, in a recent work [1] we have outlined a novel formalism and develop a computational procedure to treat the MPI process of atomic targets in strong laser fields. We treat the MPI process nonperturbatively as a decay phenomenon by solving a coupled set of the integral Lippmann-Schwinger equations. As basic building blocks of the theory we use a complete set of field-free atomic states, discrete and continuous. As a demonstration of principle, we applied the proposed procedure to a simple model of MPI from a square well potential and to the hydrogen atom. Good agreement with previously published results was achieved.

The Lippmann-Schwinger approach should enable us to provide both the total and differential cross-sections of MPI of atoms with one or two electrons. For two-electron targets, an accurate set of target states, both discrete and continuous, can be generated by the so-called convergent close coupling (CCC) method. This method has been extensively tested for processes with two electrons in the continuum such as electron scattering on atomic hydrogen [2] and low-field double ionization of helium [3].

The work is now underway to utilize the CCC basis within the Lippmann-Schwinger description of the MPI process. We have encountered, and successfully overcome, the problem of divergence of the dipole matrix elements for the free-free electron transitions. This problem can be avoided by choosing the interaction Hamiltonian in the Kramers- Henneberger (acceleration) gauge. A succession of the models of increasing accuracy is considered starting from the perturbative regime for the frozen-core He atom, relaxation of the core to include two-electron excitations and, finally, fully non-perturbative regime for one- and two-electron transitions. The latter model should enable us to describe the two-photon two-election ionization in the mode of the free-electron laser. So far, the frozen-core model produced accurate numerical results shown in the figure. Results of more sophisticated models will be presented at the conference.

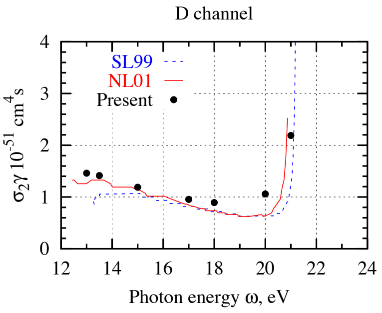

Fig. 1. Two-photon ionization cross-sections of He in the S- and D-channels. Comparison is made with literature values marked as SL99 [4] and NL01 [5]

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POSTERS

Tuesday 8/5

3. Biomolecules - Biophysics

Tu3-1

DISPERSION OF DARK BACTERIORHODOPSIN AT 800 NM

G. Szalay[1], Zs. Heiner[1,2], K. Osvay[1,3]

[1] Department of Optics, University of Szeged, P.O.Box 406, Szeged 6701, Hungary
[2] Institute of Biophysics, Biological Research Center, P.O.Box 521, Szeged, Hungary
[3] Max Born Institute, Max-Born-Str. 2A, D-12489 Berlin, Germany
osvay@physx.u-szeged.hu

Recent applications of bacteriorhodopsin (bR) are relied on the direct or indirect utilization of its optical properties. Apart from one measurement of the refractive index of a bR film in the visible [1], however, no information is available on the dispersion properties of bR. Regarding the promising role of bR in biophotonics, the lack of data becomes especially disturbing in the near infrared, where femtosecond lasers are typically available. Since bR has many photo cycles, the exact measurement should account for the appropriate state of bR, as well. Here we present the determination of the concentration dependent dispersion of dark (unexcited) bR.

In the experiment a Michelson-interferometer was constructed having bacteriorhodopsin suspended in TRIS in the sample arm, and pure TRIS in the reference arm. Since bR cannot be directly excited by light with a wavelength longer than 680 nm, the interferometer was illuminated by 800 nm, 17 fs laser pulses from a Ti:S laser oscillator. The resulting interference pattern was directed to an imaging spectrograph. The formed spectrally and spatially resolved interference (SSRI) fringes are characteristic purely for the bR in the sample arm. The spectral shift of the phase is directly deducted from the SSRI fringes [2], providing hence the relative change of refractive index within the spectral range of the laser pulse. Taking the slope of the change of refractive index at 800 nm, the dispersion, that is dn(λ)/dλ, is calculated.

The measurement has been carried out for seven concentrations of bR, each having derived from the same sample of dense bR (OD=40) prepared by the standard technique of centrifugation. At each concentration a set of forty SSRI patterns was captured and evaluated. The relative change of spectral refractive indices (Fig. 1a) is moderate, as one can expect for low concentration. For higher concentrations this can be predicted from the concentration dependent dispersion (Fig. 1b).

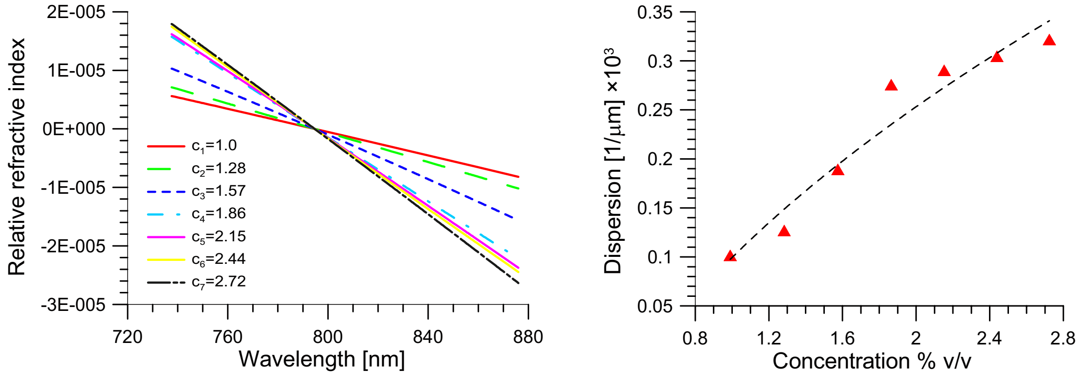

Figure 1. Relative change of spectral refraction index (a) and dispersion (b) of bacteriorhodopsin at different concentrations.

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Tu3-2

The backbone effects in intermolecular normal mode vibrations of adenine-thymine simple and double sequenced base pairs system

A. Bende[1,2] and S. Suhai[2]

[1]National Institute for R&D of Isotopic and Molecular Technologies, Molecular and
Biomolecular Physics Department, Donath Street, No 71-103, Ro-400293,
Cluj-Napoca, Romania. email: bende@s3.itim-cj.ro

[2]German Cancer Research Centre, Molecular Biophysics Department, Im
Neuenheimer Feld 580, D-69120, Heidelberg, Germany. email: S.Suhai@dkfz-heidelberg.de

Hydrogen bonding is ubiquitous in nature and governs a wide array of chemical and biological processes ranging from local structure in molecular liquids to the structure and folding dynamics of proteins. Although the hydrogen bond is well studied, its low-frequency vibrations - the large-amplitude motions involving stretching and bending along the actual hydrogen-bond coordinates - have been rarely investigated. Information about these vibrations offers exceptional insight into the potential energy surface of the interaction and so further enhances our understanding of the hydrogen bond and its impact on molecular structure and dynamics. The "C=O···H-N" type hydrogen-bond (HB) is the one of the most frequent occur rent Van der Waals (VdW) bond in the biological systems. They can be found as a main component of the DNA bases pairs interaction systems or in protein α-helix and β-sheets. In their cases, not only the cognition of molecular structures are so much important, but also their dynamics, which in essence represent their biological functionality. In our previous work we have investigated the nature of this C=O···H-N hydrogen bond in case of formamide-water and formamide-formamide systems [1], giving a detailed description for binding energies, inter and intramolecular harmonic frequencies and their anharmonic corrections.

The equilibrium structures, binding energies and vibrational harmonic frequencies of the simple and double sequenced adenine-thymine (AT) molecular structures including the sugar-phosphate backbone has been investigated in order to study the low-frequency IR spectra using B3LYP exchange-correlation potential and considering the D95* basis set. The widely used a posteriori Boys-Bernardi "counterpoise" (CP) correction scheme for basis set superposition error (BSSE) elimination, has been included in our calculations in order to take into account the BSSE effects in geometry optimisation, binding energies and the harmonic vibrational frequencies. The different intermolecular normal mode vibrations of the simple and double sequenced AT-backbone molecular systems has been compared with the classical backbone-free AT system and the change in their normal mode vibrational behaviour are discussed.

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Tu3-3

Water ionization by charged particles: Medical applications

Christophe Champion

Laboratoire de Physique Moléculaire et des Collisions,
Université Paul Verlaine-Metz,
1 boulevard Arago, Technopôle 2000, 57078 Metz, France

With the more and more regular use of ionizing radiations in medicine, it is today necessary to appraise, at best, the biological consequences of radiological examinations, and particularly to know the energy deposits induced by all the radiations commonly used in radiotherapy and even in medical imaging (light and heavy ions, electrons and positrons, X-rays and γ-rays). This implies to be able to describe, at the nanometric scale, each collision induced by ionizing projectiles, in order to quantify the full spectra of molecular damage radio-induced. To do that, numerical simulations of charged particle track-structure were developed in modeling the biological matter by water [1-2]. Actually, accurate differential and total ionization cross sections are still needed to describe with the highest degree of accuracy the charged particle crossing trough the matter. In this state of mind, we have recently developed a full-differential model dedicated to water ionization by electron, positron and light ions (H^+, He^{2+}, C^{6+}) covering a large impact energy range. The theoretical results also obtained were in good agreement with the available experimental data [3-5], what encouraged us to extend our model to other biological target molecules like DNA bases. The expected results would be of prime importance for quantification of radio-induced damages at the cellular level.

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Tu3-4

ON MAGNETORECEPTION MECHANISMS IN BIRDS

Ilia A. Solov'yov[1], Danielle Chandler[2], Klaus Schulten[2] and Walter Greiner[1]

[1]Frankfurt Institute for Advanced Studies, Max-von-Laue str. 1
60438 Frankfurt am Main, Germany

[2]Department of Physics, University of Illinois at Urbana-Champaign, and
Beckman Institute for Advanced Science and Technology.
E-mail: ilia@fias.uni-frankfurt.de

The ability of some animals, most notably migratory birds, to sense magnetic fields is still poorly understood. Two, likely co-existing, mechanisms underlying animal magnetoreception are discussed.

It has been suggested [1, 2] that animal magnetoreception is mediated by the blue light receptor protein cryptochrome, which is known to be localized in the retinas of migratory birds. Cryptochromes are a class of photoreceptor signaling proteins which are found in a wide variety of organisms and which primarily perform regulatory functions, such as the entrainment of circadian rhythm in mammals and the inhibition of hypocotyl growth in plants. Recent experiments have shown that the activity of cryptochrome-1 in *Arabidopsis thaliana* is enhanced by the presence of a weak external magnetic field, confirming the ability of cryptochrome to mediate magnetic field responses. Cryptochrome's signaling is tied to the photoreduction of an internally bound chromophore, flavin adenine dinucleotide (FAD). The spin chemistry of this photoreduction process, which involves electron transfer from a chain of three tryptophans, can be modulated by the presence of a magnetic field through the so-called radical pair mechanism based on Zeeman and hyperfine coupling. We present calculations showing that the radical pair mechanism in cryptochrome can produce an increase in the protein's signaling activity of approximately 10% for magnetic fields on the order of 5 Gauss, which is consistent with experimental results. These calculations, in view of the similarity between bird and plant cryptochromes, provide further support for a cryptochrome-based model of avian magnetoreception.

An alternative avian magnetoreception mechanism is based on the interaction of two iron minerals (magnetite and maghemite) which were experimentally found in subcellular compartments within sensory dendrites of the upper beak of several bird species [3]. The iron minerals in the beak form platelets of crystalline maghemite and assemblies of magnetite nanoparticles. We develop a theoretical model [4] to quantitatively describe the interaction between the iron-mineral containing particles. We demonstrate that depending on the external magnetic field the external pull or push to the magnetite assemblies, which are connected to the cell membrane, may reach a value of 0.2 pN. This might be principally sufficient to excite specific mechanoreceptive membrane channels leading to different nerve signals and causing a certain orientational behavior of the bird.

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Tu3-5

ANTIBODY-ANTIGEN DISSOCIATION: FRAGMENTATION OF COMPLEX MULTI-ATOMIC AGGREGATES

Elsa S. Henriques[†] and Andrey V. Solov'yov

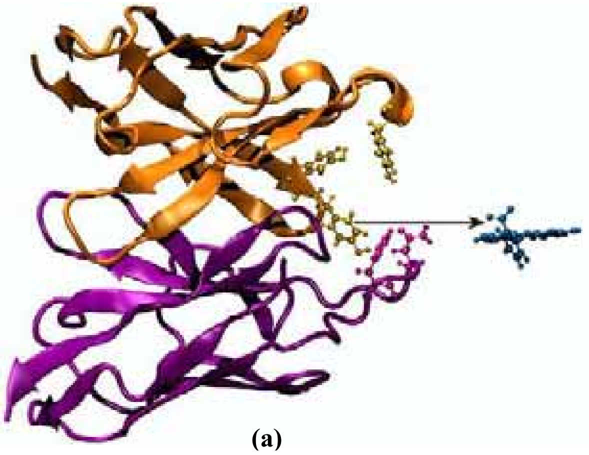
Frankfurt Institute for Advanced Studies,Max-von-Laue-Str. 1,
D-60438 Frankfurt am Main, Germany

[†] *Henriques@fias.uni-frankfurt.de*

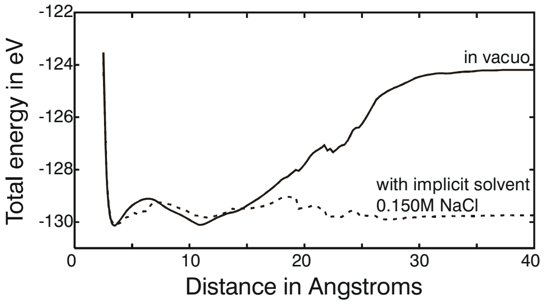
Life is driven by interactions between the molecular components of cellular machinery, and most cellular processes portray a cascade of association/dissociation events between proteins and their target molecules. The dissociation events are, in essence, a fragmentation of complex multi-atomic aggregates.

The fragmentation of multi-atomic aggregates has been extensively studied in atomic cluster physics, and the emerging key idea is that such processes can be successfully described in terms of a few collective coordinates that define the overall configuration of the escaping and parent fragments [1]. This concept also holds for similar events in more complex systems [2], and it prompted us to now address the dissociation process of an aggregate of higher complexity, a biological one.

Antibody–antigen complexes are involved in fundamental recognition processes during the body immune response. A reference example is the Fab4-4-20–fluorescein complex, and the present work reports a rational computational approach to probe its unbinding at the atomistic classical-mechanics level. The complex problem was reduced to a low-dimensional scanning along a selected distance between the antibody Fab4-4-20 and fluorescein (the antigen) as schematized in figure a. Positional and orientational coordinates of the escaping fluorescein were also assessed in order to fully characterise the unbinding. Solvent effects were accounted for by means of a continuum model. The dissociation time of the complex was derived from the calculated barrier height (figure b), in compliance with the experimentally reported Arrhenius-like behaviour. The computed results are in good agreement with the available experimental data.



(a)



(b)

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Tu3-6

AB INITIO DESCRIPTION OF PHASE TRANSITIONS IN FINITE BIO- NANO-SYSTEMS

Alexander V. Yakubovich, Ilia A. Solov'yov, Andrey V. Solov'yov
and Walter Greiner

Frankfurt Institute for Advanced Studies, Max-von-Laue str. 1
60438 Frankfurt am Main, Germany
E-mail: ilia@fias.uni-frankfurt.de

The phase transitions in finite complex molecular systems, i.e. the transition from a stable 3D molecular structure to a random coil state or vice versa (also known as (un)folding process) occur or can be expected in many different complex molecular systems and in nano objects, such as polypeptides, proteins, polymers, DNA, fullerenes, nanotubes.

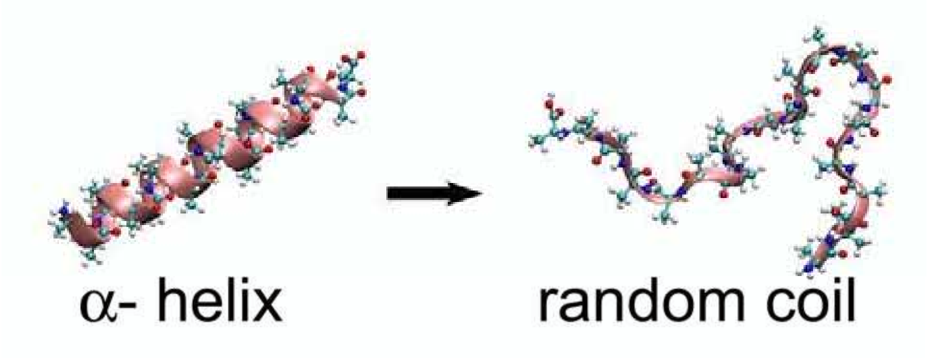

Fig. 1 The characteristic structural change of alanine polypeptide experiencing an α-helix↔random coil phase transition.

We suggest a novel *ab initio* theoretical method [1] for the description of phase transitions in the mentioned molecular systems. In particular, it was demonstrated that in polypeptides (chains of amino acids) one can identify specific, so-called twisting degrees of freedom, responsible for the folding dynamics of the amino acid chain, i.e. for the transition from a random coil state of the chain to its α-helix structure (see Fig. 1). The essential domain of the potential energy surface of polypeptides with respect to these twisting degrees of freedom can be calculated and thoroughly analysed on the basis of *ab initio* methods such as density functional theory (DFT) or Hartree-Fock method. It is shown [1] that this knowledge is sufficient for the construction of the partition function of a polypeptide chain and thus for the development of its complete thermodynamic description, which includes calculation of all essential thermodynamic variables and characteristics, e.g. heat capacity, phase transition temperature, free energy etc. The method has been proved to be applicable for the description of the phase transition in polyalanine of different length by the comparison of the theory predictions with the results of several independent experiments and with the results of molecular dynamics simulations.

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Tu3-7

QUANTUM BUILDING BLOCKS CONCEPT FOR BIOMACROMOLECULES

O. I. Obolensky, I. A. Solov'yov, A. V. Solov'yov, W. Greiner

A.F. Ioffe Physical Technical Institute, 194021 St. Petersburg, Russia
Frankfurt Institute for Advanced Studies, 60438 Frankfurt am Main, Germany

The idea of representing complex molecular structures as sets of building blocks is not new. It allows one to reduce drastically the volume of the conformational space, since fine details are integrated out producing renormalized effective interactions between the surviving collective degrees of freedom (the building blocks). The number of the degrees of freedom and accuracy of the effective interactions range widely depending on the system under consideration and on simplicity of the model. This strategy has led to significant breakthroughs in understanding structural properties of complex systems. For example, in the protein folding problem such phenomena as nucleation of the hydrophobic core or existence of a molten globule state can be explained with the building blocks concept [1]. The shortcoming of this approach is in the lack of predictive power for the *de novo* structure determination stemming from the excessive simplicity of the interaction potentials used.

We present here the formalism and the first results of quantum building blocks calculations in which the interaction potentials are calculated at an *ab initio* quantum mechanical level. We have performed density functional theory calculations of multidimensional potential energy surface for alanine-alanine interactions. In our approach the potential energy of the interaction depends on six variables, three of which describe the relative position and the other three describe the mutual orientation of the coordinate systems associated with each amino acid, see the figure. Using the quantum building blocks approach we found the global energy minimum structures of several Ala oligopeptides. The found structures are in a good agreement with our previous complete quantum mechanical analysis [2].

We acknowledge partial financial support from INTAS (contract 03-51-6170) and from European Commission (project EXCELL).

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Tu3-8

STRUCTURE OF UNFOLDED POLYPEPTIDES

O. I. Obolensky, K. Schlepckow, H. Schwalbe, A. V. Solov'yov

A.F. Ioffe Physical Technical Institute, 194021 St. Petersburg, Russia
Frankfurt Institute for Advanced Studies, 60438 Frankfurt am Main, Germany
Johann Wolfgang Goethe-Universität, 60438 Frankfurt am Main, Germany

Unfolded proteins have recently attracted a lot of attention when it became evident that the intrinsically unstructured proteins comprise a large part of the proteins being encoded in eukaryotic genomes [1]. The open question, which is important, e.g., for the protein folding studies, is how much of residual structure is actually present in the unfolded proteins. High-resolution, liquid-state nuclear magnetic resonance (NMR) spectroscopy is an ideal tool for answering this question. Several experimental observables (e.g., chemical shifts) can be used for this purpose [2]. One of such observables is the direct dipole-dipole interactions between nuclear spins (the so-called residual dipolar couplings, RDCs), e.g., between the spins of a ^{15}N and a ^{1}H nuclei. RDCs are expressed via the average orientation of internuclear vectors in an anisotropic environment (created by dissolving the polypeptide in a liquid crystal medium). As RDCs throughout the polypeptide chain are correlated, NMR spectroscopy makes it possible to deduce the persistent residual structure of the chain [3]. RDCs have been measured on a variety of unfolded proteins and small peptides.

We have developed a theoretical framework [4] suitable for describing various characteristics of unfolded polypeptides including the prediction of RDCs. The framework is rather general and can serve as a basis for determining RDCs in unfolded polypeptide chains under a wide spectrum of experimental conditions. The framework allows one to employ various models for the polypeptide chains and for aligning media in order to find RDCs with the desired degree of accuracy.

Using the framework we showed that within a simple model which approximates the alignment media as infinite planes and in which unfolded polypeptides are described within the random walk formalism, it is possible to obtain a closed-form analytical result for the RDCs. The two general features predicted by the model are (i), RDCs in the center of the chain are larger than RDCs at the ends and (ii), RDCs are larger for shorter chains than for longer chains at a given liquid crystal medium concentration. We demonstrate how these features can be explained from the general physical considerations. Experimental data available from the literature confirm the first prediction of the model, providing, therefore, a tool for recognizing fully unfolded polypeptide chains. With less certainty experimental data appear to support the second prediction as well.

We acknowledge partial financial support from INTAS (contract 03-51-6170) and from European Commission (projects EXCELL and UPMAN).

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Tu3-9

EVALUATION OF RADIOLOGY PERSONNEL PRACTICE OF Mazandaran university of Medical sciences

Seyed Ali Rahimi

Mazandaran University of Medical Sciences, Kilomer 18 KHAZARABAD Road,
Fax: +981513542473, Te l: +981513543082-9, E-mail: rahimi 201@ yahoo.com
SARI, IRAN

Background and purpose:

Radiology department that provides images with proper quality plays a vital role in diagnosis of diseases. Good image is obtained by proper technical criteria and correct Positioning. Personnel practice of radiology department has a principal role on radiographs quality. This study was carried out to determine the radiology department personnel practice in university hospitals.

Method & Material:

Data collection was made using an observational check list. Its validity and reliability was determined previously. The sample size of which was thirty-nine persons. 29 items of practice related to technical and protect ional aspects at three working shifts were observed and recorded separately.

Results:

Results showed that most of the personnel were female (61.5%), over 40 years old (59%) and technicians (53.8%). On the whole, personnel's score percentages in technical field on three shifts of morning evening and night were 47.5%, 46.2%, and 45.9%, respectively which were less than them in protect ional field (60.3%, 56A% and 55.8%, respectively). Comparison of technical protection and total scores related to individual variables showed significant difference only in organizational grades ($p<0.000l$, $p<0.05$, $p<0.000l$, respectively) Le. The mean scores of radiological technologists holding BSc and associate degrees were more than those of technologists not holding university degrees.

Conclusion:

The quality of the personnel practice is not desirable; therefore continuing education programmers are needed for personnel. Protection against radiation exposure, availability of equipment and continuous evaluation of use of equipment can be effective in dose reduction in patients.

Keywords: Radiography - Radiology Department, Hospital - Personnel, Hospital Efficiency

Tu3-10

Ion-induced ionization and fragmentation of α- and β-alanine

P. Sobocinski[1], S. Bari[1], F. Alvarado[1], R. Hoekstra[1], T. Schlathölter[1],
V. Bernigaud[2], J. Rangama[2], B. Manil[2] and B. Huber[2]

[1] KVI, Rijksuniversiteit, Zernikelaan 25, 9747AA Groningen, The Netherlands
[2] Centre Interdisciplinaire de Recherche Ions Lasers, F-14050 Caen cedex 04, France

The amino acid alanine ($C_3H_7NO_2$) is one of the 20 basic building units of all proteins in living organisms. Its two isomers α- and β-alanine differ by the position of the carboxyl (COOH) and the amino (NH_2) groups. More precisely, in α-alanine both groups are attached to the same carbon while they are bonded to different carbon atoms in β-alanine. In the latter case, the nitrogen and the three carbon atoms form a linear chain.

The aim of our work is to study the geometry-sensitivity of the dissociation process for different projectile charge states. The two isomers of alanine were therefore bombarded by slow singly and multiply charged ions, namely He^+, He^{2+} and O^{5+}. The ions extracted from the ECR ion source at KVI collide at energies of 10 keV (per charge unit) with gas-phase alanine evaporated from an oven. The collision products are extracted by means of a static electric field into a reflectron time-of-flight spectrometer. The acquisition system allows measurements in a single stop mode, giving rise to conventional mass spectra, as well as in a coincidence mode.

In general, the mass spectra obtained for α- and β-alanine are similar and exhibit three clearly defined groups of peaks. Only a few fragments are produced with significantly different cross sections. In particular, an intermediate intensity of the β-alanine parent peak at $m/q = 89$ is found while the α-alanine parent peak is absent. This indicates a greater stability upon ion bombardment of the β-alanine. Another clear difference is observed for the fragments at $m/q = 30$ and 44, whose yields drastically change when going from α- to β-alanine. The formation of the $NH_2CH_2^+$ ion ($m/q = 30$) in the case of α-alanine involves dissociation of a primary unstable fragment ($m/q = 74$) whereas in the case of β-alanine this fragment is easily formed by simple bond rupture [1]. The peak at $m/q = 30$ is therefore more pronounced for β-alanine. The peak at $m/q = 44$ is attributed for both isomers to simple bond rupture. The different yields observed at $m/q = 44$ are explained in terms of fragment stability. Indeed, the $NH_2CH_3CH^+$ ion in α-alanine is more stable than the diradical fragment ion $NH_2(CH_2)_2^+$ originating from β-alanine dissociation [2]. The different response of α- and β-alanine to ion impact manifests also in different fragment kinetic energies.

Our results are very promising in the sense that they reveal a strong geometry-dependence of the fragmentation process. To our knowledge, ion induced ionization and dissociation of amino acids has never been studied before. HCI impact might appear as an useful new tool for protein sequencing, since fragmentation involves also bonds unaffected by conventional techniques. In this context, we are planning experiments involving high charge state projectiles, such as Xe^{20+}.

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Tu3-11

Ion induced fragmentation of single nucleobases vs their clusters : How hydrogen bonding affects fragmentation

Thomas Schlathölter[1], Fresia Alvarado[1], Sadia Bari[1], Ronnie Hoekstra[1], Virgil Bernigaud[2], Bruno Manil[2], Jimmy Rangama[2], Bernd Huber[1]

[1]University of Groningen, KVI, Zernikelaan 25, NL-9747AA Groningen, [2]CIRIL, CEA-CNRS-ENSICAEN, Bd. Henri Bequerel, BP 5133, F-14070 Caen Cedex05

Recently, a large number of studies has been devoted to the investigation of molecular ionization and fragmentation dynamics underlying biological radiation damage. Most of these studies were based on gas phase collisions with isolated DNA building blocks [1] . The radiobiological significance of these studies is often questioned because of the lack of a chemical environment.

Radiation damage in living cells always involves the condensed phase where the affected molecules are surrounded by a medium. Ion irradiation studies are therefore often performed on nucleobases in the solid phase [2] and on DNA deposited on solid surfaces [3]. Such studies are hampered by the complexity of the systems under study. A natural solution to avoid these difficulties is the investigation of finite systems, which still allow intermolecular interactions, i.e. clusters of DNA building blocks or mixed clusters containing biomolecules and water. Spectroscopic techniques, which proved their value in gas phase studies, can still be used to study the interaction and dissociation dynamics of such clusters. We studied interactions of keV ions with isolated nucleobases and with nucleobase clusters by means of coincidence time-of-flight spectrometry. Significant changes show up in molecular fragmentation for very small cluster sizes already, which we attribute to the influence of intermolecular hydrogen bonding.

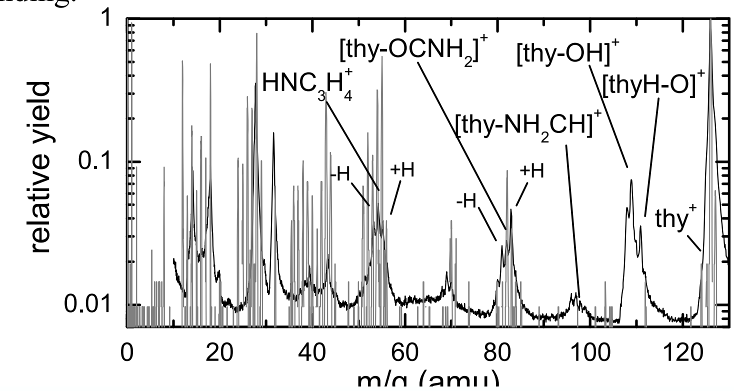

Figure 1 Mass spectra of fragmentation products for collisions of 60 keV C5+ with isolated thymine (grey) and for 50 keV O5+ with thymine.

Fig.1 shows that for instance the loss of O and OH is only observed in the presence of a chemical environment. Similar results are observed for other nucleobase clusters, as well. Note, that these channels are also seen ion induced desorption studies on thin nucleobase films [2] and can thus be regarded as fingerprints of the condensed phase.

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Tu3-12

AUTOFLUORESCENT BIOMOLECULAR SENSOR FOR EARLY CANCER DIAGNOSTICS

V.M.Kravchenko[1], O.M.Buriy[2], I.M.Kovalchuk[1], V.M.Yashchuk[1] and K.M.Kushnir[1]

[1] *Department of Physics, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine, E-mail: krav@univ.kiev.ua*

[2] *Institute of Surgery and Transplantology of the Academy of Medical Sciences of Ukraine, Kyiv, Ukraine*

A difference between fluorescence spectra of sound and affected tissues of internals of mammals opens up possibilities for luminescent diagnostics of tumour diseases. The advantages of that kind of diagnostics consist in its being non-invasive, proximate and timely, which allows one to reveal a disease at an early stage of its development.

Working out the techniques of autoflourescent diagnostics of cancer diseases of human internals requires compiling a database of intrinsic photoluminescence (PL) spectra of sound and tumour-affected tissues and developing reliable criteria for distinguishing those kinds of tissues by their spectra obtained during the optical-fiber-aided diagnostics of the human internals.

In this work we studied the intrinsic PL spectra of a few samples of the sound and the cancer-affected tissues of human stomach mucous membrane *in vitro*, obtained during surgical operations. The aim was to find the difference in the spectra which can be further used for working out the above-mentioned criteria.

The PL of the stomach tissues positioned in a quartz flask with physiological solution was excited by a pulsed UV-laser with a wavelength of 337 nm at room temperature. In the PL spectra of the sound and affected tissues one can observe a single broad band with a peak at 460-470 nm which corresponds to components of the respiratory chain of living cells (NADH molecules).

It is suggested that one of the criteria of distinguishing the sound and the cancer-affected tissues can be a ratio of the tissue PL band intensity to the scattered laser line intensity: for a sound tissue of human stomach mucous membrane that ratio is at least twice as large as for a cancer-affected tissue, which agrees with the results obtained by other authors.

Tu3-13

High resolution spectroscopic studies of organic cations

Anna M. Schulenburg[1], Frédéric Merkt[1]

[1] *Laboratorium für Physikalische Chemie, ETH Hönggerberg, CH-8093 Zürich, Switzerland*

We present high-resolution photoionisation and rotationally resolved pulsed-field-ionisation zero-kinetic-energy (PFI ZEKE) photoelectron spectra of small organic cations such as allene (C_3H_4), methyl (CH_3) and its deuterated isotopomers [1], allene and formaldehyde recorded near their adiabatic ionisation thresholds. The high resolution of up to 0.1 cm^{-1} [2] allows us to fully resolve the rotational structure of the cations which permits the determination of structural parameters. The rotational structure in these spectra provide information on the photoionisation dynamics by means of rovibronic photoionisation selection rules and angular momentum conservation rules.

In the threshold ionisation spectra of methyl rotational channel interactions mediated by the quadrupole of CH_3^+ have been observed. The rotationally resolved photoelectron spectra of allene enabled us to quantify the distortions of the cation that result from the Jahn-Teller effect. The modelling of the rovibrational line intensities of the photoelectron spectra is presented that allowed for the quantitative description of the experimental results. The spectrum of allene demonstrates that high resolution photoelectron spectroscopy is a very efficient method to obtain the rotational structure of a wide range of vibronic levels.

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Tu3-14

NUCLEAR γ-RESONANCE AT CATION-BINDING SITES IN BIOCOMPLEXES: NOVEL APPLICATIONS OF EMISSION MÖSSBAUER SPECTROSCOPY

Alexander A. Kamnev

Institute of Biochemistry and Physiology of Plants and Microorganisms, Russian Academy of Sciences, 410049 Saratov, Russia (E-mail: aakamnev@ibppm.sgu.ru)

While the absorption variant of nuclear γ-resonance (^{57}Fe Mössbauer) spectroscopy has a rich history of biological applications [1], its ^{57}Co emission variant (EMS) has remained virtually beyond that field [2]. However, its 10^4-fold higher sensitivity and the broad range of biological functions of the cobalt cation make the EMS technique highly promising for structural studies of diverse biocomplexes and metalloproteins.

To ensure EMS applicability, the following conditions have to be fulfilled: (*i*) ^{57}Co cations must be bound in proper places (e.g., at the active centres of an enzyme to be studied); (*ii*) the replacement of the native cations by $^{57}Co^{2+}$ must correspond to the physiologically relevant binding of the cation under appropriate conditions (i.e., not resulting in an irreversible deactivation of the enzyme); (*iii*) the amount of the substituted ^{57}Co cations should conform with the overall number of the cation-binding sites in the sample under study (to avoid unpredictable complications of the EMS spectra). Once these feasible prerequisites are realised [3], EMS data can provide unique information as to the chemical state, coordination symmetry and structure of the ^{57}Co species. This was for the first time illustrated using the example of a bacterial glutamine synthetase (GS, a ubiquitous key enzyme of nitrogen metabolism), having two cation-binding sites at each active centre [4]. EMS was shown to be sensitive to: (*i*) differences in the coordination of ^{57}Co(II) cations at different cation-binding sites [4], (*ii*) effects of competitive binding of activating cations other than $^{57}Co^{2+}$, (*iii*) fine structural changes induced by covalent modifications of the enzyme molecule related to its activity [5]. The results obtained are also highly promising for further studying the molecular mechanisms of enzyme–substrate biospecific interactions using EMS.

In addition, EMS can be used for monitoring real-time metabolic transformations of the $^{57}Co^{II}$ radionuclide in live bacterial cells, as compared to its purely chemical binding by dead cells [6], as well as for structural studies of cobalt biocomplexes related to the coordination of the cation and properties of its microenvironment [2, 7].

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Tu3-15

ABSOLUTE CROSS SECTIONS OF ION PRODUCTION IN ELECTRON COLLISION WITH CYTOSINE MOLECULES

, M.I.Sukhoviya, M.I.Shafranyosh, V.V. Medulych, P.M.Vichniy, L.L.Shimon, I.I.Shafranyosh

Department of Physics, Uzhgorod State University, Voloshyn st. 54, Uzhgorod 88000, Ukraine
E-mail: mshafr@tn.uz.ua; lshafr@rambler.ru

Interest in experimental studies of the processes of electron-impact ion production in the molecules of biological relevance is related, first of all, to the significance of the problem of intracellular irradiation of biological structures by secondary electrons produced in the substance in quite considerable amounts under the influence of different-type radiation. It has been shown in our preliminary experiments carried out with the heterocyclic components of the above molecules [1–2] that under electron impact different physical processes occur: i.e. molecule excitation, ionization, dissociative excitation and dissociative ionization. Physical modeling of these processes and estimation of their radiobiological consequences require knowledge of their basic characteristics – absolute ionization cross sections. Reliable data on the ionization cross sections could be obtained only in the precise experiment, in which the role of environment is minimized. Such approach was applied in this work.

Production of positive and negative ions of cytosine molecules (nucleic acid base) has been studied using a crossed electron and molecular beam technique. The method developed by the authors enabled the molecular beam intensity to be measured and the electron dependences and the absolute values of the total cross sections of production of both positive and negative cytosine ions to be determined**.** A five-electrode electron gun with a thoriated tungsten cathode was used as an electron beam source. Electron gun temperature was about 400K providing gun parameter stability during operation. Electrons having passed the interaction region were trapped by a Faraday cup kept at the positive potential. Measurements were carried out at the 10^{-7}–10^{-6} A electron beam current and the $\Delta E_{1/2}$~0.3 eV (FWHM) energy spread. Electron gun was immersed into the longitudinal magnetic field (induction $B = 1.2 \cdot 10^2$ Tl). An electron energy scale was calibrated with respect to the resonance peak of the SF_6^- ion production, the position of which determined the zero point of the energy scale.

Using the technique developed by the authors, the absolute cross sections of the positive and negative cytosine ion formation have been determined within the 0–200 eV (positive ions) and 0.4–5.0 eV (negative ions) incident electron energy ranges. It has been found that the maximal positive-ion production cross section is observed at 78 eV and reaches $7.8 \cdot 10^{-16}$ cm^2. Value of the ionization cross section obtained by us has a sense of the total cross section, i.e. it includes ion production cross sections for both initial molecules and its fragments. Formation of the primary molecular positive ion dominates. It has been found that the maximal negative-ion formation cross section is observed at 1.5 eV and is $4.2 \cdot 10^{-18}$ cm^2. Main contribution to the cross section was shown to result from the dissociative ionization cross section. It has been noted that due to the resonance mechanism of the negative cytosine ion formation just at low incident electron energies considerable disorders in the nucleic acid macromolecules are probable.

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New method to study the fragmentation processes under well controlled internal energy.

S. Martin[1], L. Chen[1], R. Brédy[1], J. Bernard[1], X. Ma[2], B.Li[1,2]

[1] Université Lyon 1 ; CNRS ; LASIM UMR CNRS 5579 ; 43 Bd du 11 Novembre
1918, F-69622 Villeurbanne, FRANCE

[2] Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000,
CHINA

Abstract: We have recently used a new method to measure the fragmentation of C_{60} and biological molecules under well controlled electronic excitation energy. This method is based on the formation of negative ions from the collision of highly positive charged ions (up to 3) [1]. The analysis of the kinetic energy of the outgoing negative ions is linked to the energy deposition on the clusters or the molecules. The fragmentation processes of C_{60} have been studied up to the C_{60}^{5+} parent ions. The excitation energies for the evaporation of C_2, asymmetrical fission and multifragmentation processes have been measured precisely and compared to the appearance energies measured by other methods such as electron, photon and atom impacts. Measurements of the excitation energies for the fragmentation of DNA bases like adenine [2] or deoxyribose show that this method can be used even for very small amount of excitation energies, typically few eV.

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Tu3-17

EXCITON DYNAMICS IN LIGHT-HARVESTING COMPLEXES AND REACTION CENTERS: CONCEPTION OF HYSTONS USED FOR SPECTRAL BROADENING AND ELECTRON TRANSFER

Vladimir S. Pavlovich

Institute of Molecular and Atomic Physics, 70 Prospect Nezalejnasty, Minsk, 220072, Belarus

A main goal of this report is to answer on the question: What are hystons and What for?

We exhibit that among the great diversity of available vibrational modes in the light-harvesting (LH) antennas and in the complexes of the reaction centers (RCs) with their protein environment is of two types, so called h_μ- and h_α-hyston modes, which produce high modulated broadening of the excitonic spectra with radically different temperature behavior [1, 2]. At the same time the h_μ- and h_α-modes initiate different activationless electron transfer (ET) processes in the RCs [1, 3].

A detailed derivation is presented for relations making it possible to describe known experimental data on the temperature effect (in the widest range 0-300 K) on the half-width of the B800, B850 absorption for LH2 antennas and the P960 and P870 absorption for RCs [4, 5] as well as on the temperature effect on the ET rate [6, 7] in the RCs for *Rps. viridis* and *Rb. sphaeroides*. Say the primary ET is considered as a resonant nonradiative transition between P* and $P^+B_A^-$ states (where P is a special pair, B_A is an additional bacteriochlorophyll in the A-branch of RC). It has been shown that the h_α-mode with frequency 130-150 cm^{-1} controls the primary ET (from P* to bacteriopheophytin H_A) [1, 3]. It has been found that the matrix element of electronic transition between the states P* and $P^+B_A^-$ is equal to 12.7 ±0.9 and 12.0 ±1.2 cm^{-1} for *Rps. viridis* and *Rb. sphaeroides* respectively [3]. It is suggested that the h_μ-mode 304 cm^{-1} governs the secondary ET (from H_A to ubiquinone) in *Rb. Sphaeroides* RC [1].

In the light of recent experimental results [8-10] an oscillation mechanism is discussed for ET from P* to B_A and then to H_A. It is suggested [3] that reorientations of water fulfill the transmission function in the ET opening the pathway for electron transport to H_A along the A-branch of the RC. Obtained results are compared to those known in literature.

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Tu3-18

On the energetics of keV ion-induced radiation damage to deoxyribose

Fresia Alvarado[1], Sadia Bari[1], Przemek Sobocinski[1], Ronnie Hoekstra[1], Thomas Schlathölter[1], Li Chen[2], Richard Bredy[2], Jerome Bernard[2], Serge Martin[2]

[1]University of Groningen, KVI, Zernikelaan 25, NL-9747AA Groningen, [2]LASIM,
Université Claude Bernard Lyon 1, 43 Bd du 11 Novembre 1918, F-69622
Villeurbanne Cedex,

Recent experiments on low energy ion-induced damage to DNA building blocks indicate that ion induced DNA damage is dominated by deoxyribose disintegration [1]. We have studied interactions of keV H^+ and He^{q+} with isolated deoxyribose molecules by means of high resolution time-of-flight spectrometry. Extensive statistical fragmentation of the molecules is observed. In contrast to studies on other DNA building blocks such as nucleobases [2], virtually complete disintegration of the molecule is observed exclusively. The fragment distribution is found to follow a power-law dependence (see fig. 1). The characteristic exponent can be used to characterize and quantify the molecular damage [3].

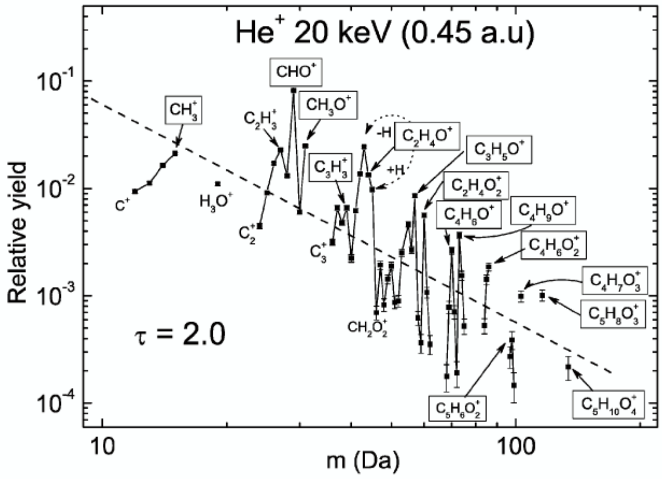

Figure 1 Yields of the various deoxyribose fragments following 20 keV He^+ impact

For a subset of collision events, where he initial and final states of the projectile are well defined (e.g. H^+ + adenine → (adenine^{2+})* + H^-), it is possible to use coincidence techniques to determine the amount of energy transferred to the molecule during the interaction process for the different fragmentation channels. This data is used to interpret the slope of the above mentioned power-law.

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Tu3-19

ELECTRON INDUCED CAPTURE DISSOCIATION OF PEPTIDE CATIONS.

Anne I. S. Holm, Preben Hvelplund, Umesh Kadhane, Steen Brøndsted Nielsen,
Subhasis Panja, Kristian Støchkel and Esben S. Worm

Department of Physics and Astronomy, University of Aarhus, Denmark

Mass spectrometry is used successfully to elucidate the primary structure of peptides and proteins, that is, the sequence of amino acids. The standard method is to induce fragmentation by collisions but the often very “rich” fragmentation spectra can be a disadvantage as too many peaks may complicate assignments. This problem has more or less been overcome with the technique electron capture dissociation (ECD), which is based on the capture of low-energy electrons by ions in the cell of a Fourier transform ion cyclotron resonance instrument. The advantage of ECD is that it leads to breakage of specific bonds in the peptide chain.

Here I will show how we in Aarhus mimic the ECD process by transfer of an electron from an alkali metal atom to a peptide dication of high translational energy. Recent experimental results from our group shed light on the mechanism behind ECD.

Tu3-20

Quantum Mechanical Self-Assembling of Artificial Minimal Cells and Control by Molecular Electronics and Spintronics Logical Devices

Arvydas Tamulis and Vykintas Tamulis

Institute of Theoretical Physics and Astronomy of Vilnius University, A. Goštauto 12, Vilnius, Lithuania

We used quantum mechanical (QM) electron correlation density functional theory (DFT) methods, *i.e.* done exact quantum mechanical experiments to investigate various self-assembled photoactive bioorganic systems of artificial minimal cells based on peptide nucleic acid (PNA) consisting of up to 800 atoms and 5 nm in diameter [1-2]. The electron correlation hydrogen bonds and Van der Waals interactions that result from the addition of water (or methanol) and fatty acid (FA) molecules play the critical role in quantum self-assembly of photosynthetic center and functioning of the photosynthetic processes in artificial minimal cells. The distances between the separated sensitizer, fatty acid precursor (pFA) and water molecules are comparable to Van der Waals and hydrogen bonding radii and therefore these nonlinear quantum interactions compress the overall system resulting in a smaller gap between the HOMO - LUMO and photoexcited electron tunneling from sensitizer (1,4-bis(N,N-dimethylamino)naphthalene or Ru(bipyridine)$_3^{2+}$) to pFA molecules which is calculated by time dependent density functional theory (TD DFT) method and differs from spectroscopic experiments only by 0.2 nm (in the value of experiment errors) that means what quantum mechanical self-assembled structures of minimal cells are very close in comparison to the realistic ones in the nature.

QM electron correlation experiments of self-assembly of artificial minimal cells show that these cells are complex systems because only entire ensembl of PNA, sensitizer, pFA, FA and water molecules is stable and perform quantum photosynthetic processes. Removing the small part of nucleobase, FA and water molecules leads to the structural changes in comparison with realistic structures and difference in comparison with the spectroscopic values of photoexcited electron tunneling from sensitizer (1,4-bis(N,N-dimethylamino) naphthalene or Ru(bipyridine)$_3^{2+}$) to pFA molecules. QM electron correlation experiments of self-assembly of artificial minimal cells removing the main part of nucleobase, FA and water molecules leads to the degradation of these cells [2]. We can state what the inclusion of ever more water, fatty acid and nucleobase molecules in the different artificial minimal cells results in a shift of the absorption spectrum to the red for the artificial protocell photosynthetic centre, leading to an ever closer approach to the real experimental value and indicates the measure of the complexity of this quantum complex system, *i.e. a* minimal protocell. It is important to say that only QM electron correlation TD-DFT experiments with minimal protocells gives results exactly comparible with spectroscopic results and all other more simplyfied QM methods such as local gradient DFTor *ab initio* Hartree-Fock gives structures and spectra far from the experimentally measured.

Implementation of quantum information bits based on spatially localized electron spins in stable molecular radicals are investigated by unrestricted DFT methods installed in the Gaussian03 package [3, 4]. The DALTON package is used for the g-tensor shift calculations of neutral radical molecules: β-diketone and syringate.

β-diketone neutral radical moiety with an attached hydrocarbon chain is suitable for construction of quantum computing processing devices because the qubit is relatively stable due to the small magnitude of g-tensor shift component that is aligned with the external magnetic field, i.e. the direction of hydrocarbon chain which provide the self-assembled monolayer an attachment of the molecule to a substrate.

TD-DFT simulations of the artificial minimal cells with implemented molecular electronics and spintronics gates done using self-assembled neutral radical molecules β-diketone and syringate show that it is possible to construct more general ContrlNOT and NAND logic functions suitable for the production of the nanobiorobots.

Results of our detailed investigations provides a collection of quantum mechanical tools including relativistic ones and applies them to the design of variety of the molecular spintronics devices which might regulate photosynthesis and growth of artificial minimal cells in the conditions of external magnetic fields, while also providing a perspective of the requirements for success in the synthesis of new forms of artificial living organisms. Quantum logic functions should control metabolic photodissociation of lipid precursor molecule absorbing additionally energy of the external magnetic fields. Results of our quantum simulations show on the possibility of experimental synthesis of quantum logically controlled artificial organisms.

Mobile molecular quantum computing element possessing ten quantum bits based on proton NMR spectra of a Fe2OEB biliverdin dimer derivative and attached to two azo-dye Disperse Orange 3 (DO3) molecular motors was designed using TD-DFT B3LYP 6-311G** model [5].

The molecular quantum computing organisms might be already were in the first stages of life emergency in the Earth or still exist somewhere in the Space.

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Tu3-21

Quantum Mechanical Modeling of Minimal Living Organisms and Programmable Nano Biorobots

Arvydas Tamulis and Vykintas Tamulis

Institute of Theoretical Physics and Astronomy of Vilnius University, A. Goštauto 12, Vilnius, Lithuania

Abstract. We used quantum mechanical (QM) electron correlation time dependent density functional theory (TD DFT) method in both the Gaussian 03 and GAMESS-US packages to investigate various self-assembled photoactive bioorganic systems of artificial minimal cells based on peptide nucleic acid (PNA) [1, 2].

The electron correlation hydrogen bonds and Van der Waals interactions that result from the addition of water and fatty acid molecules play the critical role in quantum self-assembly of photosynthetic center and functioning of the photosynthetic processes in artificial minimal cells. The distances between the separated sensitizer, fatty acid precursor (pFA) and water molecules are comparable to Van der Waals and hydrogen bonding radii and therefore we may regard these minimal cells as single electron conjugated supramolecules that we can deal with using an electron correlated TD DFT models. These nonlinear quantum interactions compress the overall system resulting in a smaller gap between the HOMO - LUMO and photoexcited electron tunneling from sensitizer to pFA molecules [3].

Our presenting quantum self-assembled model of the photosynthetic systems includes a PNA fragment which is covalently bonded to a 1,4-bis(N,N-dimethylamino) naphthalene or Ru(bipyridine)$_3^{2+}$ sensitizer molecules, pFA, fatty acid (FA) molecules constituting the 4 nm size micellar container's inner monolayer with water. The small 10 nm difference of the experimental absorption spectra peaks in comparison with our QM calculated it is possible to understand because of more water and fatty acid molecules exist in the real photosynthetic center of minimal protocells and makes possible to search for new sensitizers. The slightly shorter wavelength given by the model is also consistent with our finding that the inclusion of more water and fatty acid molecules in the models resulted in longer wavelengths for the absorption spectrum. The shift of the absorption spectrum to the red for the artificial minimal cell photosynthetic center might be considered as the measure of the complexity of this system [4].

The small 10 nm difference of the experimental absorption spectra peaks in comparison with our QM calculated confirm that our chosen method of designing single electron transfer minimal cells might be useful also for wide implementation in the nano photodevices and molecular computers.

We have performed quantum mechanical investigations of effective photosynthetic system consisting of good sensitizer Ru(bipyridine)$_3^{2+}$ working under the exciting of visible light in the region from 455.18 nm to 402.85 nm and relaxing due to passing electron from good electron donor 8-oxo-guanine-PNA molecule.

Influence of hydrogen bonded cytosine molecule result the shift of the lowest intense excited state wavelength from 455.18 nm to 456.99 nm, *i.e.* 1.81 nm to red region. The highest intense excited state shifted from 402.85 nm to 401.49 nm, *i.e.* 1.36 nm to blue region. This is usual process of splitting of spectrum of complex quantum system due to hydrogen bonding interaction with additional molecule.

TD-DFT simulations of the bioorganic complex with implemented neutral radical molecules show that it is possible to construct ContrlNOT and AND logic functions in the nanobiorobots. Quantum logic functions should control metabolic photodissociation of lipid precursor molecule.

Our quantum simulations show on the possibility of experimental synthesis of quantum logically controlled artificial organisms. The experimentally made artificial molecular quantum computing organisms might be already were in the first stages of life emergency in the Earth or still exist somewhere in the Space.

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Tu3-22

Quantum Processes of Self-Assembly, Photosynthesis and Molecular Computing in Artificial Minimal Living Cells

Arvydas Tamulis and Vykintas Tamulis
Vilnius University Institute of Theoretical Physics and Astronomy, A. Gostauto 12, Vilnius, Lithuania,
e-mail: tamulis@itpa.lt

We used quantum mechanical (QM) electron correlation interactions density functional theory (DFT) methods (*i.e.* high precision quantum mechanical simulations) to investigate various self-assembled photoactive bioorganic systems of artificial minimal living cells [1, 2]. The cell systems studied are based on peptide nucleic acid (PNA) and consisted of up to 360 atoms (not including the associated water or methanol solvent shells) and are up to 3.0-4.2 nm in diameter. The electron correlations interactions originating the hydrogen bonds and Van der Waals weak chemical bonds that increase due to the addition of a polar solvent (water or methanol) molecules, and fatty acid (FA) and precursor fatty acid (pFA) molecules play a critical role in the QM interaction based self-assembly of the photosynthetic center and functioning of the photosynthetic processes of the artificial minimal living cells. The distances between the separated sensitizer, precursor fatty acid, and water or methanol molecules are comparable to Van der Waals and hydrogen bonding radii. As a result these nonlinear quantum interactions compress the overall system resulting in a smaller gap between the HOMO and LUMO electron energy levels and photoexcited electron tunneling occurs from the sensitizer (either a 1,4-bis(N,N-dimethylamino) naphthalene or a $[Ru(bpy)_2(4,4'\text{-}Me\text{-}2\text{-}2'\text{-}bpy)]^{2+}$) to pFA molecules (notation used: Me = methyl; bpy = bipyridine). The electron tunneling and associated light absorption of most intense transitions as calculated by the time dependent density functional theory (TD DFT) method differs from spectroscopic experiments by only 0.3 or 0.2 nm, which is within the value of experiment errors [3]. This agreement implies that the quantum mechanically self-assembled structures of minimal living cells very closely approximate the realistic ones.

Quantum mechanical electron correlation experiments of self-assembly of above described artificial minimal living cells show that these cells are complex systems because only entire ensembl of PNA, and sensitizer, and pFA, and FA and water molecules is stable and perform quantum photosynthetic processes. Removing the small part of nucleobase, FA and water molecules leads to the structural changes in comparison with realistic structures and difference in comparison with the spectroscopic values of photoexcited electron tunneling from sensitizer (1,4-bis(N,N-dimethylamino)naphthalene to pFA molecules. QM electron correlation experiments of self-assembly of artificial minimal living cells removing the main part of nucleobase, and FA and water molecules leads to the degradation of these cells [2]. We can state what the inclusion of ever more water, and fatty acid, and pFA molecules, and waste pieces of the pFA molecules and nucleobase molecules in the different artificial minimal living cells results in a shift of the absorption spectrum to the red for the artificial protocell photosynthetic centre, leading to an ever closer approach to the real experimental value and indicates the measure of the complexity of this quantum complex system, *i.e. a* minimal protocell. It is important to say that only QM electron correlation TD-DFT experiments with minimal living cells gives results exactly comparible with spectroscopic results and all other more simplyfied QM methods such as local gradient DFTor *ab initio* Hartree-Fock gives structures and spectra far from the experimentaly measured.

The corresponding of experimental absorption spectra peaks and our QM calculated confirm that our chosen method of designing single electron nano photocells might be useful not only for artificial living organisms but also for wide implementation in the nano photodevices, and molecular computers.

Our goals are by using quantum mechanical experiments to predict the possibility of experimental synthesis of molecular electronics and spintronics logical elements information based artificial living organisms or nanobiorobots for nanomedicine and cleaning of nuclear, chemical and microbial pollutions.

We are creating molecular electronics logic gates regulating the photosynthesis, growing and dividing of artificial living cells and nanobiorobots [4, 5].

Implementation of quantum information bits based on spatially localized electron spins in stable molecular radicals was investigated by unrestricted time dependent functional theory methods [6, 7]. The g-tensor shift calculations of neutral radical molecules was performed for beta-diketone and syringate. beta-diketone neutral radical moiety with an attached hydrocarbon chain. Beta-diketone is suitable for construction of quantum computing processing devices because the qubit is relatively stable due to the small magnitude of g-tensor shift component that is aligned with the external magnetic field, i.e. the direction of hydrocarbon chain which provide the self-assembled monolayer an attachment of the molecule to a substrate.

TD DFT simulations of the artificial minimal living cells with implemented molecular electronics and spintronics gates done using self-assembled neutral radical molecules beta-diketone and syringate show that it is possible to construct more general ContrlNOT and NAND logic functions suitable for the production of the nanobiorobots. Designed of variety of the molecular spintronics devices will regulate photosynthesis and growth of artificial minimal living cells in the conditions of external magnetic fields, while also providing a perspective of the requirements for success in the synthesis of new forms of artificial living organisms.

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Tu3-23

DETERMINATION OF TRACE ELEMENTS OF PHYTOCOMPOSITION WITH USING HERB BY INDUCTIVELY COUPLED PLASMA OPTICAL SPECTROMETRY (HYDRIDE GENERATION)

Alena Muravitskaya, Michail Belkov

Institute of Molecular and Atomic Physics, National Academy of Sciences, 70 Nezalezhnastsi Ave., 220073 Minsk, Belarus e-mail: muravitskaya @ imaph. bas–net. by

The technique for determination of trace elements of phytocomposition based on hydride generation system by means inductively coupled plasma optical emission spectroscopy has been tested. The application of new types of optical spectrometers with Echelle-optics and semiconductor array detectors, and by the application of electronically controlled, high current generators allows to increase sensitivity and to lower limits of detection of many elements(1). Reaction rate of hydride generation have been study to optimize parameters of excitation, to raise quality of the sample decomposition, to minimize the spectral interferences. The rates are controlled with several interdependent variables: the chemical form of the hydride-forming element, the oxidation state of the hydride-forming element, the acid concentration of the sample, concentration of the reductant ($NaBH_4$) (2). Technique under consideration require of the introduction the sample and acid first before $NaBH_4$. It allows to lower power of the plasma generator, to receive more complete mineralization in the sample. Technique under consideration allows getting a linear dynamic range and detection limit about 0,1ppb for determination of selenium. The technique provides the decreasing the effect of interfering elements (Al, Fe). The accuracy of a technique has been proved to be true by definition selenium in multielement standard samples.

The determination of such elements as Fe, Mg, Al, Mn in phytocompositions was carried out in a normal mode with inductively coupled plasma. The samples have been prepared by means a method of "wet" mineralization with a nitric acid. To determine selenium 3M hydrochloric acid has been used (3). There are no statistically significant differences were obtained between the value of elements our method and X-ray-fluorescent analysis. Presented technique determination of trace elements of phytocomposition allow to study unknown herb, used in vegetable active food additives.

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Tu3-24

DIRECT FORMATION OF AMINO ACID BY UV IRRADIATION TO SIMPLE ORGANIC MOLECULES

A. Hiraya, M. Morita, Y. Harada, H. Tamaki, M. Kuwajima

Department of Physical Science, Graduate School of Science, Hiroshima University
1-3-1 Kagamiyama, Higashi-hiroshima, 739-8526 Japan

Since Miller's historical spark discharge experiment[1], a number of studies have been done to show possible prebiotic synthesis of amino acids. It has been shown that precursors of amino acids can be formed by the irradiation of high energy photon to interstellar ice[2,3]. However, despite these successful prebiotic synthesis of precursors of amino acids in simulated extraterrestrial environments, the problem of "homochirality of amino acids" has been unexplained. To find a clue to elucidate this problem, it is necessary to consider a particular reaction stage where asymmetric fields such as circularly polarized light or magnetic field contribute to enantiomer excess of amino acids. It seems natural that the molecular chirality was introduced not at the first bond-formation stage between simple molecules such as CO, N_2, NH_3 and H_2O, but at the later stage of photochemical reactions where an organic molecule is converted to other forms by addition reaction.

We have studied amino acid formation by UV irradiation to organic molecules (amines, alcohols and amides) in aqueous solution, accrete ice, and complex with Co atom. By using HPLC, small aliphatic amino acids (Gly and α-, β- Ala and α-, β-, γ-ABA) were quantitatively identified. Certain amino acids were formed in its free form before hydrolysis (direct formation), contrary to the previouse results where amino acids were detected mainly after hydrolysis (indirect formation). Direct formation of amino acids is important for enantio-selectivity. Direct D-, L-alanine formation observed for Co(III)[propylenediamine]$_3$ complex suggests the possibility of enantio-selective formation of amino acids based on magnetochiral anisotropy[4] on the metallic or metal-containing interstellar dust around pulsars that serves strong magnetic field and intense radiations in wide energy range. Species of amino acids shows dependence on starting organic molecules and also on the presence of ammonia and inorganic acids. Formation processes of identified small aliphatic amino acids were investigated with the aid of electrospray ionization (ESI) MS and MS/MS measurements of photoproducts. By identifying the amino acid precursor that has a chiral carbon atom, a new possibility is suggested for asymmetric photosynthesis of amino acid from achiral organic molecules.

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Tu3-25

INELASTIC SCATTERING AND STOPPING POWER OF ELECTRONS IN BIOMOLECULAR SYSTEMS

A. Muñoz[1], J. C. Oller[1], F. Blanco[2], P Limão-Vieira[3] and G. García[4]

[1]Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas, Avenida Complutense 22, 28040 Madrid, Spain.
[2]Departamento de Física Atómica, Molecular y Nuclear, Universidad Complutense de Madrid, 28040 Madrid, Spain.
[3] Atomic and Molecular Collisions Laboratory, CEFITEC, Department of Physics New University of Lisbon, 2829-516 Caparica, Portugal.
[4]Departamento de Física Atómica, Molecular y Agregados, Instituto de Matemáticas y Física Fundamental CSIC, Serrano 113-b, 28006 Madrid, Spain.

Models used in radiotherapy and radiation protection to assign absorbed doses are commonly based on the stopping power of radiation in the medium. However, except for the calculations of [1], values of these parameters are scarce in the literature. We propose a method to obtain reliable data for electrons in molecular systems by combining our measured and calculated cross sectional data with the corresponding experimental energy loss spectra. A recent application of this method to methane based tissue equivalent materials [2] showed important discrepancies with previous measurements. We will present results for H_2, H_2O and tetrahydrofuran (THF) which are relevant compounds to understand the radiation interaction processes in living systems.

Finally, we will compare these results with those given by a Monte Carlo simulation procedure [3] which uses as input parameters our experimental and theoretical cross sectional data

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Tu3-26

IMAGING OF ISOLATED GASEOUS BIOMOLECULES PRODUCED BY LASER DESORPTION

Authors: T L Merrigan, C A Hunniford, R W McCullough and D J Timson
Affiliation: Centre for Plasma Physics, Queen's University Belfast
Email: tmerrigan01@qub.ac.uk

This project seeks to determine the optimum parameters for the production of a gas phase target of biomolecules such as short strands of DNA. Initial work concentrates on the production of isolated molecules with future work to produce biomolecules embedded in clusters of water molecules. Such target can subsequently be used for studies of fragmentation processes induced by interactions with low energy ions, electrons, photons and radicals. Previous in-vacuo studies have used either solid phase material such as plasmid DNA deposited on a substrate or thermally evaporated DNA or RNA bases. These techniques cannot be applied to a wide range of biomolecules because of substrate effects or thermal decomposition.

The techniques of UV and IR laser desorption are well established for the generation of positive or negative ions of biomolecules. This is frequently carried out in a process known as MALDI (Matrix Assisted Laser Desorption and Ionisation) with which this group has several years experience. However, the necessity of a matrix material results in the production of plumes of desorbed material with both biomolecule and analyte components thus making it unsuitable for use as a 'clean' target. The current work intends to study several novel techniques for production of gaseous biomolecules *without* the need for a matrix.

Characterisation of the targets will be carried out by fluorescent dye tagging and laser induced fluorescence imaging of the target spatial density profiles. The production of characterized targets of biomolecular species including DNA strands will enable biological radiation damage studies investigating the underlying molecular mechanisms on a single-radiation-quantum/single-molecule level. There is considerable current interest in this topic because of its potential applications in radiation biology, diagnostic and therapeutic medicine.

Tu3-27

LOW ENERGY ION DAMAGE TO DNA

L. Sellami, S. Lacombe[1], Z. Deng, M. Imhoff, I. Bald[2], E. Illenberger[2], and **M. A. Huels***

Ion Reaction Laboratory, Dept. of Nuclear Medicine and Radiobiology, Faculty of Medicine
and Health Sciences, University of Sherbrooke, Sherbrooke, QC, Canada

Protons and heavy ions represent an efficient and volume selective mode of therapy for deep-seated and non-operable tumours, and are abundant in space environments. Moreover, low energy secondary ion fragments are ubiquitous along radiation tracks in cells where they may contribute to DNA damage, mutations, or cell death. Recent studies [1] have shown that, unlike for electron or photon tracks, highly charged energetic heavy ion collisions with DNA bases create abundant secondary ions (e.g. C^{n+}, O^{n+}, N^{n+}, n=1-3) with *hyperthermal energies reaching up to several hundreds of eV*. Here we show that atomic and molecular cations with *precisely* such low energies (1–100 eV) are capable of causing substantial damage to DNA and its components via molecular fragmentation, ionization, as well as direct and indirect physico-chemical reactions, and are thus are capable of enhancing clustered DNA lesions along ion racks in cells.

Our experimental results from condensed phase biomolecules are obtained via two techniques: (1) irradiation of condensed films with highly focused, mass and energy selected, positive and negative ion beams in the 1 – 200 eV energy range. A mass spectrometer monitors desorbing reaction products *during* ion impact; films of DNA components are evaporated *in vacuo* onto atomically clean Pt held at room temperature, and film deposition is calibrated by a quartz crystal microbalance; (2) low pressure and energy ion-plasma exposure of biomolecular solids to ions of fixed energy (variable from kT–100eV), with subsequent analysis of recovered products via HPLC, LC-MS/MS, or gel electrophoresis; target films are prepared either by spin-coating, or lyophilization techniques. We will present measurements from films of DNA/RNA components (e.g. bases, sugars, nucleosides) including radiosensitizing bromouracil, as well as double stranded DNA plasmids (3197 base pairs), exposed to various atomic and molecular cations at low energies. We find, for example, that *below 10 eV*, *reactive scattering is observed* during N^+ and N_2^+ ion irradiation of DNA/RNA sugars. N^+ ions efficiently abstract hydrogen and carbon atoms from the target molecules to form NH^- and CN^- anions. The energy threshold of CN^- desorption is found to be *5 eV*, and NH^- are observed at energies down to *1 eV* (< 0.1 eV/amu) without threshold. Furthermore, we find that *C abstraction is highly site and energy specific*. N^+ ion irradiation of 5-^{13}C D-ribose reveals that CN^- formation is highly selective for C5, which bonds to the DNA/RNA backbone phosphates. Meanwhile, hyperthermal Ar cations (2.5 eV/amu) interacting with double stranded DNA leads to single and double strand breaks, as well as fragmentation and chemical modification of nucleosides, and site specific rupture along the N1-C1 glycosidic bond, resulting in base release. *(Funded by the Natural Science and Engineering Research Council of Canada, and the Canadian Space Agency)*

*Corresponding and presenting author

[1] Permanent address: Laboratoire des Collisions Atomiques et Moléculaires, Bâtiment 351 Université Paris Sud XI 91405 ORSAY Cedex

[2] Permanent address: Institut für Chemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustrasse 3, D-14195 Berlin, Germany

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METASTABLE DECAYS OF NEGATIVE IONS FORMED UPON ELECTRON ATTACHMENT TO SMALL BIOMOLECULES AND EXPLOSIVES

A. Mauracher[1], M. Beikircher[1], S. Denifl[1], F. Zappa[1], A. Bacher[1], O. Echt[2], T.D. Märk[1], P. Scheier[1]

1 Institut für Ionenphysik und Angewandte Physik, Leopold Franzens Universität,

Technikerstrasse 25, A-6020 Innsbruck, Austria

e-mail: stephan.denifl@uibk.ac.at

2 Department of Physics, University of New Hampshire, Durham, NH 03824, USA.

Mass spectrometric studies of unimolecular, metastable decay reactions of mass selected ions have provided a wealth of information about structure, stability and energetics of these species. For positively charged ions unimolecular fragmentation has been the subject of interest for many years [1]. However, for negatively charged ions much less is known although for free electron attachment the energy balance is completely known. Capture of a free electron by a molecule generates a transient negative ion (TNI). Such a quantum state is principally unstable toward the loss of the extra electron (autodetachment). In competition to autodetachment a TNI can also dissociate into an ion and one or more neutral fragments.

Here we present a few examples for metastable decay reactions of anions formed upon electron attachment to molecules, namely explosives (2,4,6-Trinitrotoluene) and small biomolecules (DNA bases). The experimental setup consists of a Nier type ion source combined with a double focusing two sector field instrument of reversed geometry. With the experimental setup it is possible to derive the kinetic energy release of the metastable decay reactions. Unimolecular decay reactions of molecular anions can happen as late as several tens of μs after the ionization if complex rearrangement of the atoms in a molecule is necessary. For the decay reaction leading to the formation of CNO^- from dehydrogenated thymine the average kinetic energy release derived from the data amounts to 20meV. For the loss of NO from the parent anion of trinitrotoluene the average kinetic energy release is significantly larger. As for this NO loss the necessary kinetic energy of the attaching electron is close to 0eV and the electron affinity of the molecular anion is also very low, the high average kinetic energy release observed shows the explosive nature of TNT in this unimolecular reaction.

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Tu3-29

GAS-PHASE STUDIES OF THE PHOTOABSORPTION DYNAMICS IN CHROMOPHORE IONS

L. Lammich, I.B. Nielsen, H. Sand, A. Svendsen and L.H. Andersen

Department of Physics and Astronomy, University of Aarhus, Denmark

The photoabsorption of chromophore molecules constitutes the first step in the reaction of photoactive proteins to light. These proteins fulfill important functions in a variety of biological organisms and as markers in molecular biology research. Previous studies have revealed a strong influence of the environment, in particular solvents, on the behavior of the chromophore. To disentangle such disturbances from intrinsic properties of the chromophore it is therefore essential to perform photoabsorption studies on isolated molecules, that is in gas phase. To gain a full understanding of these reactions, time resolved studies are important which can yield insight in the dynamics of the underlying processes.

We present experimental techniques being used at Aarhus University to perform such studies. A keV beam of chromophore ions is produced by an electrospray ion source. These ions can be stored in the electrostatic storage ring ELISA and their response to e.g. irradiation by a pulsed laser can be followed time resolved over many msec. In the gas phase, photoabsorption in general leads to a fragmentation of the chromophore in a statistical process on a timescale depending on the energy deposited and on the properties of the molecule. The absorption cross section as a function of laser wavelength can be compared to absorption measurements in the liquid phase and in proteins. The data provide valuable input for a theoretical understanding of such systems [1,2].

For studying the initial photoresponse of the chromophore, much shorter timescales have to be addressed. To this end we use a single-pass setup employing crossed ion and laser beams. A time-of-flight technique can here be used to investigate ions fragmenting in the first microseconds after the light absorption, allowing for a separation of statistical and possible direct fragmentation pathways. Moreover, this setup has been extended to facilitate pump-probe studies employing femtosecond laser pulses. Our results on the sub-ps dynamics following photoabsorption in a GFP model chromophore will be discussed.

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Tu3-30

EPOTRAN: a full-differential Monte Carlo code for electron and positron transport in liquid water

Champion Christophe
champion@univ-metz.fr

Laboratoire de Physique Moléculaire et des Collisions,
Université Paul Verlaine-Metz,
1 boulevard Arago, Technopôle 2000, 57078 Metz, France

When biological matter is irradiated by charged particles, a wide variety of interactions occurs, what leads to a deep modification of the cellular environment. To understand the fine structure of the microscopic distribution of energy deposits, Monte Carlo event-by-event simulations are particularly suitable. However, the development of these track structure codes needs accurate interaction cross sections for all the electronic processes: ionization, excitation, Positronium formation and even elastic scattering. In these conditions, we have recently developed a Monte Carlo code for electrons and positrons in water, this latter being commonly used to simulate the biological medium. All the processes are studied in detail via theoretical differential and total cross section calculations performed by using partial wave methods. Comparisons with existing theoretical and experimental data in terms of stopping powers, mean energy transfers and ranges show very good agreements. Moreover, thanks to the theoretical description of Positronium formation, we have access, for the first time, to the complete kinematics of the electron capture process. Then, the present Monte Carlo code is able to describe the detailed Positronium history, what provides useful information for medical imaging (like Positron Emission Tomography) where improvements are needed to define with the best accuracy the tumor volumes.

POSTERS

Wednesday 9/5

1. Alignment-Orientation-Polarization

We1-1

ON THE ANGULAR DISTRIBUTION AND SPIN POLARIZATION OF PHOTOELECTRONS FROM SEMI-FILLED SHELL ATOMS

M. Ya. Amusia [1,2] and L. V. Chernysheva [2],

[1] Racah Institute of Physics, the Hebrew University, Jerusalem 91904, Israel
[2] A. F. Ioffe Physical- Technical Institute, St. Petersburg 194021, Russia

We present here the results of calculations of photoelectrons' dipole angular anisotropy and spin-polarization parameters for a number of semi-filled shell atoms and demonstrate rather peculiar features of their photon frequency dependence. We consider ionization of outer or, in some cases, next to the outer electrons in a number of elements from I, V, and VI groups of the Periodic Table. All calculations are performed in the Spin Polarized versions of one-electron Hartree-Fock (HF) approximation and with account of multi-electron correlations in the frame of the Random Phase Approximation with Exchange – SP HF and SP RPAE, respectively.

We consider the dipole angular distribution and spin polarization of photoelectrons from semi-filled subshells and from closed shells that are neighbours to the semi-filled shells. It is demonstrated that the latter affect the considered characteristics of the closed shell prominently.

We have considered also angular anisotropy and spin-polarization of photoelectrons from some excited atoms, Cr^* and Mo^* that are formed by spin-flip of one of the outer electrons *s* - electrons. At first glance almost not essential, this excitation affects the spin polarization and angular distribution of the neighbor semi-filled multi-electron shells $3d^5$ and $4d^5$ shells, respectively.

To check the accuracy and consistency of the applied SP RPAE approach and to see the role of the nuclear charge variation only, we have calculated the dipole angular anisotropy and spin-polarization parameters of 3*p* - electrons in K and compare them to Ar and K^+ that have the same configuration.

Entirely, we have calculated the angular anisotropy and spin-polarization parameters for following subshells of atoms N (2*p*), P (3*p*), Ar (3*p*), K^+(3*p*), K(3*p*), Cr(3*p*, 3*d*), Cr^*(3*d*), Mn(3*p*, 3*d*), As(3*d*, 4*p*), Mo(4*p*, 4*d*), Mo^*(4*d*), Tc(4*p*, 4*d*,), Sb(4*d*, 5*p*), Eu(4*f*).

We use Eu not only to show relatively simple behavior of considered parameters as functions of photon energy, but also to demonstrate the prominent role of 5*p* electrons in shaping the angular distribution and spin polarization of photoelectrons from the semi-filled 4*f* electrons The detailed information can be found in [1].

The peculiarities of obtained parameters as function of photon frequency are quite prominent, present a whole variety of different structure that deserve experimental investigation.

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We1-2

Molecular ionization probability measured by molecular alignment

V. Loriot, E. Hertz, A. Rouzée, B. Lavorel, and O. Faucher

Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, BP 47870, 21078
Dijon Cedex, France

We present an original application of molecular alignment for the determination of ionization probabilities induced by femtosecond (*fs*) laser pulses. It is now well established [1] that the non resonant interaction of molecules with an intense *fs* laser pulse gives rise to periodic molecular alignment under *field-free* conditions (i.e. after the end of the pulse). When the intensity of the pulse is sufficient, molecular ionization occurs as well. The approach presented here takes advantage of the coexistence of the two phenomena in order to determine absolute probabilities of single-ionization calibrated with post-pulse molecular alignment. The technique, based on the cross-defocusing of a probe pulse, has been implemented recently [2] to determine the degree of alignment induced in CO_2 with a 100-*fs* laser pulse. The measurement relies on the dependency of the refractive index upon alignment. As explained here, the cross defocusing technique yields a signal sensitive also to ionization as a result of the additional refractive index related to the density of free electrons. We show that the analysis of the global signal can provide access to ionization probabilities calibrated via the degree of field-free molecular alignment [3]. The effect is demonstrated in N_2. The ionization probabilities extracted from experimental data are in good agreement with values reported in the literature. The advantages featured by this technique are discussed.

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We1-3

Efficient Orientation of molecules

S. Guérin, D. Sugny, H.R. Jauslin

Institut Carnot de Bourgogne, UMR 5209 CNRS, BP 47870, 21078 Dijon cedex

The control of molecular alignment is of a broad interest and development of techniques to reach this goal is widely studied [1]. Orienting molecule, i.e. with the control of the direction of alignment, is a more difficult task.
Postpulse orientation can be preferred to adiabatic orientation [2]. The combination of a half cycle pulse with a laser pulse offers an efficient and long-lived postpulse orientation robust to temperature [3]. We can characterize this orientation, defining the notion of target state in a finite rotational Hilbert subspace [4].
We also show that the orientation can be enhanced by a vibrational resonant process [5].

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We1-4

Laser control of photoinduced processes.
I. Alignment and reactivity

D. Sugny, M. Desouter-Lecomte, Y. Justum L. Bomble and M. Ndong

Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne
BP 47870, 21078 Dijon, France.
Laboratoire de Chimie Physique, Unité Mixte de Recherche 8000,
CNRS et Université Paris-Sud-11, 91405 Orsay Cedex, France.

We present the control of different photoinduced processes: control of reactivity and control of molecular alignment and orientation. We consider two complementary approaches for designing the corresponding laser pulses, Optimal control theory (OCT) and adiabatic passage techniques. Note that the adiabatic processes are not used in the adiabatic limit of the order here of the nanosecond. The optimization of the different parameters (Rabi frequencies, frequency range of the chirp, duration of each pulse…) allows one to reduce the time of the control to few (or less) picoseconds. We analyse the solutions given by the two strategies both in terms of efficiency and robustness.

Control of reactivity

We consider different control scenarios in a particular region connecting three wells of the potential energy surface of the methoxy radical. The active coordinates are a bending mode and an internal rotation mode. The examples concern the control of reactivity (isomerization and passage from a delocalized state to a localized one) and the implementation of logical gates based on vibrational states [1]. The effect of the environment is also taken into account by introducing a Markovian and a non-Markovian dynamics [2].

OCT, adiabatic passage techniques and chirped pulses are also compared in a model involving non adiabatic interactions.

Control of molecular orientation and alignment

We construct target states which optimize both the efficiency of orientation (or alignment) and its duration [3]. We show how to reach these target states by using either a train of short pulses or optimal control theory to optimize the envelope of the laser pulse. We have also generalized this approach to the presence of a dissipative medium (alignment of CO molecule in an Ar gas) [4]. In this case, as the laser field cannot compensate the negative effect of dissipation, the control has to be as short as possible.

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We1-5

FIELD-FREE DYNAMIC ALIGNMENT OF DEUTERIUM WITH INTENSE FEW-CYCLE PULSES

J Wood*, E M L English*, C R Calvert†, J McKenna†, W A Bryan*, R Torres‡, I C E Turcu$, I D Williams† and W R Newell*

* Department of Physics and Astronomy, University College London, London. UK.
† School of Mathematics and Physics, Queen's University Belfast, Belfast. UK.
‡ Blackett Laboratory, Imperial College London, London. UK.
$ Central Laser Facility, Rutherford Appleton Laboratory, Oxfordshire. UK.

The ability to enforce spatial and temporal order on an initial random ensemble of molecules is a very important step along the road to experimental realization of coherent control and quantum computation. Combining a high-resolution time-of-flight mass spectrometer and a femtosecond pump-probe configuration, we map the evolution of rotational wavepackets, in room temperature D_2 molecules as a function of time and angle. The first laser pulse creates a superposition of rotational states which are then probed (Coulomb explosion imaged) by the second pulse. By varying the time delay between the initiating and imaging pulses, dephasing and revival effects [1] are observed. And by rotating the polarisation of the first pulse with respect to the second, the angular dependence is established.

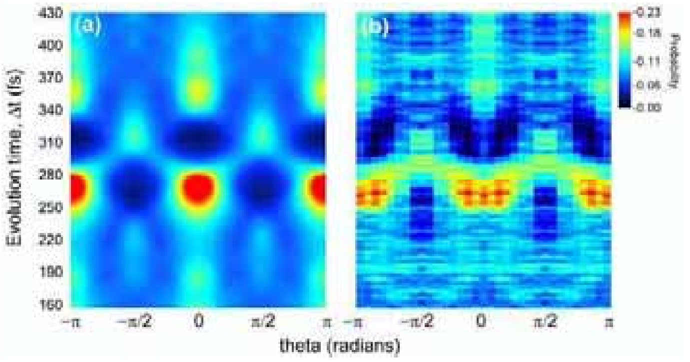

Figure 1. (a) Simulated "quantum carpet" for an initially randomly aligned ensemble of D_2 molecules at room temperature. (b) Integrated Coulomb explosion yield.

Populations of rotational states are extracted by Fourier Transform and are in excellent agreement with theoretical simulations for the deuterium molecule. The experimental data accurately follows the trends of the theoretical "quantum carpet" calculated for the experimental conditions in both terms of the position (in angular- and time-space) and relative scale of all the main features observed. This is particularly interesting as similar structures in the ionization yield were recently explained as being due to D_2^+ rotational motion [2]. Mapping the rotational wavepacket of deuterium has several direct implications, for example, such ideas are being actively sort out as a means of generating near single-cycle laser pulses via molecular phase modulation [3].

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We1-6

NEW METHODS FOR THE PRODUCTION AND DETECTION OF POLARIZED ATOMS: HYDROGEN AND CHLORINE

Dimitris Sofikitis[1,2], Luis Rubio-Lago[1], Andrew J. Alexander[3], Marion R. Martin[4], Davida J. Ankeny Brown[4], Antonis Koubenakis[1,2], Nathaniel C.-M. Bartlett[4], Richard. N. Zare[4], Theofanis N. Kitsopoulos[1] and T. Peter Rakitzis[1,2].

[1] *Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, 71110 Heraklion-Crete, Greece*

[2] *Department of Physics, University of Crete, P.O. 2208, 71003 Voutes-Heraklion, Greece*

[3] *School of Chemistry, University of Edinburgh, West Mains Road, Edinburgh, EH9 3JJ, United Kingdom*

[4] *Department of Chemistry,Stanford University,Stanford CA 94305-5080 (USA)*

Conventional methods for SPH production use involved experimental setups that produce densities of only about 10^{12} cm^{-3}, and detect the SPH non-remotely with atom polarimeters, which have limited time and spatial resolution. Recently, the production of SPH from pulsed-laser photodissociation of HCl and HBr with circularly polarized light (CPL) was confirmed indirectly via pulsed–laser detection of the halide's polarization [1]. A disadvantage of the technique is that the photodissociation process polarizes only the electronic spin of the atomic fragments leaving the nuclear spin unpolarized. At later times the polarization is shared between the electronic and the nuclear spin under the influence of the hyperfine coupling that causes a beating effect in sub-nanosecond timescales. When the electronic spin is detected in ns (or larger) timescales this beating results in an average depolarization which for the case of H atoms equals to 50%.

Here we show how SPH can be detected directly by pulsed-laser polarized fluorescence at 121.6 nm, remotely and position-sensitively on the nanosecond timescale, with detection sensitivity better than 10^{8} cm^{-3}, and with Doppler velocity resolution, which represent improvements of several orders of magnitude with respect to conventional techniques. These advances in control, sensitivity, time-resolution, and ease of use will enable pump-probe studies of SPH under single collision conditions [2].

Additionally we address the problem of the hyperfine depolarization (HFD) by demonstrating a new method to polarize independently the atom's nuclear spin. This method utilizes a similar HFD beating effect that is observed when the rotational angular momentum in molecules is polarized with a pulsed laser and without hyperfine resolution. Photodissociation at appropriate pump-probe delays "freezes" this angular momentum exchange producing atoms with their nuclear spin highly polarized. This novel method of hyperfine polarization (HFP) is demonstrated for the case of Cl atoms produced by photodissociation of HCl, and degrees of polarization of almost 75% are achieved at pump-probe delay of 150ns [3]. In combination with the high degrees of electronic spin polarization that can be obtained by the photodissociation process itself this technique can lead to the production of atoms with both their electronic and nuclear spin highly polarized. The HFP technique can be used to produce H atoms with their proton spin polarized, as predicted for the case of HF molecule, where proton polarization of 70% can be obtained at pump-probe delay of 4μs [4], making possible the production of high density SPH atoms (>10^{16} cm^{-3}), that can be produced and detected on a ns timescale, all in table-top configuration.

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We1-7

Laser induced molecular alignment of ethylene

A. Rouzée, S. Guérin, B. Lavorel, and O. Faucher

Institut Carnot de Bourgogne, UMR 5209 CNRS - Université de Bourgogne, BP 47870, 21078 Dijon cedex, France

Molecular orientation and alignment play a key role in strong field-molecule interactions, chemical reactions, and gas-phase solid interactions. For example, in chemistry, the product of a reaction can be maximized by aligning molecules, or in gas-phase solid interaction, stereodynamic effects on surface adsorption processes can be studied by guiding molecules [1]. To investigate the effects of molecular alignment on these processes, it is necessary to control the rotational degrees of freedom of the molecules. The last years, it has been established that strong non-resonant laser pulses of duration $\tau \gg \hbar /B$, with B the rotational constant of the molecule, align molecules during the interaction with the field, while impulsive pulses ($\tau \ll \hbar /B$) yield to post-pulse transient alignment revivals [2]. These effects have been studied both theoretically and experimentally, principally in linear molecules. However, lot of applications implies asymmetric top molecules. It is necessary therefore to implement experiments in order to control their rotational motions.

Here, we show that a single elliptically polarized laser pulse with appropriate ellipticity allows to align the three axes of an asymmetric top molecule. We present a theoretical model where we define the ellipticity that maximizes simultaneously the alignment of two molecular axes, and therefore the 3-D alignment. Experimentally, field free 3-D molecular alignment has been probed using the optical kerr effect in a molecular jet of ethylene. One-dimensional alignment experiments have been first conducted with linearly polarized laser pulses in order to estimate peak intensity and temperature. Then, using elliptically polarized laser pulses, we have induced and measured three-dimensional alignment of ethylene.

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Electron re-scattering in aligned H_2 and CO_2 using the R-matrix method

Alex Harvey and Jonathan Tennyson

Department of Physics and Astronomy, University College London, Gower Street,
London, WC1E 6BT, UK
`email:alexh@theory.phys.ucl.ac.uk`

Electron re-scattering in conjunction with high harmonic generation can allow for time-resolved study of nuclear and electronic dynamics at subfemtosecond timescales with Ångstrom spatial resolution [1,2]. In such experiments a molecule is ionised and the resulting electron recollided with the parent molecule by a strong laser field, either rescattering, or re-combining and emitting light. It is usual for such experiments to be performed on aligned molecules, as the alignment can modify the probability of re-collision.

Our group is modelling, computationally, electron re-scattering in aligned H_2 and CO_2 molecules. We have completed a preliminary study of re-scattering from the unaligned molecules [3].The electron—molecule scattering software we use (the UK R-matrix package) does not allow for specification of molecular alignment. A new module to add this functionality is being developed, allowing the calculation of scattering amplitudes and differential cross sections. The results will be presented at the conference.

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We1-9

Pulse shaping for optimizing field-free molecular alignment

E. Hertz, A. Rouzée, B. Lavorel, and O. Faucher

Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, BP 47870, 21078 Dijon Cedex, France

The possibility of controlling the angular distribution of molecules in space has become a subject of growing interest with a lot of challenging applications in chemical reactions, surface processing, or ultrafast optics [1]. When a molecular sample interacts with an intense ultra-short laser pulse, periodic molecular alignment is observed after the end of the pulse. Such post-pulse alignment is particularly valuable for further applications since it provides a sample of aligned molecule under *field-free* conditions. The degree of alignment that can be reached by a single ultra-short laser pulse is intrinsically limited. Experimental and theoretical efforts have thus recently concentrated on the possibility of enhancing this alignment. We present here the optimization of field-free molecular alignment by phase-shaped femtosecond laser pulse. The effect is theoretically demonstrated in O_2 at a temperature of 60 K under realistic conditions of intensity and pulse shaping. The spectral phase that optimizes the degree of *field-free* molecular alignment is designed iteratively using an evolutionary algorithm combined with a nonperturbative calculation in a feedback loop. We show that the molecular alignment under constraint of constant energy is significantly enhanced compared to a Fourier Transform Limited pulse by applying a rather simple spectral phase. The mechanism of control is analyzed. Simulations at different temperatures as well as in other molecules corroborate these results. Application to isotopic separation will be discussed.

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We1-10

Determination of atomic level polarization time decay

E.G. Kanetsyan, G.G. Adonts

"Lazerayin Tekhnika"cjc, 21Shopron St., 375090 Yerevan, Armenia
email: e_kanetsyan@yahoo.com

Intensive polarized laser radiation causes optical anisotropy of resonant atomic and molecular systems. Then the system is characterized no only by levels total population, i.e. "polarization momentum" of first order, but also by momenta of higher orders.

Polarization decay rates for the atomic multipole momenta (polarization, orientation, alignment) can be determined by means of the nonlinear polarization spectroscopy. The information on polarization momenta relaxation is obtained by examining of probe signal spectrum. However a lineshape is determined both by longitudinal and transverse relaxation.

In this paper the general theory of atomic levels polarization momenta decay time determination is developed without preliminary determination of transversal times of relaxation, any limitation on pulse duration. The essence of the method is the measurement of the time decay of probe signal polarization plane rotation, which is caused by the time-leading intensive polarized pulse.

The interaction of intense elliptically polarized light with the resonant medium consisting of identical two-level atoms with arbitrary total angular momenta is considered. The theory has been developed based on the irreducible tensorial formalism which allows to diagonalize relaxations matrix and to introduce effective decay times associated with the population relaxation as well as to the coherence relaxation between magnetic sublevels of a resonant system. atom system.

The tensor of nonlinear susceptibility of the medium with initial nonequilibrium population at the frequency of the probe signal is obtained. From the formulae it is seen that orientation vector determining hydrotropic properties of the medium depends only on the degree of circular polarization of the intense wave. In the general case of the wave elliptic polarization all tensor components are different, i.e. the medium has both hydrotropic properties and the properties of "biaxial crystal".

Studying the decay of anisotropic properties of the medium by probe signal, which delays and not overlaps the intense pulse, it is possible to determine the characteristic decay times of levels multipole momenta. It must be emphasized that the anisotropy relaxation is determined only by the longitudinal relaxation. Separation of this or that polarization momentum is possible by corresponding choice of intensive pulse polarization.

We1-11

ALIGNMENT DEPENDENCE IN STRONG-FIELD IONIZATION OF LASER-IRRADIATED MOLECULAR DIMERS

Vladimir I. Usachenko[1], Pavel E. Pyak[1] and Shih-I Chu[2]

[1] Institute of Applied Laser Physics UzAS, Tashkent, 100185, Uzbekistan.
[2] Department of Chemistry, University of Kansas, Lawrence, KS 66045-7582, USA

The orientation behavior of molecular strong-field multiphoton ionization depending on alignment of molecular axis relative to incident laser field polarization for a number of light laser-irradiated molecular dimers (H_2^+, H_2, N_2 and O_2) is addressed within the *velocity-gauge* (VG) formulation of molecular *strong field approximation* (SFA). The applied VG-SFA approach is also essentially based on the GAUSSIAN code for numerical composition of initial (laser-free) molecular state with a special Gaussian basis set extended by using the model LB_α intramolecular binding potential (which incorporates both the *exchange* and *correlation LSDA*-potentials, see, e.g., [1], for details).
The calculated molecular ionization rates Γ_{ion} were found as strongly dependent on spatial orientation of internuclear axis R_0 with respect to polarization $\boldsymbol{e}$ of incident laser field, i.e., on the angle Θ ($\cos\Theta = \boldsymbol{e}\cdot\boldsymbol{R}_0/R_0$). However, the particular form of the dependence $\Gamma_{ion}(\Theta)$ was found to be very sensitive to the orbital and bonding symmetry of the *highest-occupied molecular orbital* (HOMO) corresponding to the outermost molecular shell (normally predominantly contributing). In particular, for *Ti:sapphire* laser (ω = 1.56 *eV*) of intensity $I = 2\cdot10^{14}$ *W/cm*^{2}, the ratio $\Gamma_{ion}(0)/\Gamma_{ion}(\pi/2)$ calculated for N_2 has been found as equal to 1.7. Thus, for the appropriately composed $3\sigma_g$ HOMO the ionization rate presently calculated for N_2 proved to demonstrate correct (viz., consistent with experiment [2]) orientation dependence. The latter our result is also well consistent with the earlier alternative VG-SFA calculation [3] based on a different (viz. self-consistent Hartree-Fock) numerical procedure of $3\sigma_g$ composition, although in contrast to the respective VG-SFA findings [4] suggesting quite opposite (incorrect) orientation dependence of N_2 ionization rate. Thus, contrary to the interpretation suggested in [4], our findings demonstrate a good validity of the SFA in VG formulation for adequate description of molecular strong-field ionization. Moreover, the contradiction was reliably identified as arising due to the relative contribution from s-states well overestimated in [4] (as compared to p-states) within the particular (12s7p)/[6s4p] Gaussian basis set chosen under numerical composition of the $3\sigma_g$ HOMO using the GAMESS code.

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We1-12

CIRCULAR DICHROISM IN TWO-PHOTON IONIZATION OF ORIENTED AND ALIGNED ATOMS

M. Ya. Agre
National University of “Kyiv-Mohyla Academy”, 04070, Kyiv, Ukraine
e-mail: markag@aport2000.ru

On the basis of the reasons of symmetry and without any approximations used in atomic calculations we derive the compact invariant expression for the total probability of two-photon ionization of axial-symmetrically polarized (oriented and aligned) atoms or molecules.

After separating out the dependency on all geometrical parameters (the unit vectors **k** and **e** specifying correspondently the direction of propagation and polarization of the ionizing electromagnetic radiation, and unit vector **n** determining the direction of the orientation-alignment axis), the formula for the two-photon ionization rate can be written out in the following form:

$$\mathrm{W} = g^2 \Big\{ a_0 + b_0 \left(2 + \xi^2\right) + \rho_1^n a_1 \mathbf{k} \cdot \mathbf{n} + \rho_2^n [a_2 (1 - \xi^2)/3 + b_2 (1 + 2\xi^2)/3 \\ - |\mathbf{n} \cdot \mathbf{e}|^2 \left(a_2 + b_2\right) + \xi^2 \left(a_2/2 - b_2\right) (\mathbf{k} \times \mathbf{n})^2] + \rho_2^n c_2 \xi \mathrm{Re}[\mathbf{k} \cdot (\mathbf{n} \times \mathbf{e})(\mathbf{n} \times \mathbf{e}^*)] \Big\}. \qquad (1)$$

Here g is the density of the photon flux, $\xi = i\mathbf{k} \cdot (\mathbf{e} \times \mathbf{e}^*)$ is the degree of the circular polarization of the ionizing radiation equal to ±1 for right-hand (left-hand) circular polarization ($\xi^2 + l^2 = 1$, where $l = |\mathbf{e} \cdot \mathbf{e}|$ is the degree of linear polarization); ρ_K^n is the zeroth component of the *K*-rank state multipole for the polarized atom in the atomic system of coordinates, where z axis is directed along **n** and only the zeroth component is nonzero [1]; a_j , b_j and c_2 are the dynamic atomic parameters that one can calculate using the known approximations. The T-odd (i. e., changing sign under time inversion) pseudoscalar ρ_1^n specifies the orientation, and T-even scalar ρ_2^n specifies the alignment of the atom.

The terms linear in the degree of circular polarization ξ of eq. (1) determine the effect of circular dichroism (CD) in the total probability of two-photon ionization of oriented and aligned atomic system. Note that the CD induced by orientation is also observed in the total cross-section of photoeffect (one-photon ionization) and is determined by the same scalar combination $\xi\rho_1^n \mathbf{k} \cdot \mathbf{n}$, but CD induced by alignment is only observed in the angular distribution of photoelectrons and is not observed in the total cross-section of photoeffect [2, 3].

The CD in the total probability of two-photon ionization of aligned atoms is determined by the last term of eq. (1), which contains the T-odd combination of the vectors. It points at the T-oddness of the dynamic parameter c_2. Therefore this CD can only be observed near the resonance in two-photon ionization when the T-odd dissipative parameter (the width of resonant level) contributes to the probability of the process. A similar dissipation-induced CD manifests in the polarization peculiarities and angular distribution of light scattered by aligned atoms [4].

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POSTERS

Wednesday 9/5

2. BEC-Quantum Gases

We2-1

Generalized Mean Field Theory of Resonant Bose-Fermi Mixtures

Alexander V.Avdeenkov$^{(1,*)}$ Daniele C. E. Bortolotti$^{(2)}$, and John.L.Bohn^{2}

(1)Institute of Physics and Power Engineering Obninsk,Kaluga region,RUSSIA, 249033, (2)JILA, NIST, and Department of Physics, University of Colorado, Boulder, CO 80309-0440

Nowadays the physics of cold atomic gases and their mixtures provide extraordinary opportunities both to test theoretical models and to predict new phenomena. The most remarkable effects arise when a resonant interaction can be engineered between pairs of atoms, by means of a magnetic-field Feshbach resonance (FR). Such a tunable resonant interaction in a trapped Bose-Fermi (BF) mixture brings a variety of regimes that are defined both by the interaction strength and by the densities of the two species [1-5]

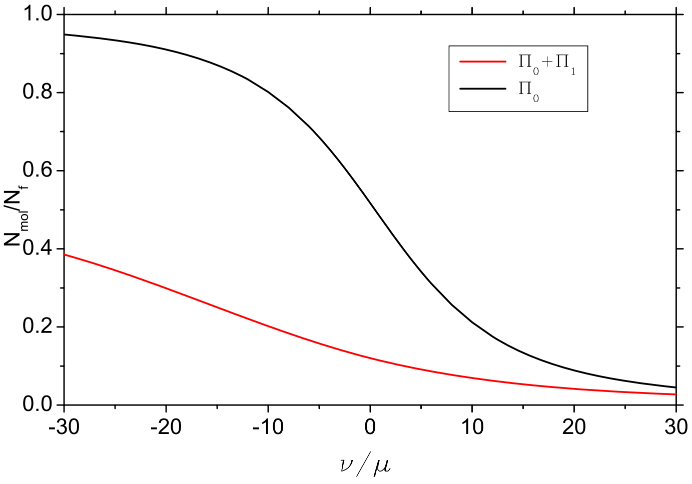

FIG. 1: Molecular population as a function of detuning normalized to number of fermions in the system. The black line represents the mean field calculation, and the red one is obtained taking full account of the two body physics, highlighting the importance of this contribution.

In the vicinity of a Feshbach resonance, one boson and one fermion can combine to make a two-body fermionic pair. This pair may be bound or not, depending on the magnetic-field detuning, and on the pair's momentum, with stability being strongly conditioned by many-body interaction in the gas. We assess this stability by identifying the poles of the many-body T-matrix. By analyzing the residues of the poles described above, we can estimate the equilibrium molecular populations as a function of detuning.

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*avdeenkov@ippe.ru

We2-2

Time-Averaged Adiabatic Potentials (TAAP) for Matter-Wave Interferometry

M. Baker, V. Bolpasi, P. Condylis, G. Konstantinidis, N. Lagos, A. Lazoudis,
I. Lesanovsky, O. Morizot, M. Pappa, A. Protopapadakis, D. Sanchez, W. von Klitzing

I.E.S.L. - Institute of Electronic Structure and Lasers
FO.R.T.H. - Foundation for Research and Technology
Vassilika Vouton, P.O. Box 1527,
Heraklion Crete 71110, Greece

Bose-Einstein Condensates have opened unprecedented possibilities for many-body physics and quantum optics. For the first time a bright source of coherent matter waves has become available which is giving rise to a new generation of atom-interferometers. This promises ultra-sensitive precision sensors for fundamental interactions such as gravitation and acceleration. However, techniques to manipulate matter-waves are still at a very early stage of development.

Here, we present our advances towards a novel type of matter-wave interferometer based on a circular matter-wave guide created with time-averaged adiabatic potentials (TAAP). [1] In the time-averaged adiabatic potential (TAAP) a radio frequency dresses a magnetic quadrupole trap to create a shell-like adiabatic trap. [3] This is then exposed to an oscillating time-averaging potential. [2] For a given quadrupole coil-configuration we can create trap shapes ranging from a ring to pancakes and double cigars, depending only on the relative frequencies and amplitudes of the modulation fields. The double trap and the ring-shaped wave-guide are of particular interest for interference experiments. The latter, for example, is ideally suited as a Sagnac interferometer. The distance between the cigars and the diameter of the ring range from a few micrometers to centimetres depending only on the radio frequency applied.

The ring trap will be used to make a Sagnac interferometer in our ongoing Bose-Einstein experiments at IESL-FORTH.

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CREATION OF SOLITONS IN ATOMIC BEC

G. Juzeliūnas[1)], P. Öhberg[2)], J. Ruseckas[1)] and M. Fleischhauer[3)]

[1)] Institute of Theoretical Physics and Astronomy of Vilnius University, Goštauto 12, 01108 Vilnius, Lithuania
[2)] Department of Physics, University of Strathclyde, Glasgow G4 0NG, Scotland
[3)] Fachbereich Physik, Universität Kaiserslautern, D-67663 Kaiserslautern,

Atomic Bose-Einstein condensates (BECs) can exhibit various topological excitations, such as vortices or solitons. Dark solitons are formed when a steep phase slip is induced in the condensate wave-function accompanied by a reduction of the condensate density in this area. Traditionally dark solitons in BECs are created using phase imprinting [1-2], where a part of the condensate cloud is illuminated by a far detuned laser pulse in order to induce a sharp π phase slip in the wave function. The subsequent dynamics can indeed develop solitons [1-2].

There are, however, some rather severe drawbacks with such a method of phase engineering. The resolution of the required phase slip is naturally restricted by the diffraction limit. Furthermore the phase imprinting does not produce a density minimum characteristic to the dark solitons in the region of the phase change. Hence completely dark stationary solitons are difficult to achieve, which consequently results in so called grey moving solitons with a shallow density dip.

It is of a significant interest to be able to create slowly moving, or even completely stationary solitons in order to test for instance the scattering properties of solitons. The shapes of the colliding solitons are preserved, and a relative spatial shift is expected. Yet the latter shift is only detectable for extremely slowly moving solitons.

Here we propose a new and robust method of creating dark solitons in atomic BECs [3]. We suggest to produce solitons by sweeping through a BEC a set of laser beams acting on the BEC atoms in the tripod configuration [3]. If the beams have proper amplitude and phase profiles, an effective magnetic field is known to be generated in the atomic BEC [4]. Creation of a soliton can then be considered as a manifestation of the Lorentz force acting on moving atoms. A topological structure of the solitons produced in this way depends exclusively on the topological structure of the laser beams applied. Furthermore the emerging phase slip is not restricted by the diffraction limit. By choosing proper laser fields one can create slowly moving multicomponent solitons of the dark-bright and dark-dark type, as well as pairs of such solitons. The latter pairs will collide and a spatial shift will show up.

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We2-4

ROUTES TOWARDS Cs ATOM BEC VIA HIGH DENSITY DIPOLE TRAP.

G. Stern, D. Sofikitis, E. Dimova, A. Fioretti, D. Comparat and P. Pillet

Laboratoire Aimé Cotton, CNRS, Bât.505, Campus d'Orsay, 91405 Orsay cedex, France

We study different routes for the production of Cs atoms Bose Einstein condensates in a crossed optical dipole trap that provides a high density atomic sample. The dipole trap is loaded either from molasses, or from magnetic trap, and the evaporating cooling process can be obtained with the variation of the optical trap's depth and dimensions, while the collisional properties of the Cs atoms can be modulated via their scattering length α with the use of a magnetic field.

Initially the atoms are prepared inside a magneto-optical trap (MOT) located in an ultra-high vacuum glass cell, loaded from a cesium vapor cell MOT using a pushing laser beam. A high power and slightly diverging laser beam has been used to optimize the transfer between the two traps with frequency red-detuned from the atomic transition. This pushing laser extracts a continuous beam of slow atoms out of the first MOT and guides them into the second one through the dipolar force [1].

The crossed optical dipole trap is realized with the use of an Ytterbium fiber laser at 1070nm. The slow divergence of the laser's focus causes atoms to remain in the uncrossed region, resulting to unfavorable conditions for the evaporating cooling process. We expel these atoms using a quadrupole magnetic field similar to the one used in magnetic traps after having them polarized in their ground state $|F = 3, m_F = +3\rangle$ using optical pumping. The dimensions of the trap can be modulated with the use of a piezoelectric motor that controls the position of a converging lens in a telescope (zoom) providing trap dimensions from 50 to 100μm in the crossed beams configuration. Optimal loading of the dipole trap can be realized with use of molasses phase or by overlapping the dipole trap with a magnetic trap [2] and is depended in the trap dimensions.

The evaporation process can be obtained by decreasing the dipole trap laser power and by adjusting the trap's dimension in order to keep it's frequency constant. We ensure that the sample is thermalized during each step of the ramp using a set of equations that take into account two-body elastic collision rate, initial power of the laser beams and trap's dimensions. Finally a magnetic field is used to drive the system in the vicinity of a Feshbach resonances to cause large variations of the value of the s-wave scattering length in order to achieve appropriate collisional properties for the evaporating cooling process [3,4]. The experiment is in process.

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We2-5

INTERACTION OF A RYDBERG ATOM WITH A TRAPPED BOSE-EINSTEIN CONDENSATE

Cenap Ates and Jan-Michael Rost

Max Planck Institute for the Physics of Complex Systems,
Nöthnitzer Str. 38, 01187 Dresden, Germany
e-mail: cenap@pks.mpg.de

The experimental realization of Bose-Einstein condensation (BEC) in atomic vapors together with quantum optical tools, which allow for a large degree of control over these systems, has opened the path for a systematic study of impurities immersed in a quantum liquid.

The presence of impurities in a quantum degenerate system can alter its physical properties drastically. In particular, the interactions of impurities with their background can be used to probe structural and dynamical properties of the host system, like, e.g., superfluidity.

One possibility to introduce impurities into a BEC is the excitation of BEC atoms to Rydberg states. They have the advantage that the BEC-impurity interaction strength can be controlled precisely by exciting atoms to specific Rydberg states.

We present a numerical study of the excitation dynamics of a Rydberg atom in a weakly interacting BEC at low temperatures and discuss differences in the dynamical behavior for varying impurity-BEC interaction.

We2-6

Multicomponent gap solitons in spinor Bose-Einstein condensates

Beata J. Dąbrowska-Wüster, Elena A. Ostrovskaya, Tristram J. Alexander,
Yuri S. Kivshar

Nonlinear Physics Centre and ARC Centre of Excellence for Quantum-Atom Optics,
RSPhysSE, The Australian National University, Canberra ACT 0200, Australia
bjd124@rsphysse.anu.edu.au

We model the nonlinear behaviour of spin-1 Bose-Einstein condensates (BECs) with repulsive spin-independent interactions and either *ferromagnetic* or *antiferromagnetic* (polar) spin-dependent interactions, loaded into a one-dimensional optical lattice potential [1]. We show that both types of BECs exhibit dynamical instabilities and may form spatially localised multicomponent structures. The localised states of the spinor matter-waves take the form of *vector gap soliton* and *self-trapped waves* that exist only within gaps of the linear Bloch-wave band-gap spectrum. Of special interest are the nonlinear localised states that do not exhibit a common spatial density profile shared by all condensate components, and consequently cannot be described by the *single mode approximation* (SMA) frequently employed within the framework of the mean-field treatment. We show that the non-SMA states can exhibits Josephson-like internal oscillations and *self-magnetisation*, i.e. intrinsic precession of the local spin. Finally, we demonstrate that non-stationary states of a spinor BEC in a lattice exhibit coherent undamped spin-mixing dynamics, and that their controlled conversion into a stationary state can be achieved by the application of an external magnetic field.

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We2-7

Ground state properties and elementary excitation of ^{85}Rb Bose- Einstein condensate : Analytical method for modified Thomas-Fermi model with large gas-parameter

Moumita Gupta and Krishna Rai Dastidar*

Indian Association for the Cultivation of Science,
Jadavpur, Kolkata-700032, West Bengal, India.

Bose-Einstein condensation in trapped gases of ^{85}Rb atoms can now be obtained in the large gas-parameter region in presence of Feshbach resonance [1] and the gas density which is characterized by peak gas parameter x_{pk} can attain the value ~ 10^{-2}. For such large gas-parameter, the first correction term to the Bogoliubov energy functional is considered to give modified Gross-Pitaevskii (MGP) equation [2]. In this work analytical expressions for the chemical potential, the density of particles and the excitation frequency of the monopole mode have been derived in Thomas-Fermi(TF) approximated approach to the MGP equation (modified TF approach) following method of higher order iteration for Bose-Einstein condensate (BEC) of atoms in spherically symmetric trap. We have also solved the MGP equation by using Runge-Kutta method for integration of nonlinear differential equation considering spherically symmetric trap. The analytical results for chemical potential and density of particles for BEC of 10^3 and 10^4 ^{85}Rb atoms in a spherically symmetric trap are in very good agreement with the numerical results from MGP equation at low as well as at large scattering length i.e, at large gas-parameter region. The frequency of monopole mode calculated using the density of particles in the ground state (found out in higher order iterative method) are also in very good agreement with the existing numerical results [3]. The difference between the analytical and numerical results decreases as the value of scattering length i.e, gas-parameter is increased.

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*krishna_raidastidar@yahoo.co.in

BEYOND MEAN FIELD: USING LASER PULSES TO PROBE PAIR CORRELATIONS IN CONDENSATES

J. Mur-Petit,[1,*] P. Naidon,[2] E. Luc-Koenig,[1] and F. Masnou-Seeuws[1]

[1]Laboratoire Aimé Cotton, CNRS and Univ. Paris-Sud, 91405 Orsay, France

[2]Atomic Physics Division, NIST, Gaithersburg, Maryland 20899-8423, USA

The formation of molecular condensates from atomic condensates by means of optical or magnetic Feshbach resonances is a topic of growing interest [1,2]. The theoretical methods required by these processes need to account for the correlations in the system, which is *beyond the validity of the mean-field approximation.*

Following the ideas of Ref. [3], we have developed a method that takes into account two-body correlations in such situations [4]. In particular, we have shown that a sudden switch-on of a photoassociation laser onto an atomic sample shall give rise to *correlated* pairs of "hot" atoms leaving the trap [5]. This leads to an *increase* in the correlation for the equal-time detection of two atoms with opposite momenta:

$$g^{(2)}(\boldsymbol{k},-\boldsymbol{k};t)=\frac{\langle\hat{a}^\dagger_{\boldsymbol{k}}(t)\hat{a}^\dagger_{-\boldsymbol{k}}(t)\hat{a}_{-\boldsymbol{k}}(t)\hat{a}_{\boldsymbol{k}}(t)\rangle}{\langle\hat{a}^\dagger_{\boldsymbol{k}}(t)\hat{a}_{\boldsymbol{k}}(t)\rangle\langle\hat{a}^\dagger_{-\boldsymbol{k}}(t)\hat{a}_{-\boldsymbol{k}}(t)\rangle}>2\,.$$

We analyze the detection of these correlations with time-of-flight measurements as in the experiments with metastable helium by the group of Chris Westbrook [6].

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[*] Also at Institut Francilien de Recherche sur les Atomes Froids (IFRAF).

E-mail: jordi.mur@lac.u-psud.fr

We2-9

DYNAMICAL INTERFERENCES AS A PROBE OF SHORT-PULSE PHOTOASSOCIATION

J. Mur-Petit,* E. Luc-Koenig, and F. Masnou-Seeuws

Laboratoire Aimé Cotton, CNRS and Univ. Paris-Sud, 91405 Orsay, France

Several experimental teams are pursuing the controlled formation of stable molecules by use of short laser pulses [1,2,3]. We have analyzed the formation of Rb_2 molecules with one such pulse applied to a cold $^{85}\mathrm{Rb}$ sample. The laser field couples a continuum level of the ground electronic state $\mathrm{X}^1\Sigma_g^+$ with bound levels in the $0_u^+(5S+5P_{1/2})$ and $0_u^+(5S+5P_{3/2})$ vibrational series. The strong non-adiabatic coupling between the two excited channels induces beatings between their populations after the end of the pulse, with characteristic timescales which we propose to use as a probe of the population of molecular levels [4].

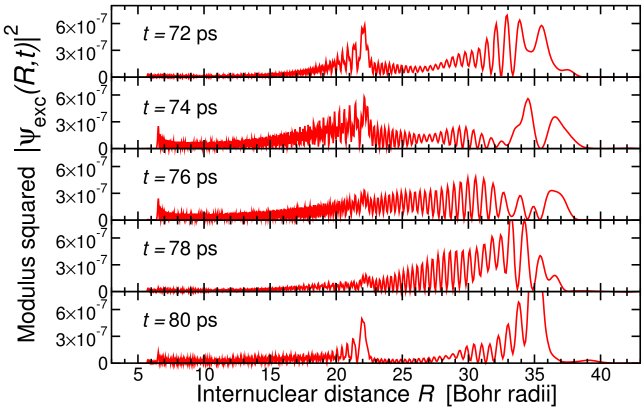

Figure: Evolution of the wavepacket in the excited channels after a photoassociation pulse of duration ≈ 10 ps was applied at time $t_P = 50$ ps to a pair of colliding rubidium atoms with an energy $E \approx k_B \times 100\ \mu$K. Note the evolution of the probability peak close to $R \approx 22a_0$, that oscillates with a timescale $T_{\mathrm{beat}} \approx 8$ ps.

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*Also at Institut Francilien de Recherche sur les Atomes Froids (IFRAF).

E-mail: jordi.mur@lac.u-psud.fr.

We2-10

GAP SOLITON SELF-FORMATION IN BOSE-EINSTEIN CONDENSATE

Michal Matuszewski[1,2], Wieslaw Krolikowski[2], Marek Trippenbach[1,3],
Yuri S. Kivshar[4]

[1]Department of Physics, Warsaw University, Hoza 69, PL-00-681 Warsaw, Poland
[2]Laser Physics Centre, Research School of Physical Sciences and Engineering, Australian National University, Canberra ACT 0200, Australia
[3]Soltan Institute for Nuclear Studies, Hoza 69, PL-00-681 Warsaw, Poland
[4]Nonlinear Physics Centre and ARC Centre of Excellence for Quantum-Atom Optics, Research School of Physical Sciences and Engineering, Australian National University, Canberra ACT 0200, Australia

We suggest an efficient method for generating matter-wave gap solitons in a repulsive Bose-Einstein condensate, when the soliton is formed from a condensate cloud in a harmonic trap after turning on a one-dimensional optical lattice. We demonstrate numerically that this approach does not require preparing the initial atomic wavepacket in a specific state corresponding to the edge of the Brillouin zone of the spectrum, and losses that occur during the soliton generation process can be suppressed by an appropriate adiabatic switching of the optical lattice. We introduce a simple analytical model that allows to get a deeper insight into the physics of the soliton generation.

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We2-11

GROUND STATES OF SPIN-3 BOSE-EINSTEIN CONDENSATES FOR CONSERVED MAGNETIZATION

H. Mäkelä and K.-A. Suominen

Department of Physics, University of Turku, FI-20014 Turun yliopisto, Finland

Since the creation of a chromium condensate [1], the interest in spin-3 condensates has increased rapidly. In its ground state ^{52}Cr is a spin-3 atom which, together with the relatively strong magnetic dipole-dipole interaction, leads to intricate ground states and rich spin dynamics. In our work we calculate the ground states and ground state phase diagrams of Bose-Einstein condensates of spin-3 atoms under the assumption of conserved magnetization [2]. We present the ground state phase diagrams pertaining to several values of magnetization, and especially concentrate on the ground states of a ^{52}Cr condensate.

We also calculate an estimate for the dipole-dipole interaction energy and show that the ground state of a ^{52}Cr condensate does not seem to depend on whether or not the dipole-dipole interaction is taken into attention. We discuss the experimental realization of a spinor ^{52}Cr condensate and point out that due to fast incoherent decay the condensate density should be decreased in order to make the lifetime of the condensate long enough for experiments. We suggest that this could be achieved by loading the condensate into an optical lattice of shallow traps [3].

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We2-12

NON-MARKOVIAN DYNAMICS IN ATOM-LASER OUTCOUPLING FROM A DOUBLE-WELL BOSE-EINSTEIN CONDENSATE

G. M. Nikolopoulos†, C. Lazarou‡ and P. Lambropoulos†

†Institute of Electronic Structure & Laser, FORTH, P.O.Box 1527, Heraklion
GR-71110, Crete, Greece

‡ Department of Physics and Astronomy, University of Sussex, Brighton BN1
9QH, United Kingdom

The development of a continuous high-flux atom laser remains one of the main goals in the field of atom optics. The most crucial prerequisite for the realization of a continuous atom laser is the pumping mechanism replenishing the trapped condensate as atoms are outcoupled from it. Up to date, perhaps the most promising scheme towards the realization of a continuous source of condensed atoms was demonstrated by the MIT group [1], and relies on the use of optical tweezers for the transport and the merging of independently produced BECs.

Motivated by these experiments, we have investigated [2] the dynamics of an effectively one-dimensional atom laser model [3], based on the merging of independently formed atomic condensates. In a first attempt to understand the dynamics of the system, we consider two independent elongated Bose-Einstein condensates which approach each other and focus on intermediate inter-trap distances so that a two-mode model is well justified. As we approach the traps, a Josephson tunneling is established between the two BECs, while atoms are coherently outcoupled. The structured atomic continuum for the free atoms is associated with strongly non-markovian phenomena which cannot be described in the framework of Born and Markov approximations. Hence, our theoretical approach relies on the discretization of the atomic continuum which, in general, allows the treatment of arbitrary forms of outcoupling and the incorporation of interatomic interactions [4]. We discuss the quasi steady-state population of the traps as well as the energy distribution and the coherence of the outcoupled atoms [2]. In addition to its relevance to the atom laser, this work pertains also to the general field of non-markovian reservoirs.

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POSTERS

Wednesday 9/5

3. Cold atoms and molecules

We3-1

Production, state selection and deceleration of cold lithium hydride

S. K. Tokunaga, J. O. Stack, J. J. Hudson, B. E. Sauer, E. A. Hinds and M. R. Tarbutt

Centre for Cold Matter, Blackett Laboratory, Imperial College London, SW7 2BW, UK

Techniques are currently being developed to form cold and ultracold molecules for applications across many fields of research [1, 2]. The applications include tests of fundamental symmetries and time variation of fundamental constants, quantum information processing, quantum chemistry and the physics of dipolar quantum degenerate gases. An important technique for producing cold molecules is Stark deceleration [3]. Molecules seeded in a gas pulse are cooled by supersonic expansion to temperatures of order 1 K, and their large centre-of-mass velocity is reduced in the decelerator by a time-varying inhomogeneous electric field. Once brought to rest, molecules can be stored in an electrostatic trap [4], and ultralow temperatures may be achievable by sympathetic cooling with ultracold atoms [5].

The lithium hydride molecule is an excellent molecule for these techniques, due to its low mass, large dipole moment and amenability to ab initio calculation. Using laser ablation and supersonic expansion, we have produced beams of cold, ground state LiH for the first time. We have built a Stark decelerator capable of bringing to rest LiH molecules in the first rotationally excited state. We have achieved efficient population transfer to this rotational state using a novel source of microwaves at 444GHz. We will describe this work, and expect to present the first results from our decelerator.

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Atom Trap Trace Analysis of Calcium Isotopes

Albert K. Mollema, Lorenz Willmann, Klaus Jungmann and Ronnie Hoekstra

KVI Atomic Physics, University of Groningen,
Zernikelaan 25, 9747 AA Groningen, the Netherlands

A magneto-optical trap (MOT) can be used to determine the abundance of extremely rare isotopes by counting the individual atoms. This technique can be applied to both long-lived rare isotopes and short-lived exotic isotopes. Our special interest is in the rare isotope ^{41}Ca which has a natural abundance of 10^{-14} to 10^{-15}. This isotope has a half-life of 103,000 years, which makes it suitable for dating ancient sea-bottom sediments. Other important applications are in biomedical research and geology.

Using laser cooling and trapping techniques we separate the rare isotopes from the more abundant isotopes (97 % of natural calcium is ^{40}Ca). The isotope shift between ^{40}Ca and ^{41}Ca on the $^1S_0$ - $^1P_1$ cooling transition is 150 MHz, while the natural linewidth is 34 MHz. Cooling of the atoms reduces the average velocity such that the Doppler broadening of the transition becomes smaller than the isotope shift.

We have trapped and detected all stable isotopes of calcium including ^{46}Ca which has a natural abundance of only 0.004 % [1]. We have been able to reach a sensitivity of our detection system such that we can detect the presence of a single atom in the trap. The average trapping time of the atoms has been increased from 20 ms to 200 ms by extending our cooling scheme with a repump laser. The repump laser effectively closes a small leak in the cooling transition, which was initially limiting the trapping time.

In contrary to even isotopes of calcium, odd isotopes posses nuclear spin and therefore hyperfine structure. We study the efficiency of applying laser cooling and trapping techniques to odd isotopes in order to be able to optimize our setup for laser cooling and trapping of ^{41}Ca, using ^{43}Ca as a pilot system.

Laser cooling and trapping experiments require laser frequency stabilisation. To do so we developed a new technique of **Li**ght **P**ressure induced **S**pectroscopy (LiPS).

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Zeeman deceleration of neutral ground state atoms

S. D. Hogan, N. Vanhaecke, M. Andrist, U. Meier, D. Sprecher, B. H. Meier
and F. Merkt

Laboratorium für Physikalische Chemie,
ETH Zurich, Switzerland

The development of general methods with which to control the translational motion of atoms and molecules in the gas phase is of particular interest in high resolution spectroscopy and studies of cold reactive collisions. Several of these techniques start from cold samples formed in supersonic expansions and aim at stopping them in the laboratory frame. So far interest has centred on the deceleration and manipulation of atoms and molecules produced in such sources using electric field gradients. The techniques employed include multi-stage Stark deceleration of polar molecules [1], optical Stark deceleration [2], and Rydberg Stark deceleration [3,4]. With the construction, in our laboratory, of a multi-stage Zeeman decelerator for neutral ground state radicals, the possibility to manipulate a wider range of species has been demonstrated [5].

The Zeeman decelerator is composed of a series of co-axial solenoids through which a pulsed gas beam propagates. By switching the current in each solenoid to generate a pulsed magnetic field as the gas pulse enters we can take advantage of the linear Zeeman interaction of a ground state atom or molecule with unpaired electrons to decelerate the gas pulse in a manner analogous to that employed in a multi-stage Stark decelerator [1]. The pulse sequences which we generate, in numerical particle trajectory simulations, and apply to the coils are completely programable and permit us to implement the concepts of phase stability as in the Stark decelerator and charged particle accelerators [6].

The results of a recent series of experiments in which we have decelerated ground state atomic hydrogen with the Zeeman decelerator will be presented. In these experiments magnetic fields of 1-2 T were pulsed in each coil for tens of microseconds, with rise and fall times as short as 5 μs. We have characterised the decelerated part of the gas pulse and studied the effect of zero field time windows, in which electron spin flips can occur, on the deceleration process.

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We3-4

QUANTUM ENGINEERING OF ULTRACOLD ATOMS IN ONE-DIMENSIONAL TRAPPING POTENTIALS

D.S. Murphy and J.F. McCann
Centre for Theoretical Atomic, Molecular and Optical Physics,
Queens University Belfast, Belfast BT7 1NN, Northern Ireland, UK
E-mail: domhnall.murphy@qub.ac.uk

The last two decades have seen considerable experimental progress in the field of atom cooling, trapping and manipulation. On the back of such advancements, scientists, both theoretical and experimental, have devoted considerable time and resource towards the exploitation of this cold atom technology, particularly in the field of quantum information processing. One exciting area of development has been the trapping and manipulation of a Bose-Einstein condensate (BEC) using an array of interfering laser beams (optical lattice) [1-6]. It has been shown that single- and two-particle effects dominate the dynamics of such cold atom/optical lattice systems [3,6].

In the current work, we investigate systems of trapped, ultracold, particles, interacting via a zero-ranged pseudopotential. Consideration is restricted to single and two-particle systems confined by one-dimensional trapping potentials. The problem of two particles interacting via a pseudopotential permits an analytic solution in certain circumstances, for example in spherically [7,8] and axially [9] symmetric harmonic trap geometries. However, more generally, such analytical solutions are not possible and one must resort to numerical techniques.

In the current study we employ a combination of analytical and numerical techniques to investigate the manipulation of the motional states of these single- and two-particle systems in different time-dependent trapping potentials. In particular, we focus on a two-well system and investigate how the control of parameters such as the barrier height and interaction strength may be used to permit control over both, the motional state of the system, and the entanglement between the two interacting particles [10,11]. Such work is of direct relevance to studies of quantum gases in quasi-1D trapping potentials [2,5] and recent studies of the Tonks-Giradeau regime [5,12,13].

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We3-5

A Scheme for Cavity Cooling of Internal and External Degrees of Freedom of Molecules.

P.W.H. Pinkse[1], G. Morigi[2], M. Kowalewski[3], R. de Vivie-Riedle[3]
[1] Max-Planck-Institut-für Quantenoptik, Hans-Kopfermannstr. 1,
D-85748 München, Germany
[2] Departament de Fisica, Universitat Autonoma de Barcelona,
E-08193 Bellaterra, Spain
[3] Department Chemie, LMU, Butenandtstr. 11, D-81377 München, Germany.

Ultracold molecules are of interest for the study of cold chemistry, cold collisions, astrochemistry and quantum information processing. Their preparation, in particular of ultracold ground state molecules, however, is still challenging. Adapted versions of laser cooling, which try to optimize optical pumping into the molecular ground state, have been proposed [1], but their efficiency is limited by the absence of closed transitions in molecules. A more viable optical avenue seems the use of cavities for cooling, which would avoid the leakage by open transitions. For instance, efficient cavity cooling of the external degrees of freedom has been proposed [2] and demonstrated for atoms [3].

In this contribution we propose to cool the internal and external degrees of freedom of molecules by suitably tailored Raman processes, where absorption of photons from a laser beams is followed by emission into the cavity resonances. On average, this removes rovibrational and translational excitations. The method relies on the enhancement of emission along resonances of a resonator, while the laser, driving the molecules, is sequentially set to different frequencies corresponding to anti-Stokes lines, in order to empty the higher excited rovibrational states of the molecules.

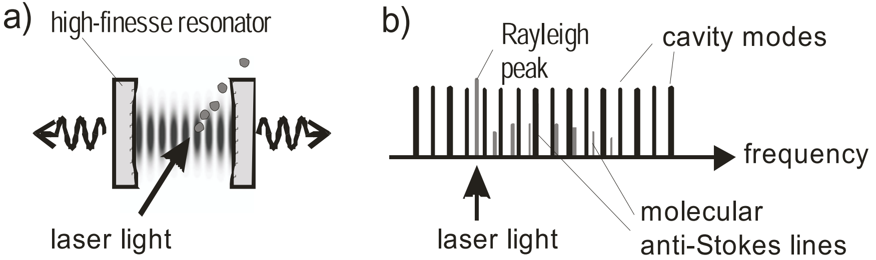

Fig. a) Schematic of the cooling setup. b) Sketch of the involved frequencies. The cavity defines a comb of resonances at which photon emission into the cavity is enhanced. The grey bars symbolize the molecular lines, which in OH extend over several 10 nm. The laser sequentially addresses several anti-Stokes lines.

The cooling efficiency is investigated numerically for the case of the OH radical, using ab initio data and taking into account the rovibrational dependence of the Raman scattering into the cavity modes.

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We3-6

CREATION OF AN ULTRACOLD MIXTURE OF FERMIONIC LITHIUM AND POTASSIUM

F.M. Spiegelhalder[1], E. Wille[1,2], G. Kerner[1], D. Naik[1], A. Trenkwalder[1], C. Aiello[1],
R. Chulia Jordan[1], G. Hendl[1], F. Schreck[1] and R. Grimm[1,2]

[1]Institut für Quantenoptik und Quanteninformation
Österreichische Akademie der Wissenschaften
Innsbruck, Austria

[2]Institut für Experimentalphysik
Leopold-Franzens-Universität
Innsbruck, Austria

Degenerate mixtures of fermionic ^{6}Li and ^{40}K provide a new, intriguing many-body quantum system, which enables the study of strongly interacting Fermi gases consisting of atoms with unequal masses. In our experiment, cold atoms from a magneto-optical trap are transferred into a crossed-beam optical dipole trap realized with a 100 W near-infrared laser. The sample is cooled down evaporatively to quantum degeneracy by lowering the trapping potential. The broad Feshbach resonance in ^{6}Li at a magnetic field of B = 834 G allows for precise tuning of the scattering length *a*. At a field of B = 764 G, we obtained a molecular $^6Li_2$ BEC (Fig. 1). At the same field we observe sympathetic cooling of bosonic ^{39}K and fermionic ^{40}K. By simultaneous absorption imaging of each atomic species at the end of each experimental cycle, we could verify the creation of ultracold mixtures of ^{6}Li-^{39}K and ^{6}Li-^{40}K. The next step will be to find inter-species Feshbach resonances at which we want to study strongly interacting gases and the formation of heteronuclear molecules.

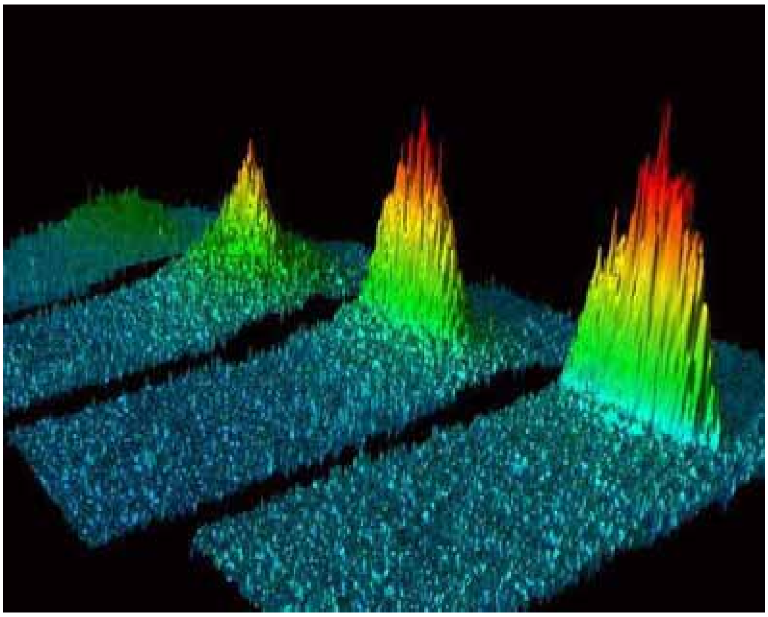

Fig. 1. Formation of a molecular BEC of about $5*10^5$ $^6Li_2$: the four time-of-flight images show the formation of a condensate peak in the centre of the initial thermal distribution.

We3-7

Coherent light transport in ultracold atomic vapors

G. Labeyrie[+], D. Wilkowski[+], R. Kaiser[+], C. Miniatura[+], D. Delande*.

[+] Institut Non Linéaire de Nice, UMR 6618 CNRS, Sophia Antipolis, France.
[*] Laboratoire Kastler Brossel, Université Pierre et Marie Curie, Paris, France.
contact : Guillaume.Labeyrie@inln.cnrs.fr

We present an overview of our results on diffusive transport of near-resonant light in ultracold atomic vapors, obtained during the past seven years. Cold atomic vapors constitute attractive new media to study light transport in the multiple scattering regime, because, among other things, of the resonant scattering cross-section and the absence of absorption. A special emphasis is put on the analysis of the *coherence* of the transport, a prerequisite to observe disorder-induced localization effects. Using the Coherent Backscattering (CBS) interference, we study three decoherence mechanisms occurring in ultracold atomic vapors, relying respectively on the internal structure[1], the residual atomic motion[2] and the nonlinearity of the atomic scatterer [3]. The experimental CBS signals are quantitatively analyzed using MonteCarlo numerical simulations, which are essential to describe e.g. the influence of the sample geometry. Theoretical models allow us to derive some analytic expressions for the coherence length L_ϕ, the typical distance over which interference effects affect the transport.

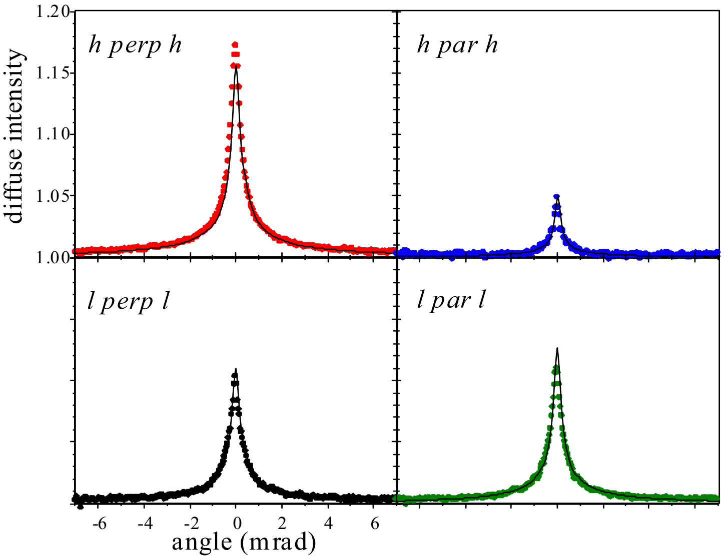

Fig.1 : CBS peaks from an ultracold cloud of Rb^{85} of optical thickness b = 26, in various polarization channels (symbols : experiment, lines : MonteCarlo simulations without adjustable parameter).

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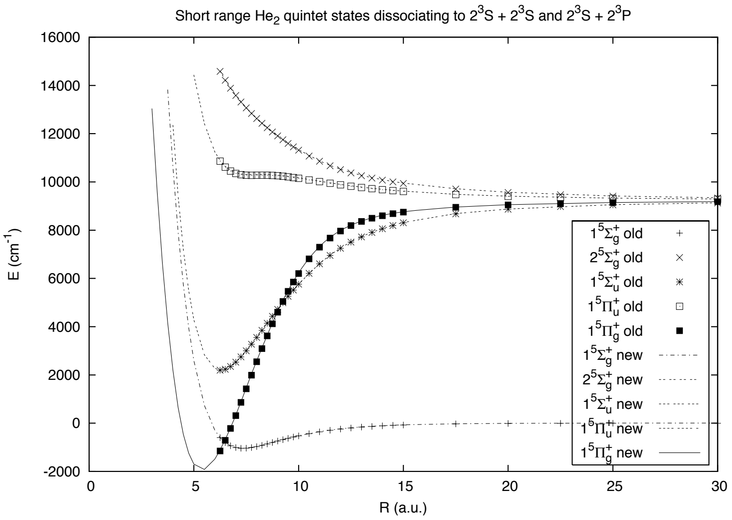
We3-8

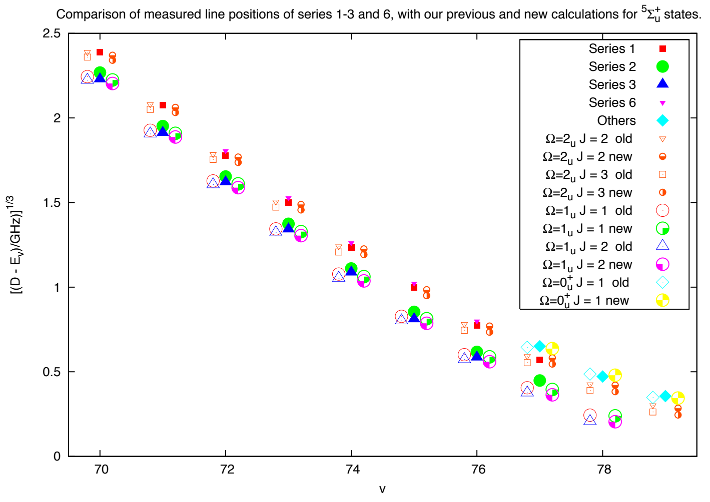
Photoassociation of metastable helium revisited

B. Deguilhem, F.X. Gadéa and T. Leininger
Laboratoire de Chimie et Physique quantique, I.R.S.AM.C, Université Paul Sabatier, 118 Route de Narbonne, F-31062 Toulouse Cedex, France
A.S. Dickinson
School of Natural Sciences (Physics), Newcastle University, Newcastle upon Tyne NE1 7RU, United Kingdom

Abstract

A theoretical study is performed for the photoassociation of metastable helium, ^{4}He*. With a new basis set better optimized, new high level (MRCI) ab initio potentials are produced, for the $^5\Sigma_g^+$ state dissociating to $2\,^3$S + $2\,^3$S and the $^5\Sigma_{g/u}^+$ and $^5\Pi_{g/u}$ states dissociating to $2\,^3$S + $2\,^3$P even for short internuclear distances. Taking into account the spin-orbit coupling so that accurate dissociation is obtained, a single channel body-fixed approximation is employed to calculate the vibrational levels below the $^3P_2$ asymptote. These new results give similar good agreement with experiment [1] to that obtained with earlier potentials [2] and confirm the vibrational assignments suggested previously.


Short range He$_2$ quintet states dissociating to 2^3S + 2^3S and 2^3S + 2^3P


Comparison of measured line positions of series 1-3 and 6, with our previous and new calculations for $^5\Sigma_u^+$ states.

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We3-9

AN ELECTRODYNAMIC TRAP FOR NEUTRAL ATOMS

Sophie Schlunk,[1,2] Adela Marian,[1] Peter Geng[1], Allard Mosk[3], Gerard Meijer[1], and
Wieland Schöllkopf[1]

[1]Fritz-Haber-Institut, Faradayweg 4-6, Berlin, Germany,
[2]FOM-Institute for Plasma Physics Rijnhuizen, Nieuwegein, The Netherlands
[3]University of Twente, Enschede, The Netherlands

We have demonstrated trapping of cold ground-state Rb atoms in an AC electric trap. It has been shown before that polar molecules can be trapped in such an AC electric trap [1]. In addition, electrodynamic trapping of Sr atoms has also been demonstrated on an atom chip [2]. Our AC trapping scheme is analogous to the Paul ion trap and it was proposed by Peik in 1999 [3]. The basic idea behind it is to create an electric field configuration that has a saddle point of constant field strength at the center of the trap and slopes of opposite signs in the axial and radial directions. Switching between the two electric field configurations gives confinement in 3D, by generating an alternately focusing and defocusing force in each direction. The calculated potential-well depths for Rb atoms are on the order of 10 μK depending on the AC-switching frequency. In contrast to static magnetic or electric traps, all (degenerate) m_F sublevels of a given hyperfine state are trapped.

In the experiment, the Rb atoms are cooled in a standard MOT loaded from a Zeeman slower. After loading the atoms in a magnetic trap, a density on the order of 10^{11} atoms/cm^3 and a temperature of about 100 μK are measured. Next, the cold Rb cloud is transferred, by physically moving the magnetic trap by 42 cm, into a second vacuum chamber housing the AC trap. We have observed trapping of about 10^5 atoms at 60 Hz switching frequency with trap lifetimes on the order of 10 s. Absorption images of the Rb cloud taken directly after switching off the AC trap at various phases of the AC cycle show round or pancake shapes reflecting the focusing and defocusing forces acting on the atoms along different directions. In addition, we have observed a strong dependence of the number of trapped atoms on the switching frequency in agreement with trajectory calculations.

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We3-10

A toolbox for the theoretical description of ultracold atomic collisions

Yulian V. Vanne and Alejandro Saenz

AG Moderne Optik, Institut für Physik, Humboldt-Universität zu Berlin,
Hausvogteiplatz 5-7, D 10117 Berlin, Germany

The theoretical description of collisions between ultracold atoms is very challenging. It starts with the requirement for a very accurate description of the interatomic potential curve which usually needs a combined theoretical and experimental input and continues with the solution of the Schrödinger equation describing scattering processes that occur on these potential curves. In the case of alkali atoms, the number of vibrational states supported be a single potential curve can easily exceed 100, and this leads to a numerically difficult description of scattering processes, especially if short-range interaction are important like in tight traps. Since a number of fascinating experiments in the field of ultracold physics of dilute atomic gases is based on magnetic-field induced Feshbach resonances, their description is also vital. We report on a recently developed program package that allows for very accurate calculations of the potential curves between (effective) one-electron atoms (of the same or different species), the solution of the nuclear-motion problem in these potential curves in the single channel case, and the treatment of the multi-channel case needed for the evaluation of magnetic Feshbach resonances.

On the basis of the electronic structure code [1] a numerical investigation of the doubly excited states of H_2 converging to the $\mathrm{H}(n{=}2)+\mathrm{H}(n'{=}2)$ limit was performed [2]. Special emphasis was put on the accurate description of the range of intermediate internuclear distances in order to correctly connect the short range with the asymptotic van der Waals regime where perturbation theory is applicable. The present non-perturbative calculation extends to internuclear separations $R = 200\,a_0$ and is sufficiently accurate to achieve a direct, smooth connection between the two extreme regimes without any need for an interpolation procedure. The high precision of the *ab initio* results revealed a long range dipole-quadrupole interaction that had been overlooked in two earlier perturbative calculations.

The multi-channel code has been tested by reproducing the known position of the Feshbach resonance in $^{87}\mathrm{Rb}_2$ with a very high accuracy. Since it is especially challenging nowadays to investigate the properties of Bose-Fermi mixtures, and being motivated by the corresponding experiment in Tübingen, a study of $^{6}\mathrm{Li}\,^{87}\mathrm{Rb}$ is presently performed. As an example of the performance of the package we present some intermediate results for this system and demonstrate the influence of magnetic field on channel functions in the vicinity of the Feshbach resonance.

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We3-11

Enhancing Raman analysis in Optical Tweezers by phase-sensitive detection.

A. C. De Luca, G. Pesce, G. Rusciano and A. Sasso

Università degli Studi di Napoli "Federico II" and CNISM –
Consorzio Nazionale per le Scienze Fisiche della Materia

Raman spectroscopy has become a powerful tool for microscopic analysis of organic and biological materials. When combined with Optical Tweezers, it allows investigating of a single, selected micrometric particle in its natural environment, therefore, reducing unwanted interferences from the cover plate. A general problem affecting either Raman spectrometers than Raman Tweezers systems is the background contribution coming from the environment surrounding the sample under investigation. This drawback is usually overcome by subtracting the acquired spectrum from a reference spectrum. In this work we report on a novel method which allows acquiring Raman spectra of trapped particles (polystyrene microspheres) free from any background contribution and without any subtraction procedure. The method is based on the use of two collinear and co-propagating laser beams: one is devoted to trapping (trapping laser), and a second one is used to excite the Raman transitions (pump laser). The trapping laser, by means of a galvomirror, moves periodically the trapped particle back and forth along one direction perpendicular to the propagation axis at a given frequency. The scattered photons are collected through the same focusing objective and spectrally analysed by means of spectrometer; the Stokes photons are then detected by a photomultiplier, and the signal sent in a lock-in amplifier for a phase-sensitive detection scheme. The purpose of the present work is to furnish a detailed description of our method and to supply a systematic study concerning the formation of the Raman signal.

The results found [1] demonstrate that this method may find valuable applications in rapid sensing of biological samples in aqueous solutions. One of the potential applications lies in studying the diffusion of molecules into micro-sized particles. This kind of application is being carried out in our laboratory.

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We3-12

Photo-associative spectroscopy of weakly bound molecules. Lu-Fano analysis.

H. Jelassi, B. Viaris de Lesegno and L. Pruvost

Laboratoire Aimé Cotton, CNRS II,
bat 505, campus d'Orsay
91405 Orsay, France

We have performed experiments on the photo-associative spectroscopy of cold rubidium atoms, below the ($5s_{1/2}$ + $5p_{1/2}$) dissociation limit, which produces weakly bound excited molecules. We have applied the trap loss spectroscopy method [1] to record the spectra, by frequency scanning a Titanium-Sapphire laser. The spectra exhibit 3 molecular vibrational series, associated to the 0g-, 0u+ and 1g symmetries. The measured energy of the molecular levels allow us to determine some properties of the molecular potentials.

Such weakly bound molecules are mainly described by the dipole-dipole atom interaction which varies, according to the molecular symmetry, either as $1/R^3$ or as $1/R^6$, where R is the inter-nuclear distance. The eigen energies of the weakly bound molecules are then very close to those given by the well-known Le Roy-Bernstein formula [2]. The discrepancies are due to the short distance behaviour of the molecular potentials, which exhibit repulsive barriers and can also include crossings between molecular potentials resulting from interactions, for example spin-orbit or spin-spin interactions. The analysis of the discrepancies reveals these interactions. We have performed the analysis by applying the Lu-Fano method on the experimental data. A quantum defect is deduced from the measurements and its variation versus the binding energy allow to characterise the interaction.

For the 0g- molecular levels we observe a linear variation of the quantum defect, which is the signature of the short range behaviour of the molecular potential. A model for the barrier allows to connect the slope to its location. [3].

For 0u+ molecular levels, we also observe the linear variation broken by some sharp variations which indicate a coupling with a neighbouring molecular series. The coupling is due to the spin-orbit interaction in the molecule. A two series model allows us to evaluate the coupling, to identify two levels of the ($5s_{1/2}$ + $5p_{3/2}$) 0u+ series and to predict the energy position and the width of its first pre-dissociated level. An experimental signal agrees with the prediction [4].

For 1g molecular levels, the resonances exhibit a structure due to the hyperfine effects in the molecule. We have shown that the energy splitting due to the hyperfine interaction can be calculated in a perturbative approach and subtracted from the data, thereby allowing an analysis by the Lu-Fano method.

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We3-13

Transport and localization in tilted and driven optical lattices

Dirk Witthaut, Friederike Trimborn, and Hans Jürgen Korsch

Department of Physics, TU Kaiserslautern, Germany

Recent experiments with ultracold atoms in accelerated optical lattices have caused a renewed interest in the quantum dynamics in periodic structures. Bloch waves, which are delocalized states leading to transport, are known since the early days of quantum mechanics. If an external static field is added, an oscillatory motion is found instead - the famous Bloch oscillations. However, transport may be reintroduced by a resonant harmonic driving [1, 2].

We present a convenient approach based on Lie-algebraic structure theory to study the dynamics in periodic structures in the tight-binding approximation. Within this framework we analyze the transport and the dispersion for a general time-periodic driving. The actual transport velocity depends on the initial momentum and the driving via multidimensional Bessel functions. Dispersion can be suppressed in leading order by the choice of an appropriate driving [3, 4].

Furthermore we investigate the dynamics in double-periodic structures, realized by ultracold atoms in two-color optical lattices or in semiconductor superlattices [5]. The ground band splits up into two minibands and the dynamics is governed by the coherent superposition of Bloch oscillations and Zener tunneling between the minibands. Combined with a suitable driving, this offers a lot of possibilities to engineer the dynamics of a matter wave [6]. A Bose-Einstein condensate in such a potential provides a clean model system to study nonlinear Zener tunneling and the dynamical instability at the edge of the Brillouin zone.

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We3-14

Sympathetic cooling of molecular ions at ultralow energies: interaction and dynamics for $MgH^+(X^1\Sigma^+)$ with $Rb(^2S)$.

M. Tacconi, E. Bodo, F.A. Gianturco

Department of Chemistry, University of Rome La Sapienza,
Piazzale A. Moro 5, 00185 Rome, Italy

So far the direct cooling methods, such as laser cooling, successfully used for numerous neutral and atomic ions could not be applied to molecular species due to the lack of closed optical transitions [1]. A very powerful and general method for the indirect cooling of neutral molecules and molecular ions is Sympathetic Cooling (SC) [2]. In principle the SC could be viewed as independent of the quantum structure associated to the internal degrees of freedom of the target system and, as a consequence of that, it could be used to cool a wider number of systems to sub milli Kelvin temperatures. However, the efficiency of the SC process actually depends on the internal level structure of the colliding complex. Aim of our work is to use the predictive power of the modern ab initio and the full quantum dynamic computational techniques to investigate the possibility of the cooling of molecular systems by thermal contact with a cold or ultracold heavy alkali atoms gas, namely Rb and Cs gas [3,4]. In this work we choose to study $MgH^+(X^1\Sigma^+)$ interacting with $Rb(^2S)$ as a model system. This system is topical because Schiller and co-worker have recently proposed an experimental scheme for the overlap of a Coulomb crystal of molecular ions with an ultracold atoms gas [5]. We have computed the potential energy surfaces for the low lying electronic states of the RbMgH ion complex at the MRCI-SD [6] level of theory by using a CASSCF wavefunction as reference and large basis sets: cc-VQZ for the Mg and H, while for the Rb the new Effective Core Potential ECP28MDF along with the companion basis set [8s7p5d3f] was used [7]. From the ab initio calculations we can see a rather complex electronic energy levels network that would allow the system to undergo charge-exchange reactions via the non-adiabatic coupling to several electronic states. Obviously we are aware of the fact that the vibronic coupling could strongly characterize the dynamical features and, consequently, the efficiency of the SC process. However, as a zeroth order approximation, we choose to limit our investigation to the study of the collisional process in a strictly adiabatic representation of the RbMgH ion electronic structure within the Close Coupling formalism of the quantum dynamics.

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We3-15

Mesoscopic Physics with Ultracold Atoms: From Confined Scattering to Rydberg Atoms in Magnetic Traps

P. Schmelcher
Physikalisches Institut, Universität Heidelberg, Philosophenweg 12, 69120 Heidelberg, Germany and Theoretische Chemie, Institut für Physikalische Chemie, Universität Heidelberg, INF 229, 69120 Heidelberg, Germany
E-mail:peter.schmelcher@pci.uni-heidelberg.de

Mesoscopic physics of ultracold atoms is discussed at hand of two different examples. We demonstrate that scattering strongly interacting particles in three dimensions (3D) can be suppressed at low energies in a quasi-one dimensional (1D) confinement. A wave-packet dynamical simulation of the collisional process is performed in harmonic cylindrical confinement by employing a fully 3D screened Coulomb interaction. An almost lossless total transmission is observed. The underlying mechanism is the interference of the s- and p-wave scattering contributions with large s- and p-wave scattering lengths being a necessary prerequisite. This low-dimensional quantum scattering effect might be probed in gases of "strongly" interacting ultracold atoms in elongated traps or in impurity scattering in strongly confined quantum wire-based electronic devices [1].

Ultracold Rydberg atoms exposed to magnetic traps such as the quadrupole field and the Ioffe-Pritchard trap are studied subsequently. A general Hamiltonian which describes the quantum dynamics of an atom in an arbitrary linear magnetic field configuration is derived. The coupled center of mass and electronic motion is solved by incorporating an adiabatic separation of the dynamics. We provide the adiabatic energy surfaces and discuss under which conditions trapped center of mass states can be achieved for Rydberg atoms. Energies and wavefunctions of the corresponding quantum hybrid states are studied thereby entering a new regime where both the external and internal motion are coupled and quantized leading to e.g. ring states. By analyzing the properties of the resulting combined motion we demonstrate that the extension of the electronic wavefunction can exceed that of the center of mass motion in a Ioffe-Pritchard trap. Such atoms cannot be considered as being point-like [2,3].

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We3-16

DETERMINATION OF THE SCATTERING LENGTH OF THE $a^3\Sigma^+$ POTENTIAL OF ^{87}RbCs

E. Tiesinga[a], M. Anderlini, and E. Arimondo[b]

Joint Quantum Institute and Atomic Physics Division,
National Institute of Standards and Technology,
100 Bureau Drive, Gaithersburg, Maryland 20899-8423, USA

We have determined the scattering length of the $a^3\Sigma^+$ potential of ^{87}RbCs based on experimental observations from the literature and the known value for the long-range dispersion coefficient. Our analysis uses quantum defect theory and analytical solutions of the Schrödinger equation for a van der Waals potential. We find that the scattering length is either 700^{+700}_{-300} a_0 or 176±2 a_0 with more confidence associated to the first value, where a_0=0.05292 nm is a Bohr radius. An independent value of the van der Waals coefficient could not be determined and the best theoretically determined C_6 value was used.

a) e-mail: eite.tiesinga@nist.gov

b) Permanent address: Dipartimento di Fisica E. Fermi, Università di Pisa, Largo B. Pontecorvo 3, I-56127 Pisa, Italy

We3-17

ELECTROMAGNETICALLY INDUCED TRANSPARENCY OF COLD Rb ATOMS IN A MAGNETO-OPTICAL TRAP

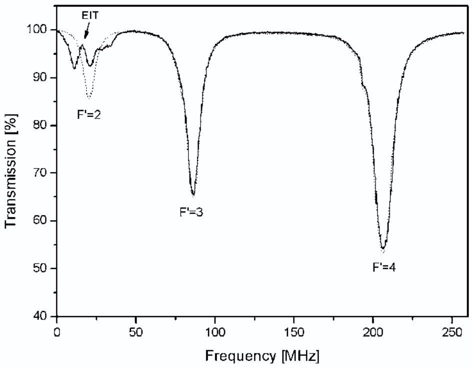
K. Kowalski[a*], S. Gateva[b], M. Głódź[a], M. Janowicz[a], J. Szonert[a], K. Vaseva[b]

[a] Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46,
02-668 Warsaw, Poland
[b] Institute of Electronics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee,
1784 Sofia, Bulgaria

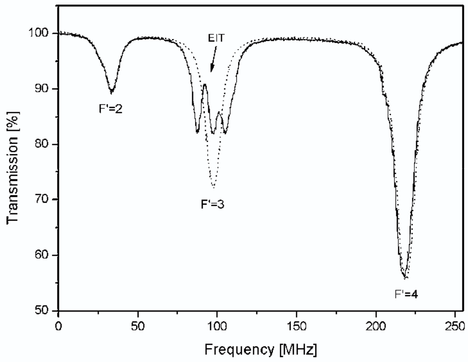
We investigate structured spectra of electromagnetically induced transparency (EIT) with the aim to prepare a medium, which could support slowing down of light pulses simultaneously at different close-lying frequencies. In this context, a multi-window EIT was communicated in the literature as produced *e.g.* (*i*) by using bichromatic coupling fields [1], or (*ii*) in a multi-level cascade scheme involving a dense hfs manifold [2].

We will present results of our experiments and theoretical predictions for various structured cascade- and Λ- type EIT spectra of cold ^{85}Rb atoms in a magneto-optical trap (MOT). Slow atoms in MOT provide an environment for spectroscopy in which both Doppler-broadening and decoherence effects are considerably reduced in a natural way. Some details of the experimental set-up (standard six-beam MOT [3] and the excitation/detection system) will also be given. The figures a) and b) examples of the registered EIT features of the kind (*ii*) are shown. The weak probe beam was tuned across the $5S_{1/2}(F=3)\rightarrow 5P_{3/2}(F'=2,3,4)$ transitions, while the frequency of the strong coupling beam was locked either to the $5P_{3/2}(F'=2)\rightarrow 5D_{5/2}$, or to the $5P_{3/2}(F'=3)\rightarrow 5D_{5/2}$ transition, respectively for a) and b). Dotted lines exhibit absorption with the coupling beam off.

a)



b)



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**Corresponding author : krkowal@ifpan.edu.pl*

We3-18

STIMULATED RAMAN TRANSITIONS IN A CO_2 LATTICE

M. G. Bason, K. J. Weatherill and C. S. Adams

Department of Physics, Durham University,
Rochester Building, Science Laboratories,
South Road, Durham DH1 3LE.
United Kingdom.

In previous work we have shown how exploiting light shift engineering enables enhanced and site specific loading into deep optical traps[1]. Next we aim to drive stimulated Raman transitions between hyperfine ground states, (labelled $| 0 >$ and $| 1 >$) in cold ^{87}Rb atoms trapped in a CO_2 optical lattice. The light for the Raman transitions is derived from the output of an electro-optic modulator (EOM) operating at 6.8 GHz. By injecting this light into another laser it is possible to lock on to one of the EOM sidebands. Repeating this process a spectrally pure output (other frequencies suppressed by > 20 dB) detuned by 6.8 GHz from the fundamental is achieved.

Combining single site loading, stimulated Raman transitions with state selective optical tweezing allows the possibility of a collisional quantum gate. By transporting part of an atomic superposition state one entangles part of an atom with atoms in neighbouring sites. The read out of the gate can be made state selective by moving either the $| 0 >$ or $| 1 >$ states of the atoms to specific detection sites.

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We3-19

Universal method for cooling/heating of the ULE Fabry-Perot cavites to the zero expansion temperature

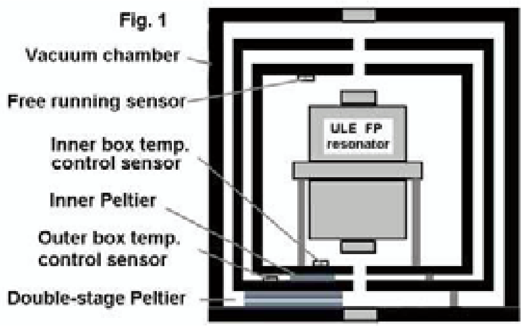
J. Alnis, A. Matveev, N. Kolachevsky, Th. Udem, T.W. Hänsch

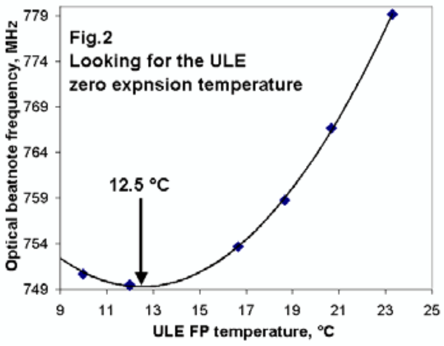
Max-Planck-Institute of Quantum Optics
Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Optical atomic clocks as a rule require a laser stabilized to a high finesse Fabry-Perot (FP) cavity with a small thermal drift rate. The best material for the FP cavity is Ultra-Low-Expansion (ULE) glass manufactured by Corning. At some temperature *Tc* around room temperature the thermal expansion coefficient of ULE becomes zero. If the ULE FP cavity temperature is stabilized at this temperature, the thermal drift of the cavity can be as low as 30 mHz/s [1].

Unfortunately the manufacturer of ULE can not measure the *Tc* accurately enough. Sometimes the *Tc* is above and sometimes below the room temperature. Cooling of the vacuum chamber with the ULE cavity is more difficult than heating, and practically cooling is not used below +15 °C as a problem arises with water condensation.

We have tried a novel approach with Peltier coolers placed inside the vacuum chamber and have demonstrated possibility to cool the ULE cavity down to +2 °C. Fig.1 shows the set-up. We use the vertically at the midplane mounted FP cavity that is self-compensating against the vibrations [1]. In the vacuum vessel there are two enclosures, the outer one is cooled down to the *Tc* and the inner one is stabilised at the same temperature as the outer enclosure, minimising heat exchange due to thermal radiation. The vacuum chamber is assembled from standard vacuum parts, and a 20 l/s ion pump achieves pressure $8x10^{-8}$ mbar even with some plastic screws and Peltier elements inside the vacuum chamber. Temperature measurements on a free running sensor gave temperature excursions of ±10 mK/day at *Tc* = +12.5 °C. We found the *Tc* of our cavity by measuring the optical beat note frequency between two FP cavities while the temperature of one of them was changed (Fig. 2). Assuming that *Tc* can be found with an accuracy 0.1 °C, the temperature change by 10 mK causes drift of 500 Hz. However, if the temperature were stabilized as usual by heating above the room temperature to +30 °C, the temperature drift of 10 mK would cause 90 kHz drift in cavity frequency. The new design with Peltier elements in vacuum appears to be very successful and will be used for building future ultra-stable FP resonators.





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Transport Properties in a Mott-like State of Molecules

D.M. Bauer, N. Syassen, T. Volz, M. Lettner, D. Dietze, S. Dürr, and G. Rempe
Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, D-85748 Garching, Germany

Ultracold gases in optical lattices are of great interest, because these systems bear a great potential for applications in quantum simulations and quantum information processing, in particular when using particles with a long-range dipole-dipole interaction, such as polar molecules.

In Ref. [1] we show the preparation of a Mott-like state of molecules. This state is a quantum state with exactly one molecule at each site of an optical lattice. The molecules are produced from an atomic Mott insulator with a density profile chosen such that the central region of the gas contains two atoms per lattice site. A Feshbach resonance is used to associate the atom pairs to molecules. Remaining atoms can be removed with laser light.

We now study the transport properties in the Mott-like state. A molecule can tunnel with an amplitude J_m to an adjacent site. If there is already another molecule at that site the molecules can collide inelastically [2], leading to loss of both molecules from the sample. This loss occurs with a rate coefficient Γ which is typically much faster than $J_m/\hbar$. The fast on-site loss leads to a suppression of tunneling. Loss from the initial state effectively occurs with a rate $\Gamma_{\text{eff}} \propto J_m^2/\Gamma$. This effect is studied experimentally at different lattice depths and the results are compared with theoretical predictions.

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We3-21

FEMTOSECOND LASER INDUCED FLUORESCENCE IN DENSE RbCs VAPOR

Nataša Vujičić, Ticijana Ban, Silvije Vdović, Damir Aumiler, Hevoje Skenderović and Goran Pichler,

Institute of Physics, Bijenička 46, 10 000 Zagreb, Croatia
contact: natasav@ifs.hr

Interest in heteronuclear alkali molecules has recently increased due to their unique features which include large permanent dipole moment and the possibility of cooling and traping by using new techniques.

High resolution absorption measurements in dense RbCs mixture are performed. Different atomic and molecular features corresponding to the Rb_2, Cs_2 homonuclear and RbCs heteronuclear molecules are observed and identified. The RbCs molecular feature with a peak wavelength at 562.9 nm belong to the triplet-triplet transition and in this work the theoretical and experimental identification of the corresponding molecular band will be presented.

The fs fiber laser (Femto Fiber Laser, Toptica) with the peak wavelength in the (545 - 630) nm range, pulse width at half maximum of 3 nm and output power of about 4 mW is used to directly excite the corresponding RbCs molecular band. The laser induced fluorescence is detected. By inspection of the theoretical potential curves in the Hund c) case and measured LIF spectra the observed molecular band is identified as a 1(a) $^3\Sigma^+ \rightarrow 4\ ^3\Sigma^+$ transition. The possible application in the ultracold hetero-molecule formation will be discussed.

We3-22

SPIN EXCHANGE SHIFTS IN MAGNETIC RESONANCE OF COLD ATOMIC HYDROGEN GAS

J. Ahokas, J. Järvinen, S. Vasiliev

Department of Physics, University of Turku, 20014 Turku, Finland

We report on a magnetic resonance study of spin-exchange effects in a cold gas of spin-polarized atomic hydrogen (H↓). The subjects of our study are three- and two-dimensional H↓ gases stabilized in a magnetic field of 4.6 T at temperatures 70-500 mK. At these conditions the thermal de-Broglie wavelength Λ_{th} is much larger than the scattering length $a \approx 0.07$ nm. Atomic collisions are in the cold collision regime, and exchange interaction leads to the shift of the resonance lines called cold collision or clock shift (CS), well known in the field of atomic frequency standards. CS of the optical 1S-2S transitions served as a main tool to detect Bose-Einstein Condensation in 3D atomic hydrogen gas [1].

Two-dimensional gas of atomic hydrogen is naturally created in the adsorbed phase on the walls of the sample container, which are covered by the superfluid helium film. ^{4}He film surface potential supports a single bound state with the adsorption energy of E_a=1.14 K. At temperatures below 100 mK surface densities of $\sigma \approx 5 \cdot 10^{12}$ cm^{-2} can be obtained by the thermal compression method [2]. Due to low mass m out-of-plane delocalization of the adsorbed atoms $l = (\hbar^2 / 2E_a m)^{1/2} \approx 0.5$ nm appears to be large compared with a. This justified the use of the scaling approach with the effective bulk density of the adsorbed gas $n=\sigma/l$ to evaluate the exchange interaction energy $E_i \approx 8\pi\hbar^2 a\sigma / ml$ and corresponding density dependent shift of the electron spin resonance lines [3].

In experiments we used electron and nuclear magnetic resonance to separate the effects of exchange and dipolar interaction on the shifts of the resonance lines [3]. We found that the CS in the 2D hydrogen gas is about 100 times smaller than it follows from the scaling approach. In a separate measurement we studied the ESR line shifts in the 3D gas and found the CS in agreement with the mean field theory. Therefore, the discrepancy in the 2D case can not be explained by imprecise knowledge of the scattering lengths, and the treatment of the collisions in 2D requires a different theoretical approach.

For the first time we performed coherent two-photon excitation of electron and nuclear zeeman transitions of atomic hydrogen. We report on the observation of the effects of electromagnetically induced transparency and opacity and coherent population trapping in the quantum 2D hydrogen gas.

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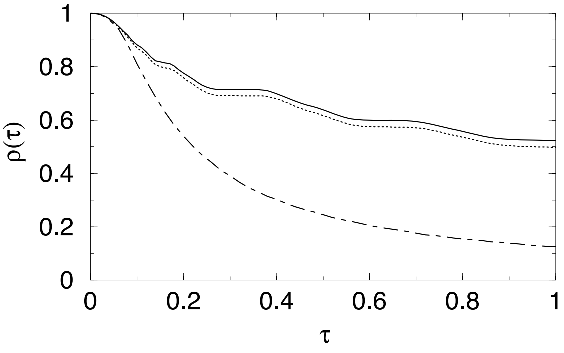
We3-23

TRAPPING AND GUIDING ULTRACOLD ATOMS WITH THE HELP OF QUANTUM REFLECTION

Javier Madroñero[1], Florian Arnecke and Harald Friedrich

Physik Department, Technische Universität München, 85747 Garching, Germany

Understanding the interaction of ultracold atoms with surfaces is a prerequisite for the design and construction of atomic waveguides and other atom-optical devices. The interaction in the close regime, i.e. when the atom is separated from the surface by few atomic units, is quite complicated and generally leads to inelastic reactions or adsorbtion. Beyond this close region the solid surfaces provide a long-range attractive potential for the atoms. For distances shorter than the wavelength of atomic transitions the interaction is the van der Waals potential, while at larger distances the retardation effects become important. At sufficiently low energies, atom-surface collisions are strongly influenced by quantum effects such as quantum reflection in the nonclassical region of an attractive atom-surface potential and dominance of low partial waves in the elastic scattering by nanospheres [1,2]. We discuss the possibilities of exploiting quantum reflection to trap atoms without the help of auxiliary fields. Accurate numerical calculations taking into account the long-distance retarded potential and the short distance van der Waals potential [3] show that the behavior of the trapped atoms between two walls can be successfully modeled by an appropriate sharp-step potential [4]. An extension of this model to higher dimensions allows us to study the confining properties of atoms in traps of more complicated geometries [5].



The surviving fraction of trapped atoms (solid line) can be successfully reproduced by a simplified step potential approximation (dotted line). Quantum reflection reduces the decay process and significantly enhances the survival probability in comparison with the free evolution (dot-dashed line).

We show that quantum reflection makes it possible to achieve a good suppression of the decay process of atoms confined in traps of different geometries. Under realistic conditions quantum reflection can enhance the survival probability by up to two orders of magnitude in a three dimensional trap or by a factor 15 in atomic wave guides.

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[1] e-mail: jmadrone@ph.tum.de

We3-24

Cold and Pure Guided Beams of Polar Molecules

P.W.H. Pinkse, L.D. van Buuren, M. Motsch, S. Pohle, T. Rieger, C. Sommer
and G. Rempe
Max-Planck-Institut-für Quantenoptik, Hans-Kopfermannstr. 1,
D85748 München, Germany

Unlike atoms, polar molecules possess a dipole moment. Once polar molecules can be cooled to the ultracold regime, where the dipole-dipole interaction dominates, new quantum phenomena can be studied. Cold polar molecules are also of interest for high-resolution spectroscopy, metrology, and quantum computation [1]. In our group we have developed a robust technique which produces up to 10^{10} s^{-1} translational cold ($T \approx 1 \ldots 5$ K) polar molecules from a 150K...300K thermal gas using velocity filtering in an electric quadrupole guide [2]. In this scheme, the distribution over the populated rotational states corresponds to a higher temperature than the translational temperature. In this contribution we show new results from two methods to reduce the number of states in the beam: (I) state filtering based on the different Stark shifts of rotational states and (II) buffer gas cooling.

(I) The low-field-seeking states of symmetric top molecules experience a strong electrostatic force in an electric quadrupole guide due to the mainly linear Stark effect. This method is now extended to asymmetric top molecules which experience a quadratic and therefore smaller Stark effect. Although the total yields are lower, the purity of the beam is higher since the number of populated states is reduced compared to thermal distribution in the source. Guiding of water and its deuterated forms (D_2O [3] and HDO) is reported. We predict that for D_2O, 80% of the guided population resides in 5 states only. The ratio of elastic to inelastic collisions is expected to be higher for asymmetric top molecules than for symmetric ones [4]. A trap loaded with asymmetric top molecules would therefore be a good starting point for evaporative cooling.

(II) We present first results with a new cryogenic source delivering a dense and slow beam of internally cold molecules to a room-temperature environment, where the access to the beam is less restricted than in a cryostat. The beam is produced by combining two powerful techniques. The translational and internal degrees of freedom of the molecules are cooled in a helium buffer gas at cryogenic temperature ($T \approx 5$ K) [5]. With an electric guide the slow buffer-gas-cooled molecules are filtered out of the (non-polar) helium and transported to a high-vacuum region [2], where they are detected. We predict that 95% of the beam will be in a single rotational state. Once the source is optimized, it can be extended to load an electrostatic trap [6] for further investigations.

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We3-25

PHOTOASSOCIATION OF COLD CESIUM ATOMS: ANALYSIS OF THE LONG-RANGE 0_g^- STATE REVISITED.

Nadia Bouloufa, Anne Crubellier, and Olivier Dulieu

Laboratoire Aimé Cotton, CNRS, bât.505, Campus d'Orsay,
91405 Orsay Cedex, France

A new interpretation of photoassociation spectra of the outer potential well of the 0_g^- ($6S_{1/2}+6P_{3/2}$) state of Cs_2 is performed, in order to solve remaining discrepancies with the intensity pattern of the spectra. The new analysis predicts a change by two units in the assignment of the vibrational levels compared to the previous work of our group [1]. The values obtained for the atomic radiative lifetimes of the $6P_{3/2}$ and $6P_{1/2}$ levels are significantly shifted from those of [1]. Special attention has been brought to the correlations between the different parameters of the fit, providing a substantially larger uncertainty on the lifetime values.

Photoassociation intensity calculations have also been performed using, for the description of the long-range part of the initial wavefunction, the accurate asymptotic ground state triplet and singlet potential curves obtained from two-colour photoassociation in our group [2]. It will be shown that these results allow us to calculate near-threshold level and resonance positions with or without magnetic field: the calculated values agree very well with the experimental results of Stanford [3]. Photoassociation intensity calculations using the new 0_g^- potential allow us to remove all discrepancies between simulated and observed intensity patterns of several 0_g^- spectra recorded in different conditions.

These results could be of interest in the perspective of the transformation of ultracold Feshbach molecules into deeply bound molecules.

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THEORETICAL STUDY OF THE OPTICAL MANIPULATION OF COLD ATOMS

Naceur Gaaloul

Laboratoire de Photophysique Moléculaire du CNRS, Bâtiment 210,
Université Paris-Sud, 91405 Orsay cedex, France.

We study the optical manipulation of ensembles of cold atoms by means of wave-packet propagation techniques. In the case of *thermal clouds*, we describe the dipolar guiding of such samples, initially trapped in a Magneto-Optical Trap, by solving the time-dependent Shrödinger equation in a semi-classical approach. Elaborated configurations are considered where the matter waves evolve under the combined effect of two laser beams and gravity. We predict a range of laser parameters which allow for the implementation of macroscopic spatial splitting [1] or atomic deflection [2]. In the case of *coherent sources of cold atoms*, *i.e.* Bose-Einstein Condensates, our study is performed by solving the time-dependent Gross-Pitaevskii equation. More precisely, the macroscopic wave function is described in different realistic three-dimensional trap geometries. Our results demonstrate the high potentialities of these optical configurations for the implementation of a coherent splitting or deflection of the condensate.

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We3-27

ULTRACOLD ATOM-ATOM COLLISIONS IN TRAP WITH TIME-DEPENDENT WAVE-PACKET METOD

V.S. Melezhik

Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research,
Dubna, Moscow Region 141980, Russia
e-mail: melezhik@thsun1.jinr.ru

In my talk in the ECAMP8 [1] an approach for treating the three-dimensional anisotropic scattering was presented and some applications for ultracold atom-atom collisions in a nonresonant laser field [2] were discussed. By using the key element of this approach, the two-dimensional DVR-like angular expansion [3,4], we have developed a time-dependent wave-packet method for quantum two-body systems with non-separable centre-of-mass and relative radial variables of the particles.

The approach is very promising in application for treating different few-body dynamics of ultracold atom-atom collisions in optical and magnetic traps. Particularly, with this technique we have found [5] that the scattering of particles strongly interacting in the free space can be suppressed at low energies in a quasi-one-dimensional confinement created by optical or magnetic trap. We suppose to discuss the advantages of the developing method as well as resent results obtained with this computational scheme for ultracold atom-atom collisions in traps.

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We3-28

AUTOIONIZATION OF SPIN-POLARIZED METASTABLE HELIUM IN TIGHT ANISOTROPIC HARMONIC TRAPS

T. J. Beams [1], G. Peach [2] and I. B. Whittingham [1]

[1] School of Mathematics, Physics and Information Technology,
James Cook University, Townsville, Australia 4811
[2] Department of Physics and Astronomy, University College London,
Gower Street, London WC1E 6BT

Spin-dipole interactions between tightly confined metastable helium atoms couple the spin-polarized |S M_S>=|22> quintet ${}^5\sum_g^+$ state to the |00> singlet ${}^1\sum_g^+$ state from which Penning and associative ionization are highly probable. This spin-dipole induced coupling results in finite lifetimes for the trap eigenstates and has been studied for spherically symmetric traps by [1] using a second-order perturbative treatment of the interaction.

We have extended these calculations to the interesting case of anisotropic harmonic traps where there arises the possibility of enhancement and/or suppression of ionization losses due to interference between the anisotropic part of the trap potential and the spin-dipole interaction which are both proportional to a second order spherical harmonic $Y_{2q}(\theta,\varphi)$. In particular we consider traps with axial symmetry about the z axis. These traps have q = 0 and an asymmetry parameter $\beta = 2(\omega_z^2-\omega_r^2)/3\varpi^2$ which ranges from β = 2 for a "pancake" trap to β = -1 for a "cigar" trap. ϖ is the mean angular frequency $\sqrt{[(\omega_z^2+2\omega_r^2)/3]}$ of the trap.

We report results for the lower eigenstates of a ϖ = 1 MHz trap. We find that the ionization is strongly suppressed and the lifetimes of the trap states significantly lengthened for highly non-spherical traps for which β approaches its extreme values.

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COLLECTIVE EXCITATIONS AND INSTABILITY OF AN OPTICAL LATTICE DUE TO UNBALANCED PUMPING

P. Domokos[1], J. K. Asbóth[1,2], H. Ritsch[2]

[1]Research Institute of Solid State Physics and Optics, Hungarian Academy of Sciences, H-1525 Budapest P.O. Box 49, Hungary
[2]Institut für Theoretische Physik, Universität Innsbruck, Technikerstr. 25, A-6020 Innsbruck, Austria

Optical lattices (OL) are perfectly periodic arrays of particles trapped by the standing wave interference pattern of several laser beams. They have important applications as model systems for solid state physics as well as for quantum information science. The back-action of the trapped particles on the trap light is carefully avoided in most OL experiments. However, it is known to give rise to intriguing phenomena in related systems, e.g., cavity cooling, mirror cooling, and optical binding. For OL's this back-action has been predicted [1] and observed [2, 3] to reduce the lattice constant d compared to the naive expectation.

We will consider the effects of optical back-action in one-dimensional OL's, brought about by tuning a hitherto neglected parameter: the relative intensity of the lattice beams. Introducing an asymmetry in the trap not only enhances the reduction of the lattice constant, but, more importantly, alters the *interaction* between the trapped particles mediated by the light. The asymmetry gives rise to traveling density waves even in the presence of arbitrarily strong viscous damping [6]. This is directly related to the wavelike excitations in other crystals driven far from equilibrium, such as arrays of vortices in a type-II superconductor [4], and trains of water drops dragged by oil [5]. These waves arise resonantly at specific values of the asymmetry, and destabilize the lattice at a critical asymmetry that decreases sharply as the lattice size is increased.

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We3-30

High sensitive detection system for weak Fr magneto-optical trap

S.N. Atutov[1], R. Calabrese[1], L. Corradi[2], A. Dainelli[2], C. de Mauro[3],
A. Khanbekyan[3], E. Mariotti[3], L. Moi[3], P. Minguzzi[4], S. Sanguinetti[4],
G. Stancari[1], L. Tomassetti[1], S.Veronesi[3]

[1]Università di Ferrara, Dip. di Fisica, via del Paradiso 12 Ferrara, I-44100, Italy
[2]INFN Lab. Naz. di Legnaro, viale dell'Università 2 Legnaro (PD), I-35020, Italy
[3]Università di Siena, Dip. di Fisica, via Roma 56 Siena, I-53100, Italy
[4]Università di Pisa, Dip. di Fisica, L.go B. Pontecorvo 3 Pisa, I-56127, Italy
email: mariotti@unisi.it

Francium atom offers a rich variety of possible fundamental studies. First of all, its atomic structure is poorly known; in this perspective, high resolution spectroscopy experiments are opportune, as a possible comparison with theory [1] and previous pioneering works [2]. Moreover, one of the most fascinating topics is that, due to Z^3 scaling and many electrons enhanced relativistic effects, Atomic Parity Violation (APV) in Fr atom is predicted to be 18 times larger than in Cs. A Magneto-Optical Trap (MOT) apparatus has been implemented, allowing the collection of a cold sample of Fr atoms, which supply to the lack of a stable Fr isotope. This constitutes the first fundamental step for atomic spectroscopy experiments on Francium [3].
Detection of the cold cloud is not trivial, basically due to the low amount of atoms we can trap. Detection is achieved using a very sensitive CCD camera and a specially conceived acquisition software, which permits to reduce the contribution of scattered light to the noise. This program evaluates in real time, from the acquired image of the trap region, the scattered light intensity level and operates a weighted subtraction of the background from the raw image. A calibration of the number of trapped atoms versus the detected power has been performed by solving optical Bloch equations for the atomic levels involved in the trapping process. Preliminary tests show a noise level that we estimate to be less than 50 Fr atoms. In te best conditions of laser intensity stability, we were able to detect a Rb MOT, that we use to test the whole apparatus, of about 80 atoms (see fig.1), with a noise level of less than 20 Rb atoms.
We are also testing the efficiency of the neutralization of the ionic beam which transports the Fr produced via nuclear reaction, from the scattering chamber to the MOT cell; this is fundamental to achieve the best conditions and the maximum number of trapped atoms.

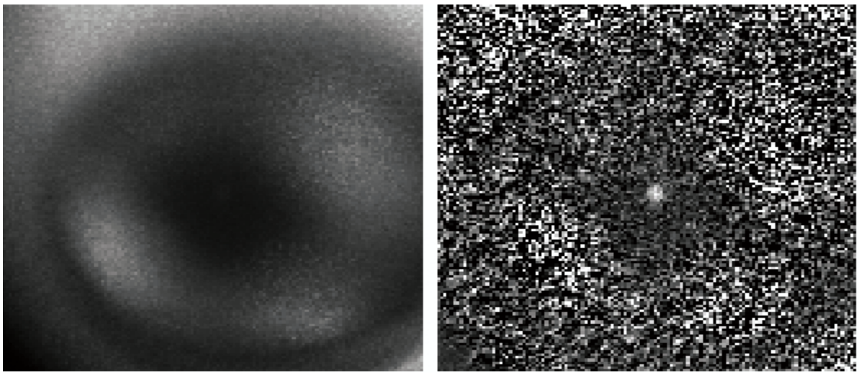

Fig.1: on the left, raw image without weighted background subtraction; on the right the same image, when improved, shows the 80 atoms Rb trap.

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We3-31

DIPOLE-DIPOLE INSTABILITY OF ATOM CLOUDS IN AN OPTICAL DIPOLE TRAP

D. Nagy[*] and P. Domokos

Research Institute of Solid State Physics and Optics
Hungarian Academy of Sciences, H-1525 Budapest P.O. Box 49, Hungary

Today, various optical trap based systems serve the study of many-body problems where the atom-atom interaction is an essential ingredient. For interatomic distances in the range of the optical wavelength, the atom-atom interaction is dominated by the radiative electromagnetic coupling. In this case one can distinguish two limits: the photon scattering is dominated (i) by spontaneous emission, e.g. in magneto-optical traps (MOT), and (ii) by stimulated emission, which occurs in far-off-resonant dipole traps (FORT). Since the MOT was the first to be able to capture dense atom clouds from vapour, it was first analyzed with respect to many-body effects [1]. The FORT operates at an extremely low spontaneous scattering rate, thus the effects of multiple spontaneous photon scattering are strongly suppressed. The mechanism of trapping relies on the process of absorption and stimulated emission of laser photons. This process polarizes the particles, hence the dipole force is accompanied by the conservative dipole-dipole coupling between atoms.

The effect of the dipole-dipole interaction is of high current interest in the ground state of a degenerate Bose gas [2-6]. Here we will consider a different regime: we will seek for the limits imposed on the FORT by the presence of the dipole-dipole coupling between *classical* particles. The energy shift induced by the neighboring polarized particles deepens the attractive potential minimum in the center of a pancake-shaped cloud. At high density the thermal motion cannot stabilize the gas against self-contraction and an instability occurs. We calculate the boundary of the stable and unstable equilibrium regions on a two-dimensional phase diagram of the atom number and the ratio of the trap depth to the temperature. The phase diagram allows for identifying possible routes to reach very large densities, eventually quantum degeneracy, in optical dipole traps.

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[*] *e-mail: nagyd_at_optics.szfki.kfki.hu*

We3-32

ATOM INTERACTIONS WITH THE EVANESCENT FIELD OF A SUBMICRON FIBRE

K. Deasy[1,2], M. J. Morrissey[1,2], T. N. Bandi[1,2], B. J. Shortt[1,2], S. Nic Chormaic[2,3]

1. Dept. of Applied Physics and Instrumentation, Cork Institute of Technology, Cork, Ireland
2. Photonics Centre, Tyndall National Institute, Prospect Row, Cork, Ireland
3. Physics Department, University College Cork, Cork, Ireland

Over the past number of years interest in the use of tapered optical fibres for manipulating and probing cold atoms has increased dramatically. It is essential that the diameter of such fibres be in the range of the wavelength of the propagating light and these can be readily fabricated by heating and pulling a single-mode fibre, ensuring the transmission of optical power within the fibre remains lossless. As the diameter decreases to the submicron range, the taper transition transforms the local fundamental mode from a core mode in the untapered region to a cladding mode in the taper waist, giving rise to a guided mode with a significant evanescent field outside the tapered area of the fibre. Recently Balykin *et al.* [1] proposed that such fibres could be used for the trapping and guiding atoms. However, unlike optical waveguides of standard diameters, many theoretical and experimental aspects of tapered fibres remain open to further investigation, which is essential for the realisation of the aims outlined in [1].

In our setup, we are currently studying the interaction between cold rubidium atoms from a magneto-optical trap (MOT) and the evanescent field created by a 780 nm probe beam propagating through a submicron fibre. Single mode, 780 nm fibre is used to produce the fibre taper, via a heat-and-pull rig with a CO_2 laser heat source [2]. The fibre is mounted within the ultra-high vacuum chamber using a Teflon feedthrough and positioned to nanometer precision using a Newscale Technologies UHV squiggle motor. This ensures that the tapered region of the fibre passes through the centre of the trapped cloud, which consists of approximately 10^7 atoms at a temperature of ~100 μK. The probe beam is modulated by ±15 MHz across the absorption line of ^{85}Rb using an AOM, prior to being launched into the fibre. The transmitted light through the fibre is detected via an avalanche photodiode.

Using the fibre eigenvalue equation it can be shown that, for a fibre of diameter 0.5 μm, the evanescent field extends approximately 0.15 μm beyond the fibre boundary. Since the MOT density is known, it is possible to determine the interaction volume between the atoms and the evanescent field. Thence, approximately 5 atoms should be affected by the field at any one time. This results in an expected absorption of ~3 pW, when the probe beam is tuned to resonance with the atoms and a probe beam with a power of tens of pW yields an acceptable signal-to-noise ratio. Switching of the MOT cooling beams during the interaction process prevents saturation of the atoms, and all data is recorded while the beams are off.

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We3-33

PRODUCTION AND QUANTUM CONTROL OF MOLECULES WITH OPTICAL AND MICROWAVE FIELDS

Svetlana Kotochigova
Department of Physics, Temple University, Philadelphia, PA 19122,
National Institute of Standards and Technology,
100 Bureau Drive, stop 8423, Gaithersburg, Maryland 20899.

We propose an association scheme to create polar molecules from ultracold atoms with a combination of optical and microwave fields. In particular, we will use an unique property of polar molecules, the nonzero permanent dipole moments that allows electric-dipole transitions between ro-vibrational levels of the ground potential. First, we propose to use microwave fields to create molecules in high vibrational states of the ground configuration followed by one optical Raman transition to form the vibrationally cold molecules. We provide values for molecular production rates for both schemes and analyze the role of the optical trapping potentials in association. In addition, we consider different scenarios that can cause loss of molecules from the lowest rovibrational states of the ground potential and propose optimal trapping frequencies and intensities to reach the experimental goals.

Controllable dipole-dipole interaction between polar molecules is an essential resource for strongly correlated many-body states. Even though polar molecules have a permanent electronic dipole moment, for any rotational state it averages to zero. We propose that a dipole moment is easily induced in a $J = 0$ state by applying a microwave field with a frequency that is close to the $J = 0$ to $J = 1$ resonance. Moreover, we investigate conditions under which the relevant states for a microwave transition have exactly the same AC Stark shift to minimize the field perturbation.

We3-34

POLARIZATION-DEPENDENT EFFECTS ON OPTICALLY PUMPED COLD CESIUM ATOMS

Yu. S. Domnin, G. A. Elkin, A.V. Novoselov, L. N. Kopylov, Yu. M. Malychev ,
V. N. Baryshev , V. G. Pal'chikov

Institute of Metrology for Time and Space at National Research Institute for Physical-Technical and Radiotechnical Measurements, Mendeleevo, Moscow Region, 141579
Russia

The theoretical and experimental study of optical pumping in cesium fountain is performed. In particular, the paper presents a possible scheme to realize a maximum population of the Cs atoms in the ground state ($F=3, M_F=0$) before entering to the microwave cavity in cesium fountain [1,2]. The efficincy of the population for thr state sublelel $F=3$, $M_F=0$ build up is calculated for two limiting cases of the optical pumping : F=3=F'=2 and F=3=F'=3.

Dynamics of an atom in a pumping laser field can be attributed to one or more basic types according to the ration between the contributions of the induced and spontaneous transitions [3,4]. On the other side, in the case of the cold and slow atoms in fountain geometry [1,2], at large interaction time compared with the spontaneous decay times, spontaneous transitions and relaxation processes cannot play a noticeable role in atomic dynamics. In such a case, it is possible to use the simplified approach using the density-matrix method [3,4].

Our theoretical calculations demonstrated a good agreement for the relationship between the experimental observations of the central Rabi resonance (0-0) with and without optical pumping (F=3-F'=2) for the horizontal type of polarization. Combining this case of the optical pumping with π – type of polarized optical pumping (F=3-F'=3), it is possible to show, that the final population efficiency can increase up to the level of ~4 times.

The presented optical pumping scheme, in principle, can be used for precise registering of the atoms in the state F=3 and, hence, for the estimation of spin-exchange frequency shift in cesium fountain.

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We3-35

Performance of an inertial sensor based on cold atoms interferometry

A. Gauguet, W. Chaibi, B. Canuel, N. Dimarcq, D. Holleville, A. Landragin

SYRTE, CNRS UMR 3630, Observatoire de Paris, 61 avenue de l'Observatoire de Paris, 75014 Paris, France.

We investigate the limits of our inertial sensor using cold atom interferometer. In contrast with previous atomic setups [1], emphasis was placed on the long term stability and compactness of the device thanks to the use of laser cooled atoms, as previously demonstrated in the field of atomic clocks. Moreover, it has been designed to give access to all six axes of inertia (three accelerations and three rotations) [2]. The expected improvement in stability will enable to consider applications in inertial navigation, geophysics and tests of general relativity (equivalence principle or Lense-Thirring effect [3]).

Cesium atoms are loaded from a vapour into two independent magneto-optical traps for 140 ms. The two cesium clouds are then launched into two opposite parabolic trajectories using moving molasses at 2.4 $m.s^{-1}$, with an angle of 8° with respect to the vertical direction. At the apex of their trajectory, the atoms interact successively with three Raman laser pulses, which act on the matter-wave as beam splitters or mirrors, and generate an interferometer of 80 ms total interaction time. The use of two atomic sources allows discriminating between the acceleration and rotation.

The sensitivity to acceleration is 8.10^{-7} $m.s^{-2}$ at one second, this correspond to a signal to noise ratio of about 50, limited by residual vibration on our isolation platform. To rotation the sensitivity is 2.10^{-7} $rad.s^{-1}$ at one second, corresponding to a signal to noise ratio of 330, limited by detection noise. These results confirm the efficient rejection of high frequency acceleration noise on the rotation. By tilting the direction of the Raman laser we had induce a controlled DC acceleration and confirm that the rejection phase shift on rotation phase shift is better than 40 dB. Measurement rotation rate is in agreement with 2% of the projection of the Earth's rotation rate. We also tested the T^2 scaling of the rotation phase shift and showed an agreement better than 1%, thus demonstrating one of advantages of cold atoms interferometer.

Currently, we carry on the characterisation of the sensor. In particular, we project to test the linearity of the scale factor with the rotation rate. In this purpose we will turn the interferometer around the vertical axis to change the value of the earth rotation rate projection. Moreover, we study the causes of drift of the rotation phase shift. Among others, we measure the effect induce by the light shift during the Raman laser pulses. These tests are crucial for the expected applications.

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We3-36

Low-Density, One Dimensional Tonks-Girardeau Gas in a Split Trap

J. Goold and Th. Busch

Physics Department, University College Cork, Cork, Ireland

Low-dimensional quantum gases are rapidly advancing from being soley theoretical concepts towards experimentally accesible systems in laboratories. Small-scale trapping potentials for low temperature samples allow the creation of degenerate fermionic or bosonic gases.

Here we investigate a low-density, one-dimensional quantum gas in the strongly interacting Tonks-Girardeau regime in a δ-split harmonic potential. Since the single particle energy eigenfunctions and eigenvalues are known exactly for all values of the splitting strength, we are able to solve the many body problem for cold fermions as well as for strongly interacting bosons using the Fermi-Bose mapping theorem.

We present a thorough investigation into the many-body properties of the fermionic as well as for the bosonic samples. Comprehensive calculations of the pair distribution functions for bosons as a function of the splitting strength show the influence of the splitting of the trap for even and odd particle numbers. We also present analytic and numerical results for the reduced single particle density matrices and investigate the degree of entropy as the splitting strength is increased.

While one of the consequences of the Fermi-Bose mapping in one-dimension is the identity of the bosonic and fermionic configuration space probabilities, both samples can be distinguished by their momentum space distributions. We have calculated the momentum distribution for all values of the splitting strength and will present a detailed comparison between the fermionic and the bosonic samples.

The large theoretical control over Tonks gases suggests its use to explore concepts of quantum information. We will show the behaviour of entanglement for two bosonic particles as a function of barrier height and outline a procedure to create entanglement in many particle systems.

We3-37

Gravitational states of cold antihydrogen atoms reflected from a solid surface

P. Froelich[a] and A. Voronin[b]

[a] *Department of Quantum Chemistry, Uppsala University, Box 518, 751 20 Uppsala, Sweden*
[b] *P.N. Lebedev Physical Institute, 53 Leninsky prospect, 117924 Moscow, Russia*

We will show that the ultracold $\bar{\mathrm{H}}$ atoms can be reflected from surfaces and will present calculations of the reflection probability as function of the temperature of the impinging atoms. We will discuss the prospects of using quantum reflection for trapping and guiding ultracold antiatoms and for probing the fundamental quantum-electrodynamical properties of antihydrogen and its gravitational interaction with matter.

Modern theories trying to unify the general relativity theory with quantum mechanics tend to doubt the universal validity of the Weak Equivalence Principle and allow the presence of finite range, non-Newtonian components in the gravitational interaction. Violations of WEP could occur as the result of difference in gravitational coupling to the rest mass and to the binding energy. WEP is now being tested for various isotops of atoms [1]. The special interest in gravitational experiments with *antiatoms* is stimulted by the fact that the non-Newtonian deviations are anticipated to be stronger for matter-antimatter than for matter-matter interaction.

We consider the interaction of antiatoms with a solid surface in the presence of gravity and investigate the possibility of exploiting such scenario for probing the gravitational interaction between matter and antimatter.

We show that sufficiently cold antihydrogen atoms falling on the solid surface are reflected (rather than annihilated) [2]. The antiatoms interact with the surface *via* purely attractive van der Waals - Casimir potential, which is sufficiently fast-changing to induce quantum reflection. We show that ultracod antiatoms, confined from below by quantum reflection *via* Casimir forces and from above by the gravitational force form meta-stable states. The quasi-stationary nature of these states is illustrated using methods of wave packet dynamics, disclosing presence of quantum revivals in the periodic motion of confined atoms. We forsee that the antihydrogen will bounce on the surface for a finite lifetime (on the order of 0.1 s) and show how the latter depends on the gravitational force (mg) acting on the antiatom. That opens the possibility of probing the gravitational properties of antimatter.

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We3-38

Ultra-thin Coherent Atom Beam by Stern-Gerlach Interferometry

F. Perales, J. Robert[1], J. Baudon, J. Grucker, J.-C. Karam, V. Bocvarski[2], G. Vassilev, M. Ducloy

Laboratoire de Physique des Lasers, Université Paris 13, Avenue J.B. Clément, 93430-Villetaneuse, France
(1) Laboratoire Aimé Cotton, Université Paris-Sud, Bât. 505, 91405-Orsay cedex, France
(2) Institute of Physics-Belgrade, Pregrevica 118, 11080 –Belgrade-Zemun, Serbia

Because of their wide range of applications, atomic beams of a high brightness, narrow aperture and large coherence, have been actively developed in recent years. Possible applications are (after slowing) loading of atomic traps and further production of Bose-Einstein condensates, coherent atom optics experiments, atomic lithography or deposition at a sub-micrometric scale. Atoms commonly used are those easiest to produce, detect and manipulate, namely alkalis (sometimes seeded in a rare-gas nozzle beam) [1, 2] and rare-gas metastable atom beams [3, 4, 5]. Other atoms have been considered, as Iron and Chromium, especially because of their magnetic properties [6, 7]. In most cases, the tools used to manipulate the external atomic motion are various 1D and 2D material masks, resonant or quasi-resonant laser beams and light standing waves, electric or magnetic fields.

Spatial resolution is generally limited by beam diffraction, an essential phenomenon of wave physics. In optics, light diffraction limits transverse energy focalisation. In wave mechanics of massive particles, wave packets also spread during the propagation in free space due to velocity-position uncertainty relations. These diffraction phenomena have consequences in both basic physics and applications. They are putting fundamental limits to the focusing accuracy in atomic and optical lithography: focusing can be improved only at the expense of field depth. In this letter, we propose a novel way of generating a matter wave which spreads very slightly as it propagates. This is obtained by fashioning an atom beam profile inside a Stern-Gerlach atomic interferometer [8]. This peculiar transverse profile (a narrow central bright fringe surrounded by a wide dark one), as provided by adequate matter refraction indices, closely resembles a Lorentzian profile which, contrary to a Gaussian profile, is much less sensitive to diffraction because of its smoother wings [9]. In spite of a size as small as a few tens of nm, this profile remains almost identical during propagation, and diverges much less than Gaussian beams. In a sense, it is the equivalent for matter waves of Bessel beams in light propagation [10]. In principle, any atoms having a non-zero spin can be used. For future applications, the metastable helium atom (He*, 2^3S_1) appears as an excellent candidate: (i) The internal energy is high, making this atom the most efficient to engrave a resist, as well as to be used as a probe since it is able to ionise any atomic or molecular species. (ii) Because of the wide energy gap between 2^3S_1 and 2^1S_0 levels (0.79 eV), which is much larger than Zeeman energies in the fields commonly used in Stern-Gerlach interferometers, He*(2^3S_1) atoms behave as particles of spin 1, which greatly simplifies the operation of the interferometer.

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We3-39

Novel Surfaces for Atom Chips

T. David, R. Salem, S. Machluf, E. Fleminger, S. Younnis, O. Arzouan, P. Petrov, V. Dikovsky, M. Rosenblit, Y. Japha, D. Groswasser, M. Keil*, and R. Folman
Department of Physics, Ben-Gurion University of the Negev, Be'er Sheva, Israel

The Atom Chip is a platform with which neutral atoms are cooled, trapped, manipulated, and measured using magnetic, electric, and optical potentials originating from a nearby surface located only microns away from the atoms. The atoms are held in ultra-high vacuum conditions and are cooled down to sub-μKelvin temperatures. Trap lifetimes are on the order of tens of seconds, allowing coherent quantum manipulation.

Applications arising from this field include ultra-sensitive sensors for acceleration, gravity and navigation devices, unique surface mapping of magnetic and electric fields, and quantum information processing and communication. However, the interaction between ultra-cold trapped neutral atoms and the nearby surface of an Atom Chip can lead to effects preventing the full realization of such devices. These effects can be classified into time-independent corrugations of the trapping potential caused by imperfections in the trapping wires (known as fragmentation), and to time-dependent noise that leads to trap loss, heating, and decoherence.

We study both types of phenomena utilizing state-of-the-art fabrication capabilities, enabling experimental and theoretical investigations of the atom-surface interaction over a wide range of geometries, temperatures, and surface materials, including alloy wires,[1] superconductors, and carbon nanotubes. New single-atom trapping and manipulation configurations are also being actively explored.[2]

This work is aimed at fundamental understanding of processes such as decoherence, and is also motivated by the practical need to develop enabling technologies for quantum sensors (*e.g.,* interferometers) and information processing.

The extreme sensitivity of ultra-cold atoms to the surface enables the use of atoms as probes for surface properties. Examples include probing carbon nanotubes, molecular/nano magnets, mesoscopic devices, and superconductors. Feasibility studies for new experiments on atom chips are also being conducted.[3,4]

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[*] `keil@bgu.ac.il`

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We3-40

Demonstration of a three-dimensional Rydberg atom trap

S. D. Hogan and F. Merkt

Laboratorium für Physikalische Chemie,
ETH Zurich, Switzerland

Recent progress in the development of methods by which to decelerate and manipulate the translational motion of Rydberg atoms and molecules in the gas phase using static and time-varying inhomogeneous electric fields has led to the experimental realisation of Rydberg atom optics elements including a lens [1], a mirror [2] and a two-dimensional trap [3]. These experiments exploit the very large electric dipole moments associated with Rydberg Stark states, and have demonstrated the possibility to stop a seeded, pulsed, supersonic beam of atomic hydrogen travelling with an initial velocity of 700 ms^{-1} within 3 mm ($\sim 5\ \mu$s) using electric fields of only a few kVcm^{-1}.

With the goal of achieving complete control of a cloud of Rydberg atoms or molecules in three-dimensions, we have recently designed and constructed a three-dimensional electrostatic trap for these particles. The design of this trap will be presented along with the results of a series of experiments in which we have used the trap to confine, in three dimensions, a cloud of atomic hydrogen Rydberg atoms in states with principal quantum numbers around $n = 30$. The dynamics of the Rydberg atoms in the trap have been investigated by pulsed field ionisation and imaging techniques. Under favourable conditions, trapping times on the order of 150 μs have been observed.

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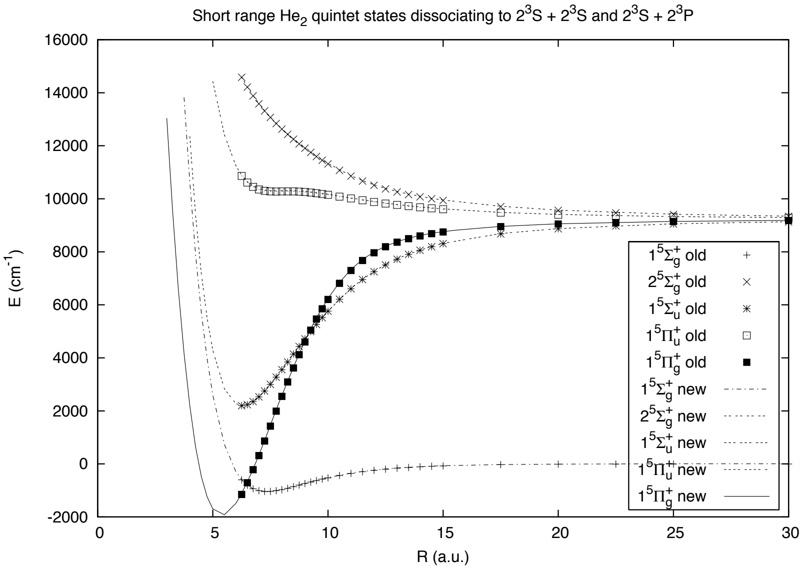
We3-41

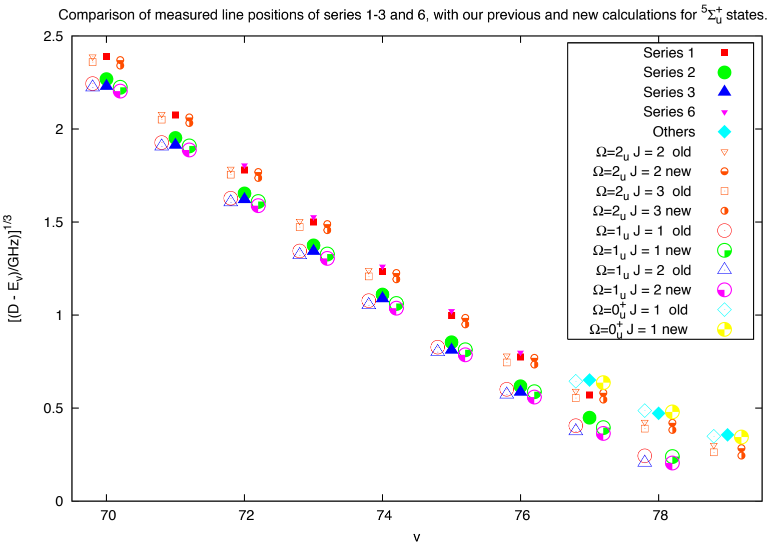
Photoassociation of metastable helium revisited

B. Deguilhem, F.X. Gadéa and T. Leininger
Laboratoire de Chimie et Physique quantique, I.R.S.A.M.C, Université Paul Sabatier, 118 Route de Narbonne, F-31062 Toulouse Cedex, France
A.S. Dickinson
School of Natural Sciences (Physics), Newcastle University, Newcastle upon Tyne NE1 7RU, United Kingdom

Abstract

A theoretical study is performed for the photoassociation of metastable helium, ^{4}He*. With a new basis set better optimized, new high level (MRCI) ab initio potentials are produced, for the $^5\Sigma_g^+$ state dissociating to $2\,^3$S + $2\,^3$S and the $^5\Sigma_{g/u}^+$ and $^5\Pi_{g/u}$ states dissociating to $2\,^3$S + $2\,^3$P even for short internuclear distances. Taking into account the spin-orbit coupling so that accurate dissociation is obtained, a single channel body-fixed approximation is employed to calculate the vibrational levels below the $^3P_2$ asymptote. These new results give similar good agreement with experiment [1] to that obtained with earlier potentials [2] and confirm the vibrational assignments suggested previously.


Short range He$_2$ quintet states dissociating to 2^3S + 2^3S and 2^3S + 2^3P


Comparison of measured line positions of series 1-3 and 6, with our previous and new calculations for $^5\Sigma_u^+$ states.

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POSTERS

Wednesday 9/5

4. Quantum Information-Cavity QED

We4-1

ENTANGLED EFFECT OF THREE-LEVEL ATOMS WITH Ξ, V AND Λ CONFIGURATIONS IN QUANTUM BIMODAL CAVITY FIELD

Ciobanu Nellu and Enaki Nicolae A.

Institute of Applied Physics, Academy of Sciences of Moldova
Chisinau MD 20-28, Republic of Moldova
nellu_ciobanu@yahoo.com

In this report a new reversible effect of three-level atom in interaction with bimodal cavity field for Ξ, V and Λ systems is proposed. We discuss the quantum mixing of two subsystems which enter in resonance in the processes of interaction. The problem consists in the possibility of realization of initial separate state of atom and electromagnetic field after the flying time through the cavity field. The quantum properties of bimodal field, which satisfy the reversible conditions for the atom flying through the cavity, were studied. In this paper the recursion relation for amplitude of electromagnetic field in decompositions on the Fock states was obtained. The exchange energy between the atom and cavity mod disentangled the state of two subsystems and the special conditions for time and proprieties of cavity field must be satisfied for realization of full separation of subsystems with initial quantum proprieties. One of examples is the reversible condition for two-level atoms, which states are mixed with cavity states of electromagnetic field during flying time through the cavity. This reversible condition can be released in the case of two undistinguished atoms crossing through the cavity simultaneously and contains with one degree of freedom more than two level radiators.

The progress in experiments with trapped atoms improves the possibilities of experimental realization of time reversibility in interaction of three-level systems with quantum bimodal cavity field. In this effect was talking into account the quantum phases of atomic electromagnetic waves function. It is well known that quantum phase's effect is used in quantum algorithms of processing information. The phase's separability between three-level atom and bimodal cavity field after interaction can be one of the candidates systems for logical information processing.

We4-2

INDIVIDUAL ADDRESSING AND ERROR RESISTANT SINGLE QUBIT GATES WITH TRAPPED YB$^+$ IONS

A. Braun, V. Elman, M. Johanning, W. Neuhauser, N. Timoney, C. Weiß,
Chr. Wunderlich

Universität Siegen, 57068, Siegen, Germany

Recently it has been shown that the simulation of one quantum system by means of observing the dynamics of another suitably tailored quantum system can be experimentally far less demanding than universal quantum computation. A system of pair-wise coupled spins described by a Heisenberg model, or a variant thereof, is particularly useful for quantum simulations that in turn are relevant, for instance, for condensed matter physics. We work on the implementation of a pseudo-spin many-body system that will serve as a well controlled prototype system and will allow for the exploration of quantum simulations: in a particular type of ion trap individual atomic ions interact via an adjustable pseudo-spin-spin coupling and, in addition, each spin is individually accessible, thus providing us with an "ion spin molecule" [1].
An important milestone towards realizing such ion spin molecules is the individual addressing of a particular spin employing a spatially varying magnetic field. We demonstrate for the first time individual addressing of ions using radio frequency radiation. Yb$^+$ ions are confined in a linear Paul trap and laser cooled such that they form a linear Coulomb crystal. Then, an rf-optical double resonance experiment is performed: The ions are optically pumped into the $|m_j|=3/2$ Zeeman states of the electronic metastable state $^2D_{3/2}$. Coherent transitions between the $|m_j|= 3/2$ and $|m_j|=1/2$ states are induced by rf radiation and the population of the $|m_j|=1/2$ states is monitored using an optical transition. Thus individual addressing of trapped ions in frequency space is demonstrated for the first time.

Another line of work with trapped Yb$^+$ ions is the implementation of error-resistant single qubit gates. In particular, we demonstrate for the first time single qubit gates with trapped ions that have been developed using optimal control theory [2] and are robust against experimental imperfections over a wide range of parameters. It is shown that errors caused by an inaccurate setting of either frequency, amplitude, or duration of the field driving a qubit transition, or a combination of these errors are tolerable (in terms of a desired accuracy, or error probability per gate) when a suitable shaped pulse is applied instead of, for instance, a single rectangular $\pi/2$-pulse [3].
Multi-qubit gates (involving two or more qubits) are usually synthesized by applying a sequence of such elementary unitary operations on a collection of qubits. Thus an essential prerequisite for fault-tolerant, scalable quantum computation with trapped ions is demonstrated here.

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We4-3

PERFECT STATE TRANSFER IN NETWORKS OF ARBITRARY TOPOLOGY AND INTERACTIONS

G. M. Nikolopoulos[†] [1], V. Košťák[‡] and I. Jex[‡]

[†]Institute of Electronic Structure & Laser, FORTH, P.O.Box 1527, Heraklion
GR-71110, Crete, Greece

[‡]Department of Physics, FJFI ČVUT, Břehová 7, 115 19 Praha 1, Staré Město,
Czech Republic

The faithful transfer of a quantum state between two distant but specified components of a quantum computer is one of the main requirements for practical quantum computation. The two components are typically parts of a larger quantum network and connected via a quantum channel (wire). Quantum wires based on systems of permanently coupled quantum objects are of particular interest as they require minimal external control. The design of such a kind of *passive* quantum wires and the problem of faithful state transfer have attracted considerable interest over the last years. As one of the main results it was demonstrated that *perfect* state transfer over passive quantum wires is possible in the context of arrays of coupled quantum dots [1] and spin chains [2-4], with mirror symmetry and nearest-neighbour (NN) interaction.

Motivated by the necessity to extent these results to more realistic scenarios, we have explored the possible forms that the system's Hamiltonian may take to be suitable for perfect state transfer (PST) [5]. Irrespective of topology and coupling configuration, we show that there are infinitely many Hamiltonians which are suitable for PST. For the sake of illustration, we demonstrate that certain Hamiltonians previously discussed in the literature can be obtained in the framework of our unified theory by setting certain restrictions and using the right parameterisation. Second, we show that our approach provides new ways for quantum wire engineering for systems of arbitrary topology and interactions beyond NN, thus generalising existing work in this context [3,4,6]. However, in contrast to [3,4,6] our approach to the problem of PST does not rely on the concept of inverse eigenvalue problems, but rather on the derivation of Hamiltonians which lead to a particular transform namely, a permutation operation.

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We4-4

Photonic phase transitions, many body spin models, and QIP in coupled cavity arrays

Dimitris G. Angelakis,[1] Marcelo F. Santos,[2] and Sougato Bose[3]

[1]Centre for Quantum Computation, Department of Applied Mathematics and Theoretical Physics,
University of Cambridge, Wilberforce Road, CB3 0WA, UK
Dept. de Física, Universidade Federal de Minas Gerais,
Belo Horizonte, 30161-970, MG, Brazil
Department of Physics and Astronomy,
University College London, Gower St., London WC1E 6BT, UK

The studies of insulator to superfluid transitions in many body systems[1] and their realization in optical lattices [2] have opened great possibilities for simulating many body systems. It is thus interesting to explore which other systems permit such phases and simulations, especially if the problem of accessibility of the individual sites is not present. Particularly arresting will be to find such phases in a system of photons which, by being non-interacting, are unlikely candidates for the studies of many-body phenomena. Here we show that a Mott phase can arise in an array of coupled high Q electromagnetic cavities between which photons can hop, when each cavity is coupled to a *single* two level system (atom quantum dot Cooper pair)[5]. In this phase each atom-cavity system has the same integral number of polaritonic (atomic plus photonic) excitations. It occurs for resonant photonic and atomic frequencies when *photon blockade* [3, 4] provides an *effective repulsion* between the excitations in each atom-cavity system. Detuning the atomic and photonic frequencies suppresses this repulsion and induces a transition from the Mott phase to a photonic superfluid. We also show that for zero detuning, the system can simulate the dynamics of a spin chain with arbitrary number of excitations and can be used to implement quantum information processing tasks[6, 7].

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HIGH-FIDELITY LOGIC GATES FOR SQUID QUBITS IN A MICROWAVE CAVITY

E. Paspalakis[1], Z. Kis[2], N. Sangouard[3], J. Janszky[2] and M. Fleischhauer[3]

[1]Materials Science Department, University of Patras, Patras 265 04, Greece
[2]Research Institute for Solid State Physics and Optics, P.O. Box 49, H-1525 Budapest, Hungary
[3]Fachbereich Physik, Universität Kaiserslautern, 67653, Kaiserslautern, Germany

Solid-state systems that make use of the Josephson effect are promising candidates for carrying out quantum computations [1]. A particular scheme of such systems is based on magnetic flux states in superconducting quantum interference devices (SQUIDs) [2-7]. In this work we propose a scheme for high-fidelity quantum logic gates for SQUID qubits. The qubits are encoded in the two lowest states of an asymmetric SQUID. To realize single- and two-qubit quantum operations, the SQUIDs are coupled to external microwave fields as well as to a common high-quality microwave cavity in a tripod-coupling scheme involving the two stable lower states, an additional lower level, and a (higher) excited state. Due to the rather large dipole moments of SQUIDs, conditions equivalent to the strong coupling regime of cavity-QED can be reached. To accommodate the parameter uncertainties inherent to any solid-state system we propose a scheme based on adiabatic passage along quasi-dark states. We find that the main limitation of an entangling gate is the absence of a third (meta)stable lower-state in the SQUID. At the same time gates that do not involve the auxiliary level, such as the swap gate, can be achieved with very high fidelities.

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Factoring numbers with ultrashort laser pulses

B. Chatel, D. Bigourd, E. Baynard, C. Meier, B. Girard,
Laboratoire Collisions, Agrégats Réactivité (CNRS UMR 5589), IRSAMC,
Université Paul Sabatier, 31062 Toulouse, France
W. Merkel, and W. P. Schleich
Insitut für Quantenphysik, Universität Ulm,Albert-Einstein-Allee 11, D-89081 Ulm,
Germany

The excitation of a two-photon transition with several intermediate states by an ultrashort laser pulse.leads to multiple interferences. These interferences are strikingly revealed when chirped pulses are used. The relative phase between the excitation paths can be changed by scanning the chirp rate ϕ''. Indeed, each path through the intermediate state $|m\rangle$ experiences a phase shift equal to $\delta_m^2\phi''$ where δ_m is the detuning between the intermediate level energy and the frequency of the two-photon transition[1]. It was recently suggested that, for equally spaced intermediate states $\delta_m = \delta_0 + m\Delta$, the sum over all paths produce a Gauss sum [2,3]. Gauss sums play an important role to factorize numbers. Scanning the chirped rate on an appropriately scaled scale results in maxima at integers value which are factors of N [3].

The factorization efficiency depends on the size of the number N to factorize and on the number of intermediate states. Moreover, the equal spacing between these intermediate states is a critical constraint. To overcome this difficulty, other alternatives have been proposed [3] and several experimental demonstrations will be given, using Rubidium atoms.

In the first example, a sequence of equally spaced ultrashort pulses is used to excite the same two-level atom. Each pulse carries the extra phase required for the Gauss sum. The pulse sequence is generated by a high resolution Liquid Crystal Device – Spatial Light Modulator (LCD – SLM, 640 pixels phase and amplitude) [4].

In a second example, a Two-photon transition is simultaneously excited by a chirped pulse and by a sequence of regularly spaced pulses. This ensures the necessary quadratic phase factor and the discrete sum.

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We4-7

Navigation in Hilbert space by quantum state reflections

P. A. Ivanov, E. S. Kyoseva, B. T. Torosov and N. V. Vitanov

Department of Physics, Sofia University, James Bourchier 5 blvd., 1164 Sofia, Bulgaria

Manipulation of superpositions of discrete quantum states has a mathematical counterpart in the motion of a unit-length statevector in an *N*-dimensional Hilbert space. Any such statevector motion can be regarded as a succession of two-dimensional rotations. But the desired statevector change can also be treated as a succession of reflections, the generalization of Householder transformations. For multidimensional Hilbert space such reflection sequences offer more efficient procedures for producing statevector changes than do sequences of rotations.

We propose a simple physical implementation of the quantum Householder reflection (QHR), $\mathbf{M}(v;\phi) = \mathbf{I} + \left(e^{i\phi} - 1\right)|v\rangle\langle v|$, in a quantum system of *N* degenerate states (forming a qunit) coupled simultaneously to an ancillary (excited) state by *N* resonant or nearly resonant pulsed external fields [1]. We use this operator as a building block in synthesizing arbitrary preselected unitary transformations. We show that the most general U(*N*) transformation can be factorized (and thereby constructed) by at most *N* - 1 QHRs and a one-dimensional phase gate. Viewed mathematically, this QHR factorization provides a parameterization of the U(*N*) group. As an example, we propose a recipe for constructing the quantum Fourier transform (QFT) by at most *N* - 1 interaction steps. For example, QFT requires a single QHR for $N = 2$, and only two QHRs for $N = 3$ and 4 [2].

We use this QHR factorization to propose a very efficient technique that connects any two arbitrary (pure or mixed) superposition states of a qunit [3]. We show that any two pure states can be linked by just a single QHR. The transfer between any two *N*-dimensional mixed states with the same dynamic invariants (e.g., the same density matrix eigenvalues) requires in general *N* QHRs. Moreover, we propose recipes for synthesis of arbitrary preselected mixed states using a combination of QHRs and incoherent processes (pure dephasing or spontaneous emission).

We extend these results to a system with lower and upper levels of arbitrary degeneracies. Then the propagators within the two sets of degenerate states are expressed by products of QHRs [4].

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We4-8

Laser control of photoinduced processes
II. Logical gates

M. Desouter-Lecomte, D. Sugny, D. Lauvergnat L. Bomble and M. Ndong

Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne,
BP 47870, 21078 Dijon, France.
Laboratoire de Chimie Physique, Unité Mixte de Recherche 8000,
CNRS et Université Paris-Sud-11, 91405 Orsay Cedex, France.

We present the control of the implementation of molecular logical gates. The aim of the control is to achieve gate operations through vibrational molecular dynamics [1, 2]. We consider two complementary approaches for designing the laser pulses able to realize the unitary transformation corresponding to a logical gate: Optimal control theory (OCT) and adiabatic passage techniques. In OCT, the optimal field is obtained by a multi target extension of the theory. Note that the adiabatic processes are not used in the adiabatic limit of the order here of the nanosecond. The optimization of the different parameters (Rabi frequencies, frequency range of the chirp, duration of each pulse…) allows one to reduce the time of the control to few (or less) picoseconds. We analyse the solutions given by the two strategies both in terms of efficiency and robustness. The effect of the environment is also taken into account by introducing a Markovian and a non-Markovian dynamics [3] and by coupling the active subspace to a small number of oscillators (up to 5) in the framework of the adiabatic coupled channels.

Simulation of the Deutsch-Jozsa algorithm

The Deutsch-Jozsa algorithm is built to illustrate the power of quantum superposed states to realize parallelism. It aims at determining by a single measure whether a binary function acting on the states of a qubit is balanced (puts different values 0 or 1 in the two states) or constant (puts equal values 0 or1). We consider a two-dimensional double well potential associated to a bending mode and an internal rotation mode of the methoxy radical. We determine laser pulses achieving the different gates of the algorithm: NOT, HADAMARD, CNOT, ACNOT.

Simulation of a quantum adder

Two strategies based on adiabatic passage [5] and on OCT are compared for different models. The first method is implemented by using electronic states while the building blocks of a quantum adder are simulated on three vibrational modes of BrCH2-COCl.

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We4-9

PERSISTENT SUPERCURRENT AS A RESOURCE FOR ATOM CHIP POTENTIAL

Tetsuya Mukai[1,3], Christoph Hufnagel[1,3], and Fujio Shimizu[1,2,3]

1. NTT Basic Research Laboratories, 3-1, Morinosato-Wakamiya, Atsugi, Kanagawa 243-0198, Japan
2. Institute for Laser Science, UEC, 1-5-1 Chofugaoka, Chofu, Tokyo 113-8585, Japan
3. CREST, Japan Science and Technology Agency, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan

An atom chip is a device to manipulate atoms near a solid surface with inhomogeneous magnetic field generated by current carrying conductors constructed on the surface. A merit of using an atom chip is its small size that realizes a strong trapping confinement with relatively small current. The shorter the distance between the potential minimum and the conductor, the potential gradient gets larger, and the atom is more easily trapped or guided in a single spatial mode. However, a shorter atom-surface distance causes a faster decoherence. It has been reported that, when atoms are trapped with normal current at room temperature, inhomogeneous structures of wires for current, technical noise of a current source, Johnson and RF noise by thermal fluctuations causes a large disturbance in the vicinity of a solid surface. For these reasons an atom chip with a smaller disturbance from the surface is strongly hoped for high-quality applications, such as on-chip guided-atom interferometers or quantum information processing devices.

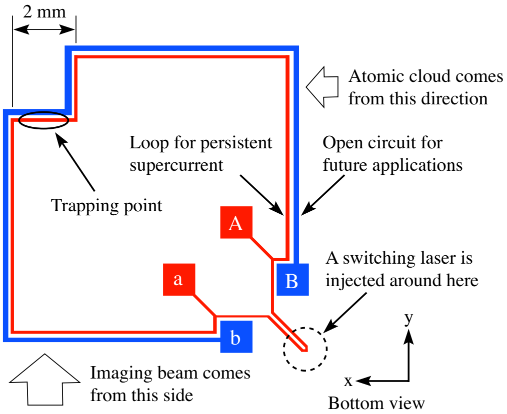

Fig. 1 The persistent supercurrent chip pattern. A persistent supercurrent is induced in the inside loop circuit. With a y-bias magnetic field a 3-dimensional trapping potential is generated at the indicated trapping point.

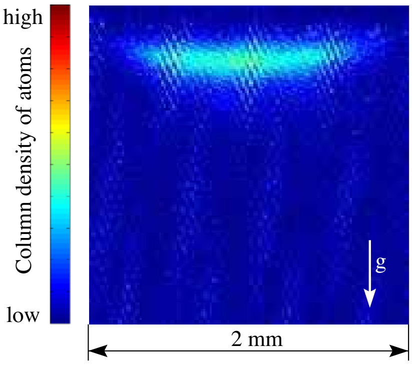

Fig. 2 Absorption image of the atomic cloud trapped in the chip potential generated by a persistent supercurrent. The induced current and the y-bias field was 2.5 A and 15 Gauss respectively.

Recently, the trapping of Rb atoms on a chip by using supercurrent instead of normal current was reported [1]. Since the resistance of a superconductor is zero, we may expect the reduction of current noise. Furthermore, the cryogenic temperature will help to reduce thermal noise and improve background pressure contributing the reduction of loss of atoms on the chip. In Ref. [1], however, the superconducting circuit was connected to the current source that was operated at room temperature. We report in this paper the first demonstration of a magnetic atom trap that is generated by a persistent current on a closed superconducting circuit and a laser-driven thermal switch to control the supercurrent [2].

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We4-10

Adiabatic Passage Technique for Quantum Information

X. Lacour, S. Guérin, H.R. Jauslin

Institut Carnot de Bourgogne, UMR 5209 CNRS, BP 47870, 21078 Dijon cedex

The perspective of a high computational power generates intense efforts to build quantum computers and their basic elements, the quantum gates.

Its implementation has to be robust, i.e insentive to fluctuations of experimental parameters and partial knowledge of the system. Adiabatic passage seems therefore to be a key process in the implementation of robust quantum computers.

We show that adiabatic passage allows one (i) to prepare a source of an arbitrary photon state [1], (ii) to entangle atoms travelling through a cavity in opposite directions [2], (iii) to generate one-qubit and two-qubit logical quantum gates [3,4,5].

We consider here qubits coded on metastable atomic states interacting with adiabatic laser pulses. The quantum gates are constructed with the use (i) of amplitude ratio of the pulses (which can be controlled by polarisation in Zeeman systems) and (ii) of static phases, since dynamical phases require the control of pulse area, and geometric phases require the control of a loop in parameter space. We propose an implementation of a controlled-unitary gate [4], where the control state can be chosen to be an arbitrary state of the control-qubit. This gate is optimised in the sense that it is faster than the equivalent one obtain by composition of elementary gates. It therefore minimizes the computational errors due to the combination of many imperfect gates. This is a key idea: some important gates have to be implemented directly, such as the SWAP gate that we propose in Ref. [5].

The use of dark states avoids spontaneous emission effects.

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POSTERS

Wednesday 9/5

5. Precision measurements

We5-1

DETERMINING THE ANTIPROTON MAGNETIC MOMENT FROM MEASUREMENTS OF THE HYPERFINE STRUCTURE OF ANTIPROTONIC HELIUM

Dimitar Bakalov(a), Eberhard Widmann(b)

(a)INRNE, Bulgarian Academy of Sciences, 72 Tsarigradsko ch., Sofia 1784, Bulgaria
e-mail: dbakalov@inrne.bas.bg
(b)SMI, Austrian Academy of Sciences, 3 Boltzmanngasse, Wien, Austria

Recent progress in the spectroscopy of antiprotonic helium [1] has allowed for measuring the separation between components of the hyperfine structure (HFS) of the (37,35) metastable state with an accuracy of 300 kHz, equivalent to a relative accuracy of 3.10^{-5}. The analysis of the uncertainties of the available theoretical results on the antiprotonic helium HFS shows that the accuracy of the value of the dipole magnetic moment of the antiproton (currently known to only 0.3%) may be improved by up to 2 orders of magnitude by measuring the splitting of appropriately selected components of the HFS of any of the known metastable states. The feasibility of the proposed measurement by means of an analogue of the triple resonance method is discussed. Independently, it is shown that the uncertainty of the magnetic moment may be reduced by one order of magnitude by the improved accuracy measurement of the difference of appropriate hyperfine transition frequencies in the (37,35) state, scheduled for the near future.

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We5-2

MATTER WAVE EXPERIMENTS WITH POTASSIUM MOLCULES

Horst Knöckel, Sha Liu, I. Sherstov, C. Lisdat, E. Tiemann

Institut für Quantenoptik, Leibniz Universität Hannover, Welfengarten 1, D 30167
Hannover, Germany
Email: knoeckel@iqo.uni-hannover.de

Matter wave interferometry has been shown by Pritchard et al. [1] to be a powerful method for investigation of collisions. We have set up a matter wave interferometry experiment with K_2 molecules [2], which is dedicated to investigate the suitability of this method for investigation of collisions between K atoms and K_2 molecules a common beam. The observed changes of the interference patterns depending on changed collision conditions can then be interpreted in terms of the interaction potential between K and K_2.

First investigations of frequency shifts by direct frequency measurements of the molecular transitions as depending on the density of the atoms in the particle beam yielded already an indication of a collision dependent frequency shift of the order of kHz [3]. The matter wave interferometry method is expected to reveal more precise results.

In a Ramsey-Bordé setup, with molecules in a supersonic particle beam, the matter wave is coherently split and recombined by laser fields. For most sensitive detection of collisions the atomic density is modulated by optically deflecting the atoms out of the particle beam with resonant laser light. The two available exits of our interferometer, with molecules either in the excited state or in the ground state, offer complementary detection schemes of the interference signal. We observe the interference patterns from the 4-beamsplitter Ramsey-Bordé setup. Under certain conditions we also observe interferences from a 2-beamsplitter Ramsey interferometer due to the transverse spacial overlap of the matter waves. The detection scheme for the ground state exit is set downstream of the particle beam sufficiently far away from the interferometer zone for a good separation of the laser induced fluorescence of both exits. The signals are in principle complementary to each other and can be recorded simultaneously, but due to additional freedom in the experiment the ground state exit gives simpler profiles of the signals.

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We5-3

Progress towards a high-precision measurement of the *g*-factor of a single isolated (anti)proton in a hybrid double Penning-trap*

S. Ulmer[1,2], K. Blaum[1,3], H. Kracke[1], S. Kreim[1], C. C. Rodegheri[1],
W. Quint[2,3], S. Stahl[4], J. Verdu[2], J. Walz[1]

[1] Physics Department, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany
[2] Physics Department, Ruprecht Karls-University Heidelberg, 69121 Heidelberg, Germany
[3] GSI Darmstadt, Planckstrasse 1, 64291 Darmstadt, Germany
[4] Stahl Electronics, 67582 Mettenheim, Germany

In our experiment we aim to measure the magnetic moment or *g*-factor of a single isolated proton stored in a cylindrical Penning-trap with a relative uncertainty of 10^{-9} or better. This will be the first direct measurement of the proton *g*-factor ever performed. Current data for the magnetic moment of the free proton are derived from theory using the measured value extracted from the hyperfine splitting of a hydrogen maser in a magnetic field. In Dehmelts famous *g*-2 geonium experiment [1] the magnetic moment of the electron was determined by means of the continuous Stern-Gerlach effect in a cryogenic Penning-trap. In our experiment we aim to apply the same method to the proton. However, the magnetic moment of the proton is 650 times smaller than the magnetic moment of the electron, which considerably complicates the measurement and bears a great experimental challenge. Therefore, different novel techniques are being developed to enhance the sensitivity of the experiment.

The detection of the spin state is carried out by coupling the magnetic moment to the axial eigenmotion of the particle in the trap via a magnetic bottle. Depending on the direction of the spin the axial frequency is shifted. The value of the frequency shift scales with the magnetic moment of the particle and the strength of the magnetic bottle. Thus we developed a novel trap design, the so-called hybrid toroidal Penning trap [2]. The cylindrical ring electrode was replaced by an electrode of toroidal shape, manufactured from ferromagnetic material, which results in a large distortion of the magnetic field lines, and thus enlarges the axial frequency jump. At the same time, the magnetic bottle perturbs the accuracy of the axial and the cyclotron frequency detection, thus a double trap design will be used, consisting of the hybrid analysis trap, where the spin state will be detected, and the cylindrical precision trap, where the precision measurement will be performed. Furthermore, a phase-sensitive detection method will be used to detect the tiny axial frequency difference between the two spin eigenstates [3].

Besides the measurement of the proton *g*-factor, in future experiments the antiproton *g*-factor will be measured. Comparison of the experimental values of both experiments will provide a stringent test of the CPT-theorem on the baryonic sector [4]. Furthermore, the hybrid trap design opens a variety of new experiments. The magnetic moments of heavier nuclei like ^{3}He or tritium could be measured as well in future experiments.

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We5-4

Visualisation of instabilities in a stable trapping area observed on Pr ions stored in a Paul trap

W. Koczorowski, G. Szawioła, A. Walaszyk, A. Buczek, E. Stachowska

Poznan University of Technology, Chair of Quantum Engineering and Metrology
ul. Nieszawska 13B, 60-965 Poznan, Poland
E-Mail: Wojciech.Koczorowski@put.poznan.pl

Ion trapping in a Paul trap requires the combination of DC and RF electric fields applied to the ring electrode. The storage conditions are stable in all spatial directions within certain ranges of the amplitudes of the voltages. These trapping ranges are visualised in a stability diagram [1].

The stability diagram is not homogeneous in terms of the trapping efficiency and storage time of the ions. It contains lines of instability to higher perturbations than quadruple ones, so-called nonlinear resonances (NR). In a NR ions can resonantly absorb energy from the trapping field. This process causes a substantial decrease of the storage time of the ions. The NR can be observed by the change of intensity of the Laser Induced Fluorescence (LIF) of the stored ions [2].

In our earlier work [3] the experimental points of the NR for Pr ions have been presented compared with theoretical predictions. In the present paper we report the imaging of the instabilities for an extended area of the stability diagram. Additionally an analysis of the obtained NR results will be given.

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We5-5

OPTICAL LATTICE POLARIZATION EFFECTS ON HYPERPOLARIZABILITY AND LATTICE-FIELD-INDUCED $^1S_0$- $^3P_0$ TRANSITIONS IN EVEN ISITOPES OF ALKALINE-EARTH ATOMS

Ovsiannikov V. D[*]., Pal'chikov V. G[+], Taichenachev A. V [#]. and Yudin V. I[#].

[*] Physics Department, Voronezh State University, Universitetskaya pl., 1, 394006, Russia,
[+] Institute of Metrology for Time and Space at National Research Institute for Physical-Technical and Radiotechnical Measurements, Mendeleevo, Moscow Region, 141579 Russia
[#]Institute of Laser Physics SB RAS, Novosibirsk, 630090, Russia
Novosibirsk State University, Novosibirsk 630090, Russia

The circular polarized laser beam of the "magic" wavelength used to produce an optical lattice for the time-frequency standard on neutral atoms may mix the $^3P_1$ state to the long living metastable state $^3P_0$ thus providing significant enhancement of the strongly forbidden $^1S_0$- $^3P_0$ clock transition in even isotopes of alkaline-earth atoms. We present a detailed analysis of various factors influencing resolution and uncertainty for this kind of optical standard, including precise estimations of the "magic" wavelengths, transition matrix elements and field induced second- and fourth – order ac Stark shifts for the ground and metastable alkaline-earth atoms.

In the second part of the paper the frequency light shift due to hyperpolarizability (i.e. terms of fourth order in field amplitude) is studied for forbidden optical transition J=0→J=0. A simple universal dependence on the field ellipticity is obtained. This result allows one to minimize the fourth –order light shift for optical lattice with "magic" wavelength. We show a principal possibility for an existence of "magic" elliptical polarization, for which the fourth-order frequency shift vanishes. The obtained results could significantly improve metrological characteristics of lattice-based atomic clocks.

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We5-6

PRECISION SPECTROSCOPY OF ANTIPROTONIC HELIUM

E. Widmann

Stefan Meyer Institut for Subatomic Physics, Austrian Academy of Sciences,
Boltzmanngasse 3, 1090 Wien, Austria

The ASACUSA collaboration is performing laser and microwave spectroscopy of antiprotonic helium ($\bar{\mathrm{p}}\mathrm{He}^+$), a metastable three-body system consisting of a helium nucleus, an antiproton and an electron, at the Antiproton Decelerator (AD) of CERN. In laser spectroscopy measurements, the transition energies of antiprotons between highly excited states of $\bar{\mathrm{p}}\mathrm{He}^+$ *((n,L)~33…39)* have been measured with increasing precision up to relative accuracies of $\sim 10^{-8}$ in the last few years [1-3]. Parallel to this, the accuracy of 3-body QED calculations has improved accordingly. By comparing theory and experiment we could extract a value for the antiproton-to-electron mass ratio of $M_{\bar{p}}/m_e = 1836.152674(5)$ (rel. error 3 ppb) [3]. By combining our result with measurements of the antiproton charge-to-mass ratio, we were able to set separate limits on the relative difference of proton and antiproton charge *M* and mass *Q* of $\left|Q_p + Q_{\bar{p}}\right| / \left|Q_p \approx \right| M_p - M_{\bar{p}} \left| / \right| M_p \leq 2 \times 10^{-9}$, a factor 250 improvement over our earlier measurements at LEAR.

The hyperfine splitting in $\bar{\mathrm{p}}\mathrm{He}^+$ has been measured for the first time in 2001 with a precision of 3×10^{-5} [4]. Due to the large angular momentum of the antiproton ($L_{\bar{p}} \approx 35$), the hyperfine structure consists of a dominant splitting caused by the interaction of $L_{\bar{p}}$ with the electron spin S_e and a smaller splitting due to the interaction of the antiproton magnetic moment $\mu_{\bar{p}}$ with the other moments. The two observed transitions are in agreement with QED calculations at a level of 6×10^{-5}, which corresponds to the theoretical accuracy. The agreement gives a limit on the antiproton *orbital* *g*-factor of $\left|g_l^{\bar{p}} - 1\right| < 6 \times 10^{-5}$ [4]. The difference of the two transition frequencies is directly related to the value of the *spin* magnetic moment $\mu_{\bar{p}}$, which so far is known to only 0.3%. ASACUSA has started a new measurement with the goal of increasing the experimental precision by an order of magnitude, which would lead to a determination of $\mu_{\bar{p}}$ to 0.1%.

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We5-7

NEW PECULIARITIES OF SATURATED-ABSORPTION AND MAGNETO-OPTICAL RESONANCES IN ELLIPTICALLY POLARIZED LIGHT FIELDS

D.V. Brazhnikov, A.V. Taichenachev, A.M. Tumaikin, V.I. Yudin
Institute of Laser Physics, SB RAS, pr. Lavrent'eva 13/3, Novosibirsk, 630090 Russia
Novosibirsk State University, ul. Pirogova 2, 630090 Russia
E-mail: llf@laser.nsc.ru

S.A. Zibrov, Ya.O. Dudin, A.G. Radnaev, V.V. Vasil'ev, V.L. Velichansky
P.N. Lebedev Physical Institute, RAS, Leninskiy pr. 53, Moscow, 117924 Russia

Methods of modern high-resolution laser spectroscopy [1] are applied in numerous scientific and technical problems (e.g., frequency and time standards, magnetometers). Investigations are carried out to optimize the parameters of nonlinear resonances (width, amplitude, amplitude-to-width ratio, shift) with respect to the gas pressure and temperature, light intensity and etc. So far relatively small attention is paid to the systematic study of polarization aspect of interaction between atoms or molecules with electromagnetic field. Often such investigations are confined to the simplest cases – linear and circular polarizations.

In the present paper we theoretically and experimentally demonstrate a significant influence of polarization parameters of light fields on some resonance properties in two cases: saturated-absorption resonance in counterpropagating waves and magneto-optical resonance of electromagnetically induced absorption (EIA) in traveling wave. The former presents a spectroscopic signal as forward wave absorption versus wave frequency in presence of backward light beam. A new polarization effect is revealed leading to asymmetry and shift of the resonance when at least one of the fields has elliptic polarization (Fig.1a).

In the case of magneto-optical EIA resonance the signal is absorption of traveling wave as the function of external static magnetic field. Here, for instance, the resonance amplitude can increase by more than an order of magnitude when the polarization changes from linear to optimal elliptic (Fig.1b).

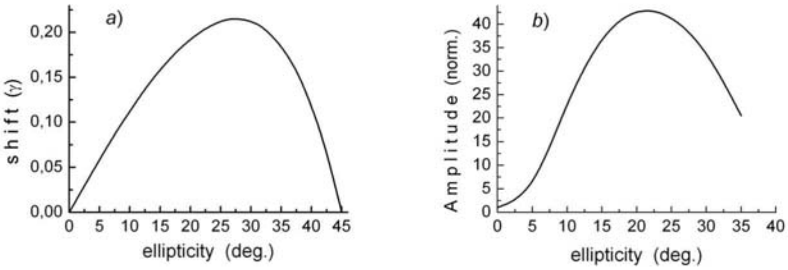

Fig.1. *a)* Calculated shift of the saturated-absorption resonance versus the ellipticity of backward wave, with linear polarized forward wave. *b)* Amplitude of magneto-optical EIA resonance versus the ellipticity of traveling light wave.

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We5-8

LINE BROADENING BY OPTICAL PUMPING IN THE WEAK EXCITATION LIMIT

E. Saks[1], I. I. Beterov[3], P. Spels[1], I. Sydoryk[1], K. Miculis[1], A. Janovs[1],
N. N. Bezuglov[2], I. I. Ryabtsev[3], A. Ekers[1]

[1] Inst. of Atomic Physics and Spectroscopy, Univ. of Latvia, LV-1586 Riga, LATVIA
[2] V. A. Fock Institute of Physics, St. Petersburg State University, 198904 St. Petersburg, RUSSIA
[3] Institute of Semiconductor Physics, SB RAS, 630090, Novosibirsk, RUSSIA

A spectral line broadening mechanism due to optical pumping in the excitation spectrum of Na($3p_{3/2}$) state in a supersonic atomic beam is described. Such beam represents an absorbing medium with anisotropic absorption coefficient, and it is affected by effects of radiation trapping (RT) and optical pumping (OP). Conventional knowledge tells that the linewidths are affected by saturation broadening, when strong laser excitation sources are used, and RT, when density of atoms in the beam is sufficiently high to lead to multiple reabsorption events of spontaneous photons. In our study, we chose a beam with low atom density ($n_{3S} < 10^{10}$cm^{-3}) and low excitation laser intensity, thus eliminating both line-broadening mechanisms. At the same time, the transit time of atoms through the laser beam (τ_{tr} = 1.9 μs) by more than 100 times exceeds the spontaneous lifetime of the $3p_{3/2}$ state (τ_{3p} = 16.2 ns), thus ensuring strong optical pumping even when laser intensity is kept 50 times lower than the saturation intensity (Rabi frequency $\Omega_{sat} \approx 1/\tau_{3p}$). Thus, upon excitation of the $3s_{1/2}(F''=2)\rightarrow 3p_{3/2}$ (F'=1,2,3) transition the population is being pumped from the ground state HFS level F'' = 2 to F'' = 1, and this effect is noticeable beginning from Rabi frequencies $\Omega \geq \Omega_{sat}\sqrt{\tau_{3p}/(\tau_{tr}\Lambda(F',F''=1))}$. The factor $\Lambda(F',F''=1)$ gives the branching coefficient for the transitions from level F' to the level F'' = 1, and it is equal to 5/6, 1/2, and 0 for F' = 1, 2, and 3, respectively. Figure 1 shows that OP strongly reduces the intensity of the component associated with the excitation of F' = 2 level and increases the linewidth, while there are no changes in the right hand side peak corresponding to the excitation of F' = 3, which is expected because excitation of this level is not affected by optical pumping due to the selection rules.

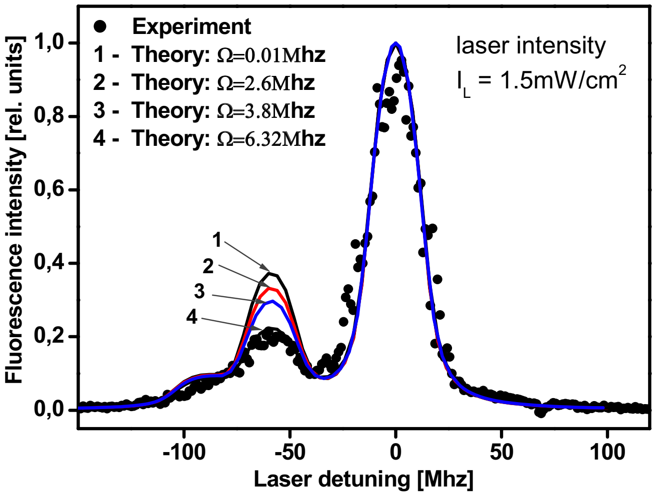

Fig. 1. $3s_{1/2}(F''=2)\rightarrow 3p_{3/2}$ (F'=1,2,3) laser excitation spectrum in a collimated Na supersonic beam at various laser Rabi frequencies.

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We5-9

COMPARISON OF DOUBLE RESONANCE MAGNETOMETERS BASED ON ATOMIC ALIGNMENT AND ORIENTATION

A. Weis, G. Di Domenico, G. Bison, P. Knowles, M. Loutsch, and H. Saudan

Physics Department, University of Fribourg, Switzerland

We present an experimental and theoretical study of the intrinsic magnetometric sensitivity of optical/radio-frequency double resonance magnetometers in which *circularly* or *linearly* polarized laser light is used in the optical pumping and detection processes. Circularly polarized light produces an atomic orientation (vector magnetization) [1], while linearly polarized light produces an atomic alignment (tensor magnetization) [2,3]. The former leads to signal modulations at the Larmor frequency ν_L, while in the latter case the signal is modulated both at ν_L and at $2\ \nu_L$. We refer to the two types of magnetometers as DROM and DRAM (double resonance orientation/alignment magnetometer).

Using model calculations based on the irreducible tensor formalism we have derived algebraic expressions of the line shapes for all three cases in the case of low laser power. A semi-empirical extension of these expressions to larger laser power has allowed us to predict the rf and laser power levels which yield an optimal magnetometric sensitivity of the DROM and DRAM devices. The experimental optimization in a spherical (14 mm radius) paraffin-coated Cs vapor cell is in excellent agreement with the theoretical modeling. We have further varied the vapor density to find the optimum intrinsic sensitivities δB_{min} given in Table 1.

	modulation	T_{opt}	δB_{min}
DROM	ν_L	42°C	9 fT/Hz$^{1/2}$
DRAM	ν_L	31°C	29 fT/Hz$^{1/2}$
DRAM	$2\ \nu_L$	34°C	28 fT/Hz$^{1/2}$

Table 1: Intrinsic magnetometric sensitivities of Cs vapor based DROM and DRAM devices with optimized laser power, rf power, and cell temperature. All measurements were performed in the same cell pumped by a laser locked to the D_1(4-3) transition.

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We5-10

^{3}HE METASTABILITY EXCHANGE OPTICAL PUMPING STUDIES AT HIGH MAGNETIC FIELD

A. Nikiel [1], T. Pałasz [1], M. Suchanek [2], M. Abboud [3], A. Sinatra [4], Z. Olejniczak [1,5], T. Dohnalik[1], G. Tastevin [4], P-J. Nacher [4]

[1] M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland
[2] Department of Physics, Agricultural University, Kraków, Poland
[3] Present address : Faculté des Sciences, Université Saint Joseph, Beirut, Lebanon
[4] Laboratoire Kastler Brossel, Ecole Normale Supérieure, Paris, France
[5]Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland

Systematic studies of the metastability exchange optical pumping (MEOP) process in ^{3}He gas [1] at high magnetic fields (0.45, 0.9, 1.5, and 2 T) and various ^{3}He gas pressures are performed. The performances of different optical pumping lines are compared to determine the most efficient line, with respect to achievable value of steady state nuclear polarization as well as production rate. The impact of experimental parameters such as laser power, beam profile, and shape of the pumping cell is evaluated. By control of the rf discharge intensity in the cell, the density of metastable state atoms and the plasma-induced nuclear relaxation rate can be varied, and their effects on MEOP efficiency is also investigated.

For these experiments, a highly sensitive optical method based on probe absorption measurements on the 2^3S-2^3P line has been implemented [2]. The high accuracy of measurements allows a quantitative comparison with recently developed models, for improved physical understanding of MEOP and relaxation processes.

We report selected MEOP results that show that, at fixed pressure, nuclear polarizations increase with the applied magnetic field strength. For instance, polarizations exceed 50 % at 67 mbar and 2 T, which represents a substantial improvement over a standard low-field MEOP [3]. This suggests that some relaxation channel, that severely limits the efficiency of MEOP at high pressure, is reduced at high field. Our systematic studies fully confirm and complement the first and surprising 1.5 T results [4-6]. Moreover, the present results suggest that even better efficiency can be expected at higher magnetic field, and urge for investigations at higher pressures.

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We5-11

I.C.E.: A BOSON-FERMION ATOM INTERFEROMETER FOR MICROGRAVITY

RA Nyman, G Varoquaux, J-F Clément, J-P Brantut, T Bourdel, A Aspect, P Bouyer
Institut d'Optique, Campus Polytechnique, RD 128, 91127 Palaiseau, France

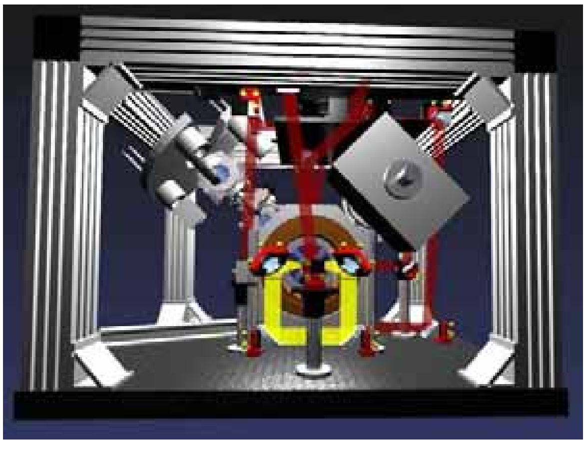
N Zahzam, Y Bidel, A Bresson.
ONERA, Chemin de la Hunière, 91761 Palaiseau, France

F Pereira Dos Santos, A Landragin
LNE-SYRTE, Observatoire de Paris, 61 avenue de l'Observatoire, 75014 Paris,France

M Rouzé, L Mondin, J Mignot
CNES, Centre Spatial de Toulouse, 18 Av. Edouard Belin, 31401 Toulouse, France

An atom interferometer for inertial sensing in micro-gravity is under construction, as part of the I.C.E. (*Interférométrie Cohérente pour l'Espace*) collaboration [1]. A mixture of quantum degenerate gases, bosonic ^{87}Rb and fermionic ^{40}K, will be used in order to find the optimal conditions for precision and sensitivity of inertial measurements. Quantum degeneracy will be achieved by an all-optical route, using a compressible crossed-beam design. Magnetic Feshbach resonances will be used both to aid during evaporative sympathetic cooling and to control interactions during interferometry experiments. Thus a range of quantum fluids will be available: simple bosons, fermions, molecules or Cooper pairs.

Micro-gravity will be realised in parabolic flights lasting up to 20s in an Airbus. A compact, transportable vacuum system has been built, and used for laser cooling and magneto-optical trapping. On-board laser systems based on frequency-doubled telecommunications fibre lasers have been developed. The laser technology is due to be tested in micro-gravity conditions in March 2007 to create a small magneto-optical trap. The full apparatus is intended to produce high-precision acceleration measurements using Raman-pulse beam splitters. We will report on in-flight results as well as progress towards ground-based production of degenerate Bose and Fermi gases.



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We5-12

RESONANT FEMTOSECOND PULSE-TRAIN EXCITATION OF RUBIDIUM ATOMS

D. Aumiler, T. Ban, S. Vdović, N. Vujičić, H. Skenderović and G. Pichler

Institute of Physics, Bijenička 46, Zagreb, Croatia

Mode-locked femtosecond (fs) lasers are a powerful tool for the frequency comb generation [1]. In a system with the relaxation time greater than the laser repetition period, the system interacts with the pulse train rather than with the single pulses [2]. Pulse train in time domain corresponds to the frequency comb in the frequency domain. Frequency comb consists of a regularly spaced series of sharp lines $f_n = nf_r + f_0$, where n is a large integer, f_r is the laser repetition rate and f_0 is the carrier-envelope offset frequency.

In our recent papers [3,4] a mode-locked femtosecond laser was used to physically map the laser frequency comb into the velocity comb of the excited Rb atoms at room temperature. Resonant excitation of the rubidium atoms by discrete frequency comb optical spectrum results in the comb-like velocity distribution of the excited state hyperfine level populations and velocity-selective population transfer between the Rb ground state hyperfine levels. Modulations in the hyperfine absorption line profiles are observed as a direct consequence of the velocity-selective optical pumping induced by the frequency comb excitation. The fs pulse-train excitation of a Doppler-broadened rubidium vapor was investigated theoretically in the context of the density-matrix formalism.

In the present work we expand the theoretical model presented in our previous papers to directly calculate the probe laser absorption and show preliminary results which support the experimental findings. We show how the strong probe laser can influence the resonant interaction of Rb atoms with the fs frequency comb. A full density matrix treatment of resonant fs pulse-train excitation of Rb atoms is applied to the case when the probe laser is tuned to Rb D_1 resonance line at 795 nm. We will show how a combined theoretical and experimental approach can be used for a direct visualization of the frequency comb by physical mapping of the optical frequency comb to the atom-velocity comb. Additionally, the possible application for absolute frequency determination of the frequency comb will be discussed.

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We5-13

Experimental Demonstration of the Fluctuation-Dissipation Theorem in a Thermal Rubidium Vapor

G. E. Katsoprinakis, A. T. Dellis and I. K. Kominis

Department of Physics, University of Crete, Heraklion 71103, Greece
and
Institute of Electronic Structure and Laser,
Foundation for Research and Technology, Heraklion 71110, Greece

Spin noise sets fundamental limits to the attainable precision of measurements using spin-polarized atomic vapors and therefore merits a careful study. On the other hand, it has been recently shown that spin noise contains useful physical information about the atomic system, otherwise accessible via magnetic-resonance type experiments. We here show in yet another manifestation of the fluctuation-dissipation theorem, that spin noise reveals information on the spin-coherence dissipation properties of the atomic system, described by $1/T_{2}$, the transverse spin relaxation rate. We present the first high-resolution measurements of spin noise at low magnetic field, leading to an accurate comparison of the extracted relaxation rates with the ones inferred from traditional magnetic-resonance type measurements in optical pumping experiments.

We5-14

FEMTOSECOND LASER FREQUENCY COMB TREATMENT OF VELOCITY GROUPS BY USING ATOMIC HYPERFINE FILTER WITH PURE RUBIDIUM ISOTOPES

Goran Pichler, Ticijana Ban, Damir Aumiler, Hrvoje Skenderović, Nataša Vujičić and Silvije Vdović

Institute of physics, Bijenička 46, Zagreb, Croatia

When femtosecond laser passes the cell filled with pure rubidium 85 isotopes the frequency comb content will be modified due to absorption of comb lines within ^{85}Rb Doppler broadened lines. At slightly elevated temperatures the absorption within the cell will remove all comb lines overlapping spectral region of hyperfine spectral lines of 85 isotopes. In this way modified frequency comb passing through the second rubidium cell with natural abundances of rubidium isotopes will act only on ^{87}Rb atoms, leaving ^{85}Rb atoms unaffected. A weak cw scanning probe laser copropagating with the femtosecond pulse train in the second cell will experience peculiar absorption profile only at ^{87}Rb hyperfine lines. The $5\ ^2S_{1/2} \rightarrow 5\ ^2P_{1/2,3/2}$ fs pulse train excitation of a Doppler broadened Rb four-level atomic vapor will be essentially modified by using atomic filter at different rubidium atom densities. This effect could be applied in different subsequent experiments. Basic physics has been described in [1,2], and the development of the experimental methods and theoretical description applied to Rb and Cs atoms is presented in references [3-6].

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We5-15

STRONGLY INTERACTING ATOMS IN OPTICAL LATTICES

Servaas Kokkelmans, Johan Mentink

Department of Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB
Eindhoven, The Netherlands

Optical lattices allow for a large amount of control over the physical parameters of interacting atoms. Using a Feshbach resonance, interactions can be tuned by changing the magnetic field, while the depth and geometry of the lattice can be adjusted via the laser field. Precise values for the interaction strengths of rubidium could be derived by studying coherent collisional spin dynamics in optical lattices [1,2]. These high precision measurements provides challenges for finding agreement with current state-of-the-art interaction potentials and models, and also for finding accurate descriptions for the optical lattice which include (resonant) binary interactions.

we derived a new solution for two interacting atoms in an optical lattice. In the single site approximation, we start with the exact solution of the Busch model [3], with each lattice site treated as an harmonic oscillator. Subsequently we treat lattice effects beyond the harmonic oscillator approximation as a perturbation. This way we effectively derived Wannier-like solutions for a pair of interacting atoms, with the interaction modeled exactly. This allows us to model the interactions for all values of the scattering length. We also investigated effects of the lattice confinement on the relative wavefunction.

We applied this model to the Mainz experiment [1,2] with spin dynamics for f=1 and f=2. The interaction energy is computed as the difference between two-atom energy levels with and without interaction. We find that our model describes the experiment well, within experimental and theoretical error bars.

Apart from applying our model to spin dynamics, we are in a good position to analyze future optical lattice experiments where the interactions are made very strong by utilizing Feshbach resonances. It is also a starting point for a description of photoassociation in an optical lattice.

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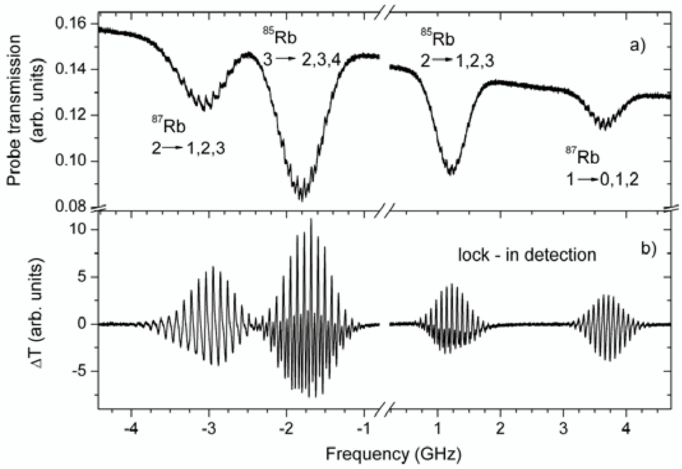
We5-16

ENHANCED SENSITIVITY RUBIDIUM VELOCITY COMB MEASUREMENTS

T. Ban, S. Vdović, D. Aumiler, H. Skenderović, N. Vujičić and G. Pichler

Institute of Physics, Bijenička 46, Zagreb, Croatia

An experimental technique with enhanced sensitivity for the rubidium atom velocity comb observation will be presented. Rubidium atom velocity comb, observed as modulation of probe cw laser transmission, is a result of the velocity selective optical pumping induced by the resonant frequency comb excitation of Rb atoms. Resonant excitation of the rubidium atoms by discrete frequency comb optical spectrum results in the comb-like velocity distribution of the excited state hyperfine level populations and velocity-selective population transfer between the Rb ground state hyperfine levels. Decrease of the effective relaxation time of the Rb system is observed in the strong probe case, leading to the gradual change from the frequency comb excitation to the pulse by pulse excitation. We expand the theoretical model presented in our previous papers [1,2] to directly calculate the probe laser absorption and show preliminary results which support the experimental data.



Measured probe transmission for the Rb vapor at room temperature in the case when the fs laser is tuned to $5^2S_{1/2} \rightarrow 5\ ^2P_{1/2}$ transition at 795 nm.

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We5-17

HIGH RESOLUTION LASER SPECTROSCOPY OF Cs-VAPOUR LAYERS WITH THICKNESS COMPARABLE TO THE WAVELENGTH OF THE IRRADIATING LIGHT

S. Cartaleva[1], K. Koynov[2], S. Saltiel[2], D. Sarkisyan[3], D. Slavov[1], P.Todorov[1], K.Vaseva[1]

[1]Institute of Electronics, Bulgarian Academy of Sciences, 72 Tzarigradsko Shosse bld, 1784 Sofia, Bulgaria
[2]Sofia University, Faculty of Physics, 5 J. Bourchier boulevard, 1164 Sofia, Bulgaria
[3]Institute for Physical Research, National Academy of sciences of Armenia, Ashtarak-2, Armenia

The high resolution single beam spectroscopy of thin alkali-vapor layers, made possible recently through the development of Extremely Thin Cells, is very advantageous for study of the interesting effects in atomic absorption and fluorescence appearing when the vapor-layer thickness can be precisely controlled in an interval around the wavelength λ of the irradiating light. The usage of extremely (in one dimension) thin cell leads to strong anisotropy of atom light interaction time. Atoms with velocity component normal to the cell walls give smaller contribution to the absorption and fluorescence signals than those flying parallel to the walls. Interesting coherent effects are observed in absorption profiles changing their width periodically, with minima for thickness odd λ/2. At the same time the width of the fluorescence profiles increases monotonically with the cell width.

We present experimental and theoretical study of absorption and fluorescence spectra for Cs-atomic-layers with thickness $L = m\lambda$, where $m = 0.5, 1, 1.5, 2, 2.5, 3$. The influence of the light intensity on the individual hyperfine optical transitions of the D_2 line of Cs is examined in details. For low light intensity, experimentally observed absorption spectra are in agreement with the previously developed theory related to the collapse and revival of Dicke-type coherent narrowing of hyperfine optical transition profiles. Based on the Optical Bloch Equations, a theoretical model is developed and attempt is made for quantitative comparison of theory with the experiment. With the enhancement of irradiating light intensity and $L>\lambda/2$, more complicated absorption spectra are observed where the coherent Dicke narrowing is accompanied by absorption drop in a narrow spectral interval, for all hyperfine optical transitions. The experimental study of the fluorescence behavior shows that for the open transitions suffering hyperfine or/and Zeeman optical pumping, narrow dip in fluorescence is observed superimposed on the top of the sub-Doppler-width fluorescence profile. However for the fluorescence, completely different behavior is observed in case of closed transition. Here, dip in the fluorescence is not observed at any of the used cell thicknesses or light intensities. The developed model is in very good agreement with the experimental observations.

The presented results contribute to the further advancement of our knowledge not only in fundamental studies of saturation and optical pumping in transient regime, but also in practical aspect, since it provides information about the behavior of one-dimension-confined atomic ensemble.

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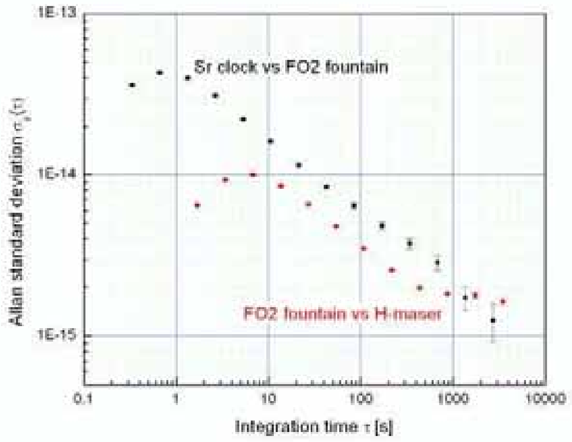
We5-18

^{87}Sr OPTICAL LATTICE CLOCK USING SPIN-POLARIZED ATOMS

X. Baillard, M. Fouché, R. Le Targat, P. Westergaard, A. Lecallier, F. Chapelet,
S. Bize, P. Rosenbusch, M. Abgrall, P. Laurent, Y. Lecoq, G.D. Rovera, A. Clairon,
P. Lemonde
LNE-SYRTE, Observatoire de Paris, 61 Avenue de l'Observatoire, 75014 Paris,
France

B. Lipphardt, G. Grosche, H. Schnatz
Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig,
Germany

We present a new accuracy evaluation of the LNE-SYRTE optical lattice clock with ^{87}Sr atoms. The interrogation is now achieved with spin-polarized atoms in the (F=9/2, m_F=9/2) or (F=9/2, m_F=-9/2) Zeeman sub-state. Using a pi-polarized clock laser, we alternate cycles where the 9/2 → 9/2 and -9/2 → -9/2 transitions are probed, strongly decreasing the uncertainty on the magnetic field effects for this measurement. The frequency measurement was made thanks to a femtosecond frequency comb based on a fiber laser, and referenced to the three atomic fountains FO1, FO2 and FOM at LNE-SYRTE. The resulting accuracy of the Sr clock is in the low 10^{-15} range. An experimental standard Allan deviation is plotted on the figure. The stability of the measurement at 1s is 5.10^{-14}, with roughly equal contribution of the Sr clock and of the fountain.
We also made a measurement of the frequency for the ^{88}Sr bosonic isotope, using a static magnetic field to allow the transition. The evaluation of the systematic effects and a comparison with the fermionic isotope will also be discussed.



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We5-19

High-resolution spectroscopy of formaldehyde for diagnostics of guided cold molecules

P.W.H. Pinkse, M. Motsch, M. Schenk, M. Zeppenfeld, and G. Rempe
Max-Planck-Institut-für Quantenoptik, Hans-Kopfermannstr. 1, D85748 München, Germany

Optical manipulation of cold polar molecules necessitates a molecule with strong electronic transitions, preferably in a spectral region accessible with standard cw-laser techniques, and a large Stark shift for efficient electric guiding and trapping. Slow beams of up to 10^{10} s^{-1} formaldehyde molecules with velocities around 50 m/s have been produced [1]. We envision doing state-selective detection of these molecules by depletion spectroscopy, optically pumping molecules into unguided states. Alternatively, molecules can be removed from the beam by exciting them in predissociating states.

Formaldehyde (H_2CO) exhibits a rich ultraviolet spectrum between 280 and 360 nm [2]. Based on the calculated populations of selected states of up to 5% in the guided beam, and the fact that formaldehyde predissociates with over 90% probability under UV excitation, we estimate that depletion spectroscopy is feasible. In order to be able to perform this technique, precise knowledge of its energy levels is prerequisite. Although formaldehyde is a well-studied molecule, being among the simplest poly-atomic molecules, literature data is not accurate enough to precisely predict the UV frequencies of individual rovibrational transitions originating from guided states. For this reason, room-temperature absorption spectroscopy of the weak $\tilde{A}^1A_2 \leftarrow \tilde{X}^1A_1$ transition is performed in a multi-pass setup at H_2CO pressures of 50 Pa. A frequency-doubled cw dye laser allows higher resolution than previous studies relying on pulsed dye lasers [3] and makes it possible to identify the desired transitions. Comparison between calculations based on available rotational constants and our measurement indicates the necessity to include sixth-order centrifugal distortion coefficients.

In order to predict the limits of this and other spectroscopic methods, we are also interested in the natural linewidth of the studied transitions. One of the main obstacles for measuring these is Doppler broadening. Doppler broadening can be circumvented by saturation spectroscopy, but applying this method to weak transitions can be a significant challenge. We employ a number of experimental techniques to obtain Doppler-free signals of lines in the $\tilde{A}^1A_2 \leftarrow \tilde{X}^1A_1$ transition.

In this contribution, the spectroscopic measurements will be presented as well as progress towards state-dependent detection of electrostatically guided formaldehyde molecules.

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We5-20

PRECISION ELECTRONICS FOR PRECISION EXPERIMENTS

S. Stahl and S. Djekic

stahl-electronics, Kellerweg 23, 67582 Mettenheim, Germany

Highly sophisticated and customized electronic components are needed for challenging experiments in ion beam lines and ion traps. Our company has specialized in supplying scientific experimental groups with customized electronics dedicated to their needs.

The product portfolio comprises precise voltage supplies for ion optics and ion trapping, cryogenic assemblies for cryogenic experiments, and consulting service concerning ion trap development. Examples are: a highly sensitive single ion detection system [1] for FT-ICR at SHIPTRAP/GSI Darmstadt, a planar trap structure for Quantum Computing [2] (collaboration of Universities of Mainz, Ulm, Camerino/Italy) and substantial instrumental improvements for g-factor measurements of HCI (highly charged ions) [3] and protons/antiprotons [4], [5] at University of Mainz and FLAIR/HITRAP/GSI Darmstadt.

Outstanding highlights of recent developments are ultra stable multi-channel voltage sources of 10^{-7} short term stability, and low noise $T = 4.2$ K suited GaAs based low temperature electronics for non-destructive detection of single ions (HCI, protons/antiprotons). The latter is meanwhile successfully used by several research groups worldwide .

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We5-21

EVIDENCE FOR LASER-INDUCED RELAXATION IN METASTABILITY EXCHANGE OPTICAL PUMPING OF ^{3}HE

M. Batz[1], W. Heil[1], P.-J. Nacher[2], G. Tastevin[2]

[1] Johannes Gutenberg-Universität, Institut für Physik, Mainz, Germany
[2] Laboratoire Kastler Brossel, Ecole Normale Supérieure, Paris, France
contact : batz@uni-mainz.de

Gaseous ^{3}He can be efficiently spin polarised by metastability exchange (ME) optical pumping (OP), using a rf discharge to excite the ground state atoms into the 2^3S metastable state, and performing OP on the 2^3S-2^3P transition with a 1083 nm laser. Despite recent successful MEOP investigations at high magnetic fields and gas pressures [1,2], the best performances are obtained at a few mT and below 1 mbar with maximum polarisations reaching 90% so far [3,4].
In order to understand current limitations of ^{3}He MEOP, and to gain deeper insight into relaxation mechanisms in ^{3}He plasmas, we perform systematic studies of 2^3S-2^3P$_0$ pumping below 30 mT. The ground state polarisation M is measured optically using an accurate and highly sensitive method that operates at arbitrary magnetic field, based on the comparison of absorption signals simultaneously recorded for two light polarisations of a weak probe laser at 1083 nm [5]. The time evolution of M is monitored as a function of gas pressure (0.65-2.6 mbar), discharge intensity, pumping line, and pumping power (0-5 W). An OP model [5,6] is used to compute the laser-driven populations in 2^3S and 2^3P states, and the corresponding evolution of M under the combined action of OP, ME, and relaxation processes.
Pump absorption and polarisation growth rates measured at M=0 provide accurate relaxation-independent data that are used to test and quantitatively validate the OP model. During polarisation build-up, however, experimental growth rates decrease faster than expected, and systematically lower steady-state polarisations are measured. To account for the observed discrepancies, relaxation rates must be used in the model that exceed those measured in the plasma (when the pump is turned off) by up to two orders in magnitude. The required additional relaxation rates are found to be proportional to the absorbed laser powers.
The actual relaxation rates can be directly inferred from pump absorption measurements in the particular case of C_8 pumping (2^3S, F=1/2 – 2^3P$_0$). For this single-component excitation, the net loss of angular momentum is simply equal to the difference between the deposited one (absorbed power) and the stored one (nuclear polarisation growth). Potential contribution of laser-enhanced relaxation processes, such as radiation trapping or collisions with metastable He_2^* molecules (more likely formed from the excited 2^3P state), will be investigated.

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We5-22

HYPERFINE STRUCTURE OF THE ONE- AND TWO-PHOTON TRANSITION LINES IN HD$^+$

Dimitar Bakalov(a), Vladimir I. Korobov(b), Stephan Schiller(c)

(a)INRNE, Bulgarian Academy of Sciences, 72 Tsarigradsko ch., Sofia 1784, Bulgaria,
e-mail: dbakalov@inrne.bas.bg
(b)BLTP, Joint Institute of Nuclear Research, Dubna 141980, Russia
(c)IEP, Heinrich-Heine University, 40225 Duesseldorf, Germany

High precision laser spectroscopy on ultracold hydrogen molecular ions has recently been proposed, aimed at improving the precision of the level energies and of the electron-to-proton mass ratio, and for tests of time-independence of particle mass ratios. To enable the interpretation of spectroscopic data an accurate knowledge of the spin structure of the transition lines in the lower ro-vibrational states of HD$^+$ with orbital momentum $L \leq 4$ and vibrational quantum number $v \leq 4$ is required. Using the recent results on the hyperfine structure of these states [1], obtained with a Breit-type spin interaction Hamiltonian, we evaluate the one- and two-photon transition rates for transitions between the hyperfine components of the lower ro-vibrational states of HD$^+$.

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From Newton to Casimir and back: fundamental physics using Atomic Beam Spin Echo.

M.F.M. DeKieviet[1]
[1] *Physics Department, Heidelberg University,*
Heidelberg, Germany
E-mail:maarten@physi.uni-heidelberg.de

The quantum mechanical nature of (empty) space has far-reaching consequences in many branches of physics, ranging from (sub-)atomic physics to cosmology. The existence of electromagnetic vacuum fluctuations, for example, manifests itself most impressively in the Casimir force [1], a stochastic and feeble force, so hard to measure properly, that it was considered to be solely of academic interest for a long time. With the current revolution in nano-technology, however, there is a rising, yet even economic need for a quantitative understanding. I will present an experiment, in which the Casimir-Polder force between a *single* atom and the surface of a solid is determined quantitatively to better than the 1% level. It is based on the Atomic Beam Spin Echo method developed in Heidelberg [2], an atom interferometry method, in which we combine the exclusive surface sensitivity of thermal atom scattering with the resolution of in-beam magnetic resonance techniques. This technique will be introduced and its high resolving power (down to sub-neV) shown in some simple scattering experiments. Subsequently, I will turn to the phenomenon of quantum reflection and show how it may depend very sensitively on the long-range details of some *attractive* atom-surface interaction. Utilizing quantum reflection as a tool, we have been able to clearly identify the Casimir and the van der Waals branches for a variety of surfaces [3]. Finally, the potential of Atomic Beam Spin Echo is addressed in particular with respect to testing fundamental questions in physics concerning the Casimir force and beyond. I will show on-going measurements focussing on the dependency of the working of the vacuum fluctuations on temperature, geometry and spectral properties of the solid. For example, our data show the Casimir interaction can be significantly altered by heating the surface, or by using specifically nano-crafted ones. As an outlook, I will describe two possible experiments that may have the sensitivity for detecting parity violation in light atoms, respectively for testing gravity beyond Newton's law.

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We5-24

A Ca^+ SINGLE ION FOR FREQUENCY METROLOGY IN THE OPTICAL RANGE

C. Zumsteg, C. Champenois, G. Hagel, M. Houssin, M. Knoop, M. Vedel and F. Vedel

PIIM UMR6663 Université de Provence-CNRS
Centre de Saint Jérome, Case C21, 13 397 Marseille Cedex 20, France
fern@up.univ-mrs.fr

Among the atom candidates for an optical frequency standard, a single Ca^+ ion is extremely attractive. The electric quadrupole transition at 729 nm proposed as frequency reference (clock transition) has a natural linewidth below 200 mHz corresponding to a quality factor of 2×10^{15}; the wavelengths of the required lasers all lie in the visible domain. A single Ca^+ ion, cooled in a miniature radiofrequency trap and confined in the Lamb-Dicke regime, is an almost perfectly isolated atomic system suited for long interrogation times. The main contribution to the systematic uncertainty of this frequency standard, at the 9×10^{-16} level, is the Stark effect due to black body radiation at room temperature, provided the quadrupole shift is cancelled out. Stability is limited by the quantum projection noise and is expected to reach $2.5\times10^{-15} / \sqrt{\tau}$.[1] The Ca^+ ion is expected to outperform the best microwave atomic frequency references, and to be competitive with other atomic optical frequency references.

Probing of the clock transition of a single ion is carried out using quantum jump statistics which requires interrogation times of several seconds to avoid power broadening. The line width of the probe laser (local oscillator) should reach the hertz level for a duration at least as long as the interrogation time to take full advantage of the quality factor of the clock transition. Our local oscillator is a lab-built titanium-sapphire laser pumped with 5 W of laser radiation at 532 nm, stabilised onto an invar reference cavity. Measurement by an auto-correlation technique yields a linewidth below kHz with a resolution limited by the length of our optical fibre (10 km). Absolute stabilisation of the clock laser on an ultra-stable high-finesse ULE cavity is under way.

To record the clock signal, the discrete Doppler frequency profile must be reduced to only few bands. To this purpose, the ion should be localized to better than 120 nm (Lamb-Dicke regime) by laser cooling and optimization of the trapping field.

The ultra-narrow quadrupole transition, combined with the two cooling lasers, can also be used to create three-photon coherent population trapping in a dark state[2]. This provides a robust method to create a coherent superposition of the two metastable states. The dark line can be employed for frequency metrology thanks to the (first order) Doppler-free geometry of the laser beams.

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JONES EFFECT ON ATOMS WITH DOUBLET STRUCTURE OF LEVELS

V.V. Chernushkin, P.V. Mironova and V.D. Ovsiannikov
Department of Physics, Voronezh State University, Voronezh, Russia
E-mail: albert@phys.vsu.ru

Magnetoelectric birefringence, which was predicted by Jones [1] and first observed in liquids [2], may also become a useful tool for the high-precision spectroscopy of atomic systems [3]. In the case of resonance with an excited D-level, the dipole-forbidden bilinear Jones effect on a medium of free atoms in their ground S-states may become significantly stronger than the dipole-allowed Kerr and Cotton-Mouton effects [4], quadratic respectively in electric and in magnetic field. In this paper we present an account for the influence on the Jones amplitude of the resonant-level fine structure.

The Jones effect is determined by the bilinear in the static fields amplitude of the Rayleigh scattering of a monochromatic wave, which for the frequency $\omega = E_{nD_J} - E_{nS_{1/2}} - \varepsilon_J$ in resonance ($|\varepsilon_J| \ll \omega$) with the D-level doublet substates of the total momentum $J = 3/2, 5/2$, may be written as (taking into account only the terms with the second-order resonance singularities)

$$U = AQ\left(\frac{7}{(\varepsilon_{3/2})^2} + \frac{47}{(\varepsilon_{5/2})^2} - \frac{4}{\varepsilon_{3/2}\varepsilon_{5/2}}\right)[\varphi_0 + \varphi_1], \tag{1}$$

where the constant factor $A = F^2F_0B/1500$ is proportional to the product of the square laser field F^2, static electric field F_0 and magnetic field B. For atoms with the singlet structure of levels, the resonance detuning $\varepsilon_{5/2} = \varepsilon_{3/2} \equiv \varepsilon$ and the double-resonance fractions in parentheses combine into $50/\varepsilon^2$ [4]. The polarization-dependent factors are

$$\varphi_0 = (\mathbf{e}_0 \cdot [\mathbf{n} \times \mathbf{e}_B]); \qquad \varphi_1 = \mathrm{Re}\{(\mathbf{e}_0 \cdot \mathbf{e})\,(\mathbf{e}^* \cdot [\mathbf{n} \times \mathbf{e}_B])\},$$

where $\mathbf{e}_B$ and $\mathbf{e}_0$ are the unit vectors of the magnetic and electric fields, $\mathbf{e}$ and $\mathbf{n}$ are the unit polarization and wave vectors of the laser wave. In addition to birefringence, the imaginary part of the detuning $\varepsilon_J = \Delta_J + i\Gamma_J/2$, which equals to the resonance level width Γ_J, may cause the dichroism effects. The factor Q is a product of the radial matrix elements for the first-order quadrupole and second-order dipole radiation transition between the ground $nS_{1/2}$ and resonance $n'D_J$.

The Jones birefringence appears, when $\mathbf{e}_0 = \mathbf{e}_B$, being directly proportional to the difference $\Delta U^{(J)} = U^{(+)} - U^{(-)}$ between the amplitude (1) for $\mathbf{e} = \mathbf{e}^{(+)}$ and $\mathbf{e} = \mathbf{e}^{(-)}$, where $\mathbf{e}^{(\pm)} = (\mathbf{e}_0 \pm [\mathbf{n} \times \mathbf{e}_0])/\sqrt{2}$ [4].

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High-accuracy mass and *g*-factor measurements on highly-charged ions in Penning traps*

K. Blaum[1,2], J. Alonso[1,2], I. Bergström[3], T. Fritioff[3], H.-J. Kluge[2], Sz. Nagy[1],
W. Quint[2], B. Schabinger[1], R. Schuch[3], A. Solders[3], M. Suhonen[3], G. Werth[1]

[1] Physics Department, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany
[2] GSI Darmstadt, Planckstr. 1, 64291 Darmstadt, Germany
[3] Atomic Physics, AlbaNova, Stockholm University, 10691 Stockholm, Sweden

Highly-charged ions (HCI) confined in Penning traps allow for high-accuracy mass measurements, as well as for the determination, via a measurement of the Larmor and the cyclotron frequencies of a single stored ion, of the *g*-factor of the bound electron in hydrogen-like and lithium-like ions. This is demonstrated by the performance of the Penning trap mass spectrometer SMILETRAP in Stockholm, and the *g*-factor experiment Mainz, respectively [1-3]. Accurate mass values contribute, among other things, to astrophysics, to metrology, and to tests of quantum-electrodynamics. *g*-factor measurements on $^{12}C^{5+}$ and $^{16}O^{7+}$ allowed to extract a new value for the mass of the electron m_e with a four-fold improved accuracy. Presently, a *g*-factor experiment on $^{40,48}Ca^{17+,19+}$ is under preparation order to perform stringent tests of bound-state quantum-electrodynamics, to check for isotope shifts and to test the multielectronic models used by theoreticians.

Efficient storage, cooling, and detection of HCI in ion traps are prerequisites for such high-accuracy experiments in which down to a single stored particle can be observed. The contribution summarizes recent results and technical developments from Stockholm and Mainz and reports on possible mass and *g*-factor measurements at the Highly-charged Ion TRAP (HITRAP) project, which is presently being built up at GSI Darmstadt to perform a number of unique experiments with very heavy, stable or radioactive ions up to hydrogen-like U^{91+}.

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We5-27

ATOM INTERFEROMETRY EXPERIMENTS WITH LITHIUM

M. Jacquey, A. Miffre (a), M. Büchner, G. Trénec and J. Vigué
Laboratoire Collisions, Agrégats, Réactivité, IRSAMC
UMR 5589 CNRS - Université Paul Sabatier Toulouse 3
118 Route de Narbonne ; 31062 Toulouse cedex, France
(a) LASIM, Université Claude Bernard Lyon I and CNRS UMR 5579
10, Rue A.M. Ampère; 69622 Villeurbanne Cedex, France

We have built a Mach-Zehnder atom interferometer [1]: a supersonic beam of lithium seeded in argon produces a lithium wave with a 1065 m/s mean velocity, corresponding to a54 pm de Broglie wavelength. Atom diffraction on laser standing waves serves as mirrors and beam-splitters. The distance between consecutive standing wave is about 600 mm, so that the maximum distance between the two atomic beams is close to 100 μm. Thanks to a strong collimation, this distance is sufficient to separate the two beams by a "septum", as shown in figure 1. In this way, a perturbation can be applied on only one of the two interfering atomic beams and the interference signals probe the effects of the perturbation.

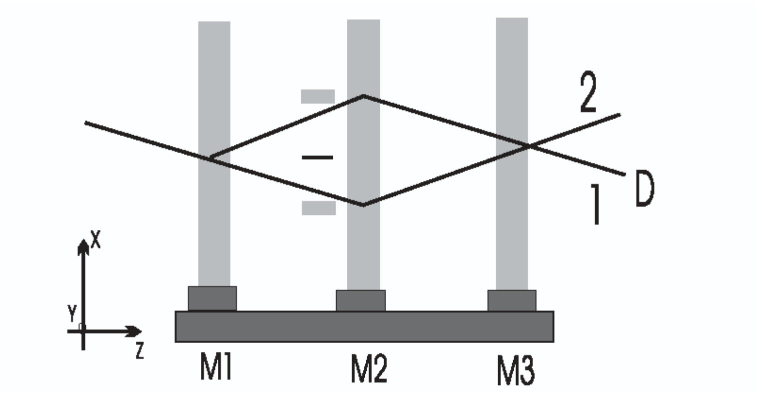

Figure 1: schematic drawing of our Mach-Zehnder atom interferometer.

We have made two such experiments which will be described in the poster:

- we have applied an electric field on one of the two interfering beams [2,3] and we have thus measured the static electric polarizability of ^{7}Li with an improved accuracy, $\alpha = (24.33 \pm 0.16)\times 10^{-30}$ m^3=164.2 ± 1.1 a.u. This result is in excellent agreement with the most accurate calculations.
- we have introduced a low density gas and measured the index of refraction of this gas for lithium atomic waves as a function of the lithium mean velocity and of the gas density [4]. The refraction index clearly exhibits glory oscillations, as predicted by theory.

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POSTERS

Thursday 10/5

1. Atomic and Molecular Astrophysics

Th1-1

RELATIVISTIC CORRECTION TO LYMAN AND WERNER BAND SYSTEMS OF HYDROGEN MOLECULE

E.A.Pazyuk[1], A.N.Drozdova[1], V.V.Meshkov[1], A.V.Stolyarov[1], M. Tamanis[2]

[1]Department of Chemistry, Moscow State University, Leninskie gory 1/3, 119992, GSP-2, Moscow, Russia
[2]Department of Physics, University of Latvia, Rainis Blvd. 19, Riga LV-1586, Latvia

Superstring theories predict a time dependent of the electron-proton mass ratio $\gamma= m_e/m_p$ and fine structure constant $\alpha=e^2/\hbar c$. A possible cosmological variation of the dimensionless γ and α values could be discovered by means of the wavelengths difference of nowadays laboratory spectra λ^{lab} for the Werner $X^1\Sigma^+_g \rightarrow C^1\Pi_u$ and Lyman $X^1\Sigma^+_g \rightarrow B^1\Sigma^+_u$ band systems of hydrogen molecular and the absorption spectra of quasars λ^{obs} with a large redshift [1,2].

We have performed extensive *ab initio* calculation of the wavenumbers and transition probabilities for rotationally resolved $X \rightarrow C,B$ spectrum of H_2 in the framework of non-adiabatic approximation based on highly accurate Born-Oppenheimer potential curves, adiabatic correction functions [3] as well as radial, angular and electronic coupling matrix elements [4]. Relativistic corrections to the states treated were estimated within the Cowan-Griffin approach by computing expectation values of the mass-velocity and 1-electron Darwin integrals. The rigorous close-coupling approach was used to approximate the strong local perturbation effect between the low-lying $(1\text{-}6)^1\Sigma_u^+$ and $(1\text{-}4)^1\Pi_u$ states. The weak regular intramolecular interactions with the rest higher excited bound and embedding continuum Rydberg's states were accounted by using of the analytical quantum-defect theory [5].

The work was supported by the Russian Foundation for Basic Researches (grants 06-03-32330).

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Th1-2

TRANSITION FREQUENCY SHIFTS WITH FINE STRUCTURE CONSTANT VARIATION FOR Fe II

K. V. Koshelev[1,2], S. G. Porsev[1], I. I. Tupitsyn[3],
M. G. Kozlov[1], D. Reimers[2], and S. A. Levshakov[4]

[1] Petersburg Nuclear Physics Institute, Gatchina, Russia
[2] Hamburger Sternwarte, Universität Hamburg, Hamburg, Germany
[3] St.Petersburg State University, Petrodvorets, Russia
[4] Ioffe Physico-Technical Institute, St. Petersburg, Russia

Recently discovered acceleration of the universe is usually regarded as evidence for the existence of dark energy. Cosmological evolution of the dark energy may cause variations in coupling constants, such as the fine-structure constant α. Different models predict different behavior of the coupling constants and it is extremely important to measure α at different redshifts. Because of the relativistic effects in atoms their transition frequencies depend on αZ, where Z is atomic number. Therefore, one can study space-time variation of α by comparing atomic frequencies for distant objects in the universe with their laboratory values. To do that one needs to calculate the so called q-factors for the atomic transitions which are defined as follows:

$$\omega = \omega_{\mathrm{lab}} + qx, \quad x \equiv (\alpha/\alpha_{\mathrm{lab}})^2 - 1\,.$$

Generally q-factors scale with atomic number as Z^2. That allows to look for α-variation by comparing transition frequencies of heavy and light ions. However, this method is subjected to different systematic effects and one need to do large scale averaging over many lines of different ions from different objects to eliminate systematic errors. That is why it is particularly interesting to find atoms, where q-factors for different transitions have different signs. In Ref. [1] it was shown, that the line 1608 Å in Fe ɪɪ has large negative q-factor, while other observed lines have positive q-factors. This fact was used in [2,3] to suggest the single-ion method, which is less sensitive to systematics and allows to measure α for a given astrophysical object.

Here we report new calculations of the q-factors for Fe ɪɪ with more accurate account for relativistic effects and electronic correlations. We found, that Breit corrections to q-factors are smaller than correlation corrections.

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Th1-3

THE FERRUM-PROJECT: EXPERIMENTAL AND THEORETICAL TRANSITION RATES OF FORBIDDEN [ScII] LINES AND RADIATIVE LIFETIMES OF METASTABLE ScII LEVELS

Hartman H.[1], Gurell J.[2], Lundin P.[2], Schef P.[2],Hibbert A.[3], Lundberg H.[4],
Mannervik S.[2], Norlin L-O.[5] and Royen P.[2]

[1]Lund Observatory, Lund University, Box 43, SE-221 00 Lund, Sweden
[2]Department of Physics, Stockholm University, AlbaNova University Center,
SE-106 91, Stockholm, Sweden
[3]Department of Applied Mathematics and Theoretical Physics, The Queen´s
University of Belfast, Belfast BT7 1NN, Northern Ireland
[4]Department of Physics, Lund Institute of Technology, Box 118, SE-221 00, Lund,
Sweden
[5]Physics Department, Royal Institute of Technology, AlbaNova University Center,
SE-106 91, Stockholm, Sweden

In many plasmas, long lived metastable levels are primarily depopulated by collisions. In low-density regions, however, radiative decays through forbidden transition channels will be more important and can be observed. If the atomic transition data is known, these lines are indicators of physical plasma conditions and can be used for abundance determination [1]. Transition probabilities can be derived by combining relative intensities between the decay channels, so called branching fractions (BFs), and the radiative lifetime of the common upper level [2]. We use this approach for forbidden [ScII] lines along with new calculations.

Neither BFs for forbidden lines nor lifetimes for metastable levels are easily measured in the laboratory. Therefore, astrophysical BFs measured in Space Telescope Imaging (STIS) spectra of the strontium filament of Eta Carinae are combined with lifetime measurements using a laser probing technique [3-4] on a stored ion beam at the CRYRING facility in Stockholm, Sweden. These lifetimes are used to derive the absolute transition probabilities (A-values). New theoretical transition probabilities and lifetimes are calculated using the CIV3 code.

We report experimental lifetimes for the ScII levels $3d^2\ {}^3P_{0,1,2}$ with lifetimes 1.28, 1.42 and 1.15 s respectively and transition probabilities for lines from these levels down to the ground state $3d4s\ a^3D$. New calculations for these forbidden [ScII] lines and metastable lifetimes are also presented.

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Th1-4

INFRARED EMISSION SPECTRUM OF INTERSTELLAR MOLECULAR HYDROGEN FORMED ON THE SURFACE OF DUST

Junko Takahashi

Meiji Gakuin University, 1518 Kamikurata, Totsuka, Yokohama 244-8539, Japan
E-mail: juntaka@law.meijigakuin.ac.jp

It is thought that H_2 should be mainly formed by the recombination of two H atoms on the surface of dust grains in interstellar space. The energy distribution of the product H_2 were investigated theoretically and experimentally [1,2,3]. It was found that H_2 should be highly vibrationally and rotationally excited in the ground electronic state via the formation pumping mechanism. It means that the H-H bond energy should be redistributed into the vibrational, rotational, and translational energies of the product H_2 and the energy absorbed by dust through the H-surface interaction. The formation pumping to the rovibrationally excited levels in the ground electronic state should be followed by the spontaneous radiative cascade transitions to the lower rovibrational energy levels.

In the present work, we investigated the pure effects of the formation pumping in the infrared emission spectrum of interstellar H_2. We built up our formation pumping models for H_2 newly formed on icy mantles, carbonaceous dust, and silicate dust [4]. Then, we calculated the infrared emission spectra of interstellar H_2 with our formation pumping models. We solved the master equations including the spontaneous rovibrational transitions, the formation and UV pumpings, and the photodissociation process. We considered the cold interior of an interstellar cloud under a weak ultraviolet (UV) radiation field at the early stage evolving from an atomic cloud to a molecular one, where it is dominated by the H_2 formation process on the surface of dust grains. The uniform density and the gas temperature were taken to be 10^3 cm^{-3} and 10 K, respectively.

It was found that the resulting infrared H_2 emission spectra dominated by the formation pumping could be discriminated from those dominated by the UV pumping and that it could depend on the property of the dust. It was also found that the fluxes of the most intense emission lines arising from the formation pumping should be strong enough to be detectable. This suggests that the infrared emission spectrum of H_2 might be detectable even in the interstellar regions without a source of UV pumping or dynamical excitation [5]. Moreover, the infrared H_2 emission arising from the formation pumping could be a new probe that shows us the spot where an interstellar cloud is evolving from an atomic to a molecular one.

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Th1-5

COLLISIONAL EXCITATION OF AMMONIA BY HELIUM AND MOLECULAR HYDROGEN IN SPACE

E. Scifoni, P. Valiron, A. Faure, C. Rist

Laboratoire d'Astrophysique de Grenoble, University Joseph Fourier, Grenoble, France

From its first detection in the interstellar medium, in 1968 [1], as a first polyatomic molecule, ammonia has been the object of many studies through both theoretical [2] and experimental [3] means. In fact, its large abundance there (also in a rich variety of isotopical forms), its inversion-splitting occurrence in the range of 1 cm^{-1} and its typical collisions-dominated population of levels, as a symmetric top molecule, have made it a very good probe of various temperatures and gas densities.

Collisions with hydrogen molecules are of particular interest since H_2 is the most abundant colliding partner in the dense interstellar medium. However, for simplicity, most of the studies were carried on NH_3 interacting with atomic helium, because the excitation effect of this atom, in the temperature range of interest, was assumed very similar to the para-H_2 one [2]; while only a few works directly explored the NH_3–H_2 system. Futhermore, the inversion motion of the ammonia in the collision was never taken explicitely in account, except in a study involving Argon as the colliding partner [4], where only small effects of that on the results were found.

After more than 30 years however a persistent disagreement between the theoretical works and some double resonance experiments [3] is still object of debate while a full dimensional study has never been performed on the latter system.

In the present work we analyze the dependence of the expansion coefficients of the potential both for a recent PES of NH_3-He [5] and for a new NH_3–H_2 one computed by one of us, with respect to the inversion coordinate, and their coupling matrix elements with the vibrational states. In both cases we discuss the importance of a detailed treatment of the movement with respect to the delta function approssimation used by [2].

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Th1-6

RECENT ADVANCES IN CALCULATING COLLISIONAL RATES FOR ASTROPHYSICS

Faure A.[1], Valiron P.[1], Wiesenfeld L.[1], Tennyson J.[2], Dubernet M.L.[3],
Kokoouline V.[4], Greene, C. H.[5]

[1]Laboratoire d'Astrophysique, UMR 5571 CNRS, Université Joseph Fourier, BP 53,
38041 Grenoble Cedex 09, France
[2]Department of Physics & Astronomy, University College London, Gower Street,
London WC1 E6BT, UK
[3]Observatoire de Paris-Meudon, UMR 8112 CNRS, 5 place Jules Janssen, 92195
Meudon Cedex, France
[4]Department of Physics, University of Central Florida, Orlando, FL 32816, USA
[5]Department of Physics & JILA, University of Colorado, Boulder, CO 80309-0440,
USA

E-mail: afaure@obs.ujf-grenoble.fr

Collisional rate coefficients are essential for modelling energy exchange processes responsible for thermal balance and molecular line formation in astronomical environments. Despite some recent progress in laboratory measurements of state-to-state rates, astrophysical models still rely heavily on theoretical estimates owing to the wide range of temperatures and transitions needed. We will present recent rate coefficient calculations for the rotational (de)excitation of astronomically important molecules colliding with both neutrals (He and H_2) and electrons. The influence of inaccuracies in the interaction potentials will be illustrated in the case of H_2O+H_2 [1, 2]. The precision of the quasi-classical trajectory (QCT) method will be discussed by comparison with full quantum close-coupling calculations for H_2O+H_2 [3] and HC_3N+H_2 [4]. The importance of closed-channel effects near rotational thresholds will be analyzed in the case of electron-H_3^+ collisions [5]. Astrophysical applications of the calculated rates will be finally presented.

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Th1-7

THEORETICAL STUDY OF STARK WIDTH AND SHIFT PARAMETERS OF Pb III TRANSITIONS

C. Colón[1], A. Alonso-Medina[1], F. Fernández[2], C. Rivero[3], A. Zanón[4],
J. Madueño[2] and J. Albeniz[2]

[1]Dpto. Física Aplicada, EUIT.Industrial, Universidad Politécnica de Madrid (UPM), Madrid, Spain
[2]Dpto.Química Industrial y Polímeros, EUIT. Industrial (UPM), Madrid, Spain
[3]Dpto. de Tecnologias Especiales, ETSI. Telecomunicación(UPM), Madrid, Spain
[4]Dpto.Matemática Aplicada, EUIT. Industrial (UPM), Madrid, Spain
e-mail. cristobal.colon@upm aurelia.alonso@upm.es

Data on atomic properties are relevant not only to spectroscopy, these values are also of interest in a variety of other fields in physics and technology. Measurements of Stark-broadening parameters provide means for diagnosis laboratory and astrophysical plasmas. Stark broadening data for a large number of transitions in many atomic and ionic spectra are needed for the modelling of stellar plasma, the investigation of its physical properties and abundance determinations. When calculating opacities of large-scale plasmas of stellar atmospheres, the Stark-broadened line profiles of resonance transitions are of the utmost importance because they give a relatively large contribution to radiative energy transport. In order to provide astrophysicists with the relevant data needed for the theoretical modelling of stellar spectra and stellar atmospheres, we made an effort to determine the relevant Stark broadening parameters with the semi-classical formalism of Pb III.

In this work we present theoretical calculated Stark widths for 54 lines arising for $6s^2$-6snp, 6sns-6snp and 6snd-6snp lines of Pb III.

The data have been obtained using Griem´s semiclassical calculations. Stark widths are presented as functions of temperature for an electron density of 10^{17} cm^{-3}.

The atomic matrix elements were obtained using relativistic Hartree-Fock calculations and configuration interaction in an intermediate coupling (IC) scheme. The Cowan code was selected for this purpose.

To provide level energies for our calculations, the table of Moore has been used. The relatively good agreement between experimental transition probabilities and our theoretical results obtained with this method shows that our IC mixing accounts the correlation effects. We use the effective Gaunt factors proposed by Niemann et al.

The theoretical values obtained in this work are compared with the experimental ones recently published by Alonso-Medina and C. Colón. The calculated values are in good agreement with the experimental data. We have studied the dependence of the Stark width on principal quantum number for several series.

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Th1-8

ELECTRON-ION RECOMBINATION FOR ASTROPHYSICS

I.Orban[1], Z. Altun[2], S. Böhm[1], P.Glans[3], E. Lindroth[1], and R. Schuch[1]

[1] Atomic Physics, Fysikum, AlbaNova Physics Centre, S-106 91 Stockholm, Sweden
[2] Dept of Physics, Marmara University, Turkey,
[3] Dept. of Engineering, Physics and Mathematics, Mid Sweden University, Sweden

Silicon is among the most abundant elements in the Universe and recombination plays an essential role in the energy balance and diagnostics of astrophysical plasma. However, very few experimental data exist for Si. Therefore, we measured the recombination spectra of Na-like Si, using the CRYRING heavy ion storage ring at the Manne Siegbahn Laboratory in Stockholm and for H-like, He-like, Li-like, and Be-like Si with the new Electron Beam Ion Trap (EBIT) facility at AlbaNova, Stockholm University. In the storage ring experiment [1], the recombined Si^{2+} ions were detected after the first dipole magnet following the electron cooler. The collision energy between electrons and stored ions was changed over the centre-of-mass energy range of 0-20 eV, this covered the Dielectronic Recombination (DR) resonances up to the limit of the $Si^{3+}(3s) + e^- \rightarrow Si^{2+}(3dnl)$ series. Transition energies, calculated using the Rydberg formula, are presented in figure 1 by vertical bars. Details of resonances, calculated by Many Body Perturbation Theory (MBPT) [2] are shown by the solid line. For the high-n DR resonances, results of an AUTOSTRUCTURE [3] calculation were used. Calculations for Na like systems are extremely complex and large discrepancies with certain approaches, but also with hitherto tabulated values were found [4].

In the EBIT experiment, the recombination was measured by detecting X rays, tagged with the electron-beam energy. The electron-ion centre-of-mass energy was scanned in a range of 1.2 – 2.9 keV which covered the dielectronic recombination resonances with K shell electron excitation.

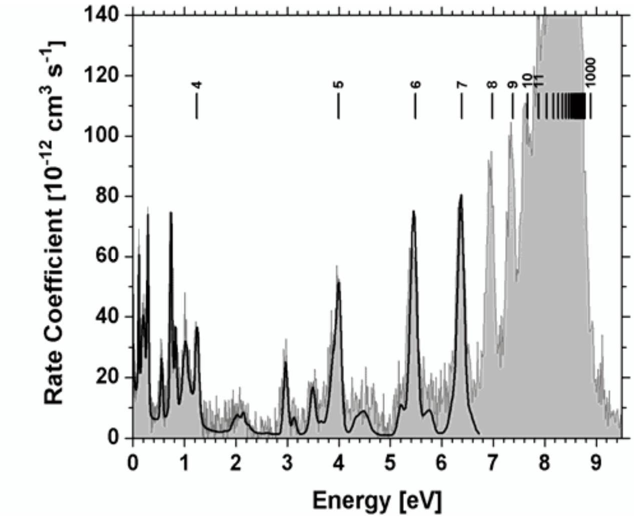

Fig. 1. Experimentally derived recombination rate coefficients for Si^{3+} (shaded area) and the MBPT results (solid curve).

At the conference, absolute recombination rate coefficients will be compared with different theoretical calculations for a conclusive test. The temperature dependent rate coefficients will be presented and compared to several theoretical models.

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POSTERS

Thursday 10/5

2. Atomic and Molecular Spectroscopy

Th2-1

VUV SPECTROSCOPY AND PHOTOPHYSICS OF ACETONITRILE

Sydney Leach[1], Martin Schwell[2], Hans-Werner Jochims[3], Helmut Baumgärtel[3]

[1]LERMA, Observatoire de Paris-Meudon, 92195 Meudon, France
[2]LISA, Universités Paris 7 & 12, 61 Avenue du Géneral de Gaulle, 94010 Créteil, France
[3]Institut für Physikalische und Theoretische Chemie der Freien Universität Berlin, Takustr.3, 14195 Berlin, Germany

Acetonitrile, CH_3CN, is one of the possible building blocks of biomolecules. It has been observed by radioastronomy in several sites of the interstellar medium, in comets, (its release on the Deep Impact encounter with comet 9P/Tempel 1, has been suggested by I.R. emission spectroscopy), and in the atmosphere of Titan. Acetonitrile has also been detected in the Earth's stratosphere and troposphere. The VUV spectroscopy and photophysics of acetonitrile, which inform on the possibilities of photodestruction and photoionization processes, are thus of direct interest for radioastronomy or infrared searches of CH_3CN in protected astrophysical sites, as well as for exobiology and atmospheric studies of the Earth and other Solar system objects.

In the present work we carried out the following measurements on acetonitrile, using monochromatised synchrotron radiation as the photon excitation source: 1) the absorption spectrum between 6 and 20 eV, which allowed us to reinterpret, or assign for the first time, a number of valence and Rydberg transition bands and to establish the absorption cross sections over the spectral range studied ; 2) the dispersed fluorescence spectra between 250 and 700 nm excited at various photon excitation energies between 10 and 16 eV ; 3) fluorescence excitation (FEX) spectra for emission bands of CN (B-X) and (A-X) transitions and, for the first time, of CH (A-X), over the photon excitation range 8-20 eV; 4) the photoionization quantum yield between 11 and 22 eV, never previously measured for acetonitrile. The observations are discussed in terms of specific photodissociation and photoionization processes. The results provide information on the photodissociation rates of acetonitrile by solar flux and interstellar radiation, as well as on the lifetimes of acetonitrile in planetary atmospheres. Comparison of photodissociation rates with rates of chemical reactions destroying acetonitrile in the Earth's and other planetary atmospheres as well as in other astrophysical sites will be discussed. The information provided by the photoionization quantum yields as a function of excitation energy is shown to be of potential use in cosmochemical modelling.

Th2-2

High resolution LIF spectroscopy of the NaCs B(1)$^1\Pi$ state and construction of the potential energy curve

J.Zaharova[1], O.Docenko[1], M. Tamanis[1], R.Ferber[1], A.Pashov[2], H.Knöckel[3] and E.Tiemann[3]

[1] Department of Physics and Institute of Atomic Physics and Spectroscopy, University of Latvia, Rainis Boulevard 19, LV-1586 Riga, Latvia
[2] Sofia University, Department of Physics, 5 James Bourchier Boulevard, 1164 Sofia, Bulgaria
[3] Institut für Quantenoptik, Universität Hannover, Welfengarten 1, 30167 Hannover, Germany
E-mail: tamanis@latnet.lv

The NaCs molecule is one of the prospective objects for the production of ultracold polar molecules. A number of electronic states of NaCs has been studied recently by Fourier transform spectroscopy [1, 2]. In the present report we will focus on the B(1)$^1\Pi$ state. This state can be exploited in a production of cold alkali molecules in the a$^3\Sigma^+$ state through photoassociation via the 3s+5p atomic asymptote, and this state is considered in proposed schemes for efficiently transforming cold a$^3\Sigma^+$ state molecules into the X$^1\Sigma^+$ (v = 0) level via coupled B(1)$^1\Pi$~c(2)$^3\Sigma^+$~ b$^3\Pi$ excited states [3].

Rich spectroscopic information about the B$^1\Pi$ state was obtained during the study of the first triplet state a$^3\Sigma^+$ of the NaCs molecule [2] when the laser induced fluorescence (LIF) from the B$^1\Pi$ state to the a$^3\Sigma^+$ and the X$^1\Sigma^+$ states was recorded by a high resolution Fourier transform spectrometer . Here we present the B$^1\Pi$ state analysis which is based on these data.

NaCs was formed in a heat pipe oven. The B$^1\Pi \rightarrow$ X$^1\Sigma^+$ LIF was induced by a single-mode CR-599 dye laser (DCM dye). LIF spectra were recorded by a Fourier transform spectrometer (Bruker IFS-120 HR) with a typical resolution of 0.015 – 0.03 cm^{-1} [2]. Due to the presence of argon buffer gas in the heat pipe we were able to observe rich rotational relaxation spectra. This allowed us to enlarge the data set for the B$^1\Pi$ state significantly and to obtain information about Λ-splitting in the B$^1\Pi$ state and numerous local perturbations. The vibrational levels of strong perturbation regions giving fluorescence to a$^3\Sigma^+$ state were excluded from the analysis. The data field of the levels included in the final fit consists of 492 levels with vibrational quantum number from v'=0 to 7 and of 42 levels with v' = 9 – 25.The range of rotational quantum numbers was from J'=5 to 168. Direct fit of a pointwise potential energy curve to the level energies is realized using the inverted perturbation approach [4]. The obtained empirical potential reproduces the level energies included in the fit for v'= 0 – 7 with experimental accuracy stated as about 0.02 cm^{-1}, and the deviations of the other levels , with a few exceptions, do not exceed the 1cm^{-1}.

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Th2-3

COMPUTATION OF THE MOLECULAR FINE STRUCTURE OF DIPOLAR ALKALI MOLECULES

Johannes Deiglmayr[1], Mireille Aymar[2], Olivier Dulieu[2] and Fernand Spiegelman[3]

[1] Physikalisches Institut, Albert-Ludwig-Universität Freiburg,
79104 Freiburg im Breisgau

[2] Laboratoire Aimé Cotton, CNRS, bât.505, Campus d'Orsay,
91405 Orsay Cedex, France

[3] Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Paul Sabatier,
Bât. 3R1B4 - 118, route de Narbonne, 31062 Toulouse Cedex 4, France

Recently the production of ultracold heteronuclear molecules in their electronic ground state either via photoassociation [1] or Feshbach resonances [2] has been achieved. Such heteronuclear molecules, if deeply bound, have a significant permanent electric dipole moment leading to strong, long-range, and alignment dependent intermolecular forces, which offer control by external electromagnetic fields.

We have calculated the *R*-dependent polarizabilities for all heteronuclear dimers in the ground state using a quantum chemistry method based on pseudopotentials for the core representation and effective core polarization potentials, as described in ref. [3].

We also follow a new approach to include spin-orbit coupling in our calculations of molecular potentials: starting from adiabatic potential curves resulting from a full configuration interaction, a diabatization procedure is used to introduce the spin-orbit operator in suitable representation. First results will be shown for Cs_2 and other Cs heteronuclear compounds.

These new insights will be used to find efficient routes to produce and stabilize polar molecules, to model the dynamics of a dipolar gas in an optical dipole trap and to explore external field dependent scattering properties.

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HIGH RESOLUTION FOURIER TRANSFORM SPECTROSCOPY OF ATOMIC NIOBIUM

Ipek K. Öztürk[1], Alev Er[1], Gönül Başar[1], Günay Başar[2], Sophie Kröger[3]

[1]Istanbul University, Faculty of Science, Physics Department,
34118 Vezneciler, Istanbul, Turkey
e mail:ikanat@istanbul.edu.tr
[2]Technical University of Istanbul, Faculty of Science and Letters,
Physics Engineering Department, 34469 Maslak, Istanbul, Turkey
[3]Technische Universität Berlin, Institut für Atomare und Analytische Physik,
Hardenbergstr.36, 10623 Berlin, Germany

[4]Andrey Jarmola, [4]Maris Tamanis, and [4]Ruvin Ferber

[4]Department of Physics and Institute of Atomic Physics and Spectroscopy,
University of Latvia, Rainis Blvd. 19, Riga LV-1586, Latvia

In recent years the fine and hyperfine structure of atomic Niobium has been the subject of several experimental and theoretical investigations (see [1] and references therein). On the experimental side, all recent work has been performed using laser spectroscopic methods, which are restricted in the wavelength range accessible to the lasers currently in use. Recently, the spectrum of Nb is recorded in the wavelength region from 330 nm to 800 nm with a high resolution Bruker IFS 125HR Fourier transform spectrometer in Riga lab with resolution 0.02 cm^{-1} from a hollow cathode discharge. These data enable us to determine many magnetic dipole hyperfine constants, which had been unknown up to now.

Here, results are presented for the lines in the wavelength region from 400 nm to 430 nm connecting the $4d^4(^5D)5s\ ^6D$ ground state term with levels of the two terms $4d^4(^5D)5p\ ^6F$ and $4d^4(^5D)5p\ ^6P$. The hyperfine constants A of the upper levels are extracted from the complex line profiles with a least-squares-fit precedure assuming a Doppler profile and using the hyperfine constants of the lower levels, which have been previously measured with high precision [2]. With only one exception, all A constants can be validated by several lines originating from the same upper level.

Riga team acknowledges support from ERAF grant No. VPD1/ERAF/CFLA/05/APK/2.5.1. /000035/018 and LZP grant No. 04.1308. A.J. is grateful for support from ESF grant.

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Th2-5

High resolution ultra-violet absorption cross sections of sulphur dioxide at 200K

D. Blackie (1), R. Blackwell-Whitehead (1), G. Stark (2), J.C. Pickering (1), J. Rufus (1), A. Thorne (1), P.L. Smith (3),

(1) Imperial College London, UK
(2) Wellesley College, USA
(3) Harvard-Smithsonian Center for Astrophysics, USA,
Douglas.Blackie01@ic.ac.uk

Sulphur Dioxide plays an important role within the complex chemistry of both the upper atmosphere of Venus and the volcanically active Jovian moon Io. The lack of high resolution laboratory studies has prevented the full, accurate determination of absorption cross sections which are the basis for reliable photochemical models.

High resolution laboratory measurements of SO_2 absorption cross sections are essential to resolve the complex and congested SO_2 spectrum. However, using the Imperial College UV Fourier Transform Spectrometer new high resolution ($\lambda/\delta\lambda \sim 450{,}000$) measurements have been recorded over a range of temperatures and pressures.

As part of an on-going series of measurements, current laboratory work focuses on photoabsorption cross sections of SO_2 at 200K across the wavelength range 220 – 325 nm. These measurements not only compliment previous room temperature measurements obtained at Imperial College in the 190 - 220 nm and 220 – 328 nm ranges [1][2], but also coincide with the wavelength regions being recorded by the Venus Express mission through the UV-IR spectrometer SPICAV [3]. Our new measurements will allow accurate analysis of the chemical processes in the upper atmosphere of Venus.

These absorption cross section measurements will be the first to be acquired at this temperature and pressure. Preliminary results will be presented.

This work was supported in part by NASA Grant NNG05GA03G, PPARC (UK), and the Leverhulme Trust.

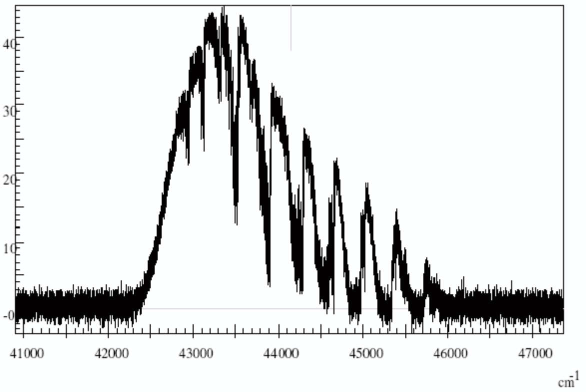

Figure 1: The absorption spectra of SO_2 within the region 42800 - 45800 cm^{-1} as recorded on a high resolution Fourier Transform Spectrometer using a Xeon arc lamp continuum source.

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Th2-6

HYPERFINE STRUCTURE CONSTANTS OF THE 7, 9, 10D$_{5/2}$ STATES OF CESIUM

M. Auzinsh[1], K. Bluss[1], R. Ferber[1], F. Gahbauer[1],
A. Jarmola[1], M. S. Safronova[2], U. I. Safronova[3], and M. Tamanis[1]
[1]Department of Physics and Institute of Atomic Physics and Spectroscopy,
University of Latvia, Rainis Blvd. 19, Riga LV-1586, Latvia
[2]Department of Physics and Astronomy, 223 Sharp Lab,
University of Delaware, Newark, Delaware 19716, USA
[3]Physics Department, University of Nevada, Reno, Nevada 89557, USA
jarmola@latnet.lv

We present new hyperfine structure (hfs) constant *A* values of the 7, 9, and 10D$_{5/2}$ states of cesium obtained from electric-field-induced level-crossing signals and precise calculations of the tensor polarizabilities α_2. Unlike the case of Cs *n*D$_{3/2}$ states where atomic parameters could be determined directly from the positions of well resolved level-crossing resonances [1], the *n*D$_{5/2}$ states contain so many closely spaced magnetic sublevel crossings (see Fig. 1) that resolved resonances can no longer be observed (see Fig. 2). Therefore, to describe the experimental signals, a detailed theoretical model is essential. To determine the hfs constants *A,* we fit measured level-crossing signals with calculated curves obtained from a theoretical model based on optical Bloch equations. With the tensor polarizability α_2 fixed, these fits yielded the hfs constant *A*. To provide reliable α_2 values, relativistic many-body calculations have been performed [2]. The values we obtained for the hyperfine constants of the 7, 9, and 10D$_{5/2}$ states are -1.56(9), -0.43(4), and -0.34(3) MHz, respectively.

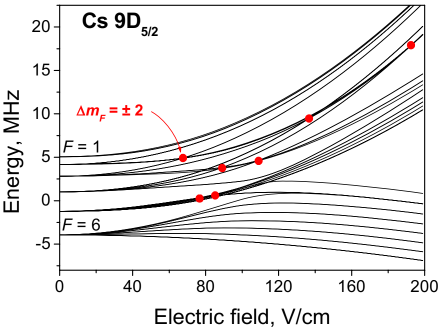

Fig. 1.

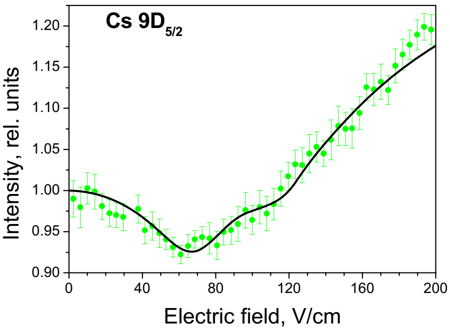

Fig. 2.

We acknowledge support from NATO Grant SfP-978029, Latvian National Research Programme in Material Sciences grant Nr. 1-23/50, Latvian University Grant Y2-22AP02, National Science Foundation Grant No. PHY-04-57078, and DOE-NNSA/NV Cooperative Agreement DE-FC08-01NV14050. K.B., F.G., and A.J. thank the European Social Fund for support.

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Th2-7

ON THE STARK BROADENING OF TWO Xe II LINES FROM THE MULTIPLET 5d [3] – 4f [4]^o

S. Djurović[1], R. J. Pelaez[2], M. Ćirišan[1], J. A. Apparicio[2] and S. Mar[2]

[1]Faculty of Sciences, Department of Physics, Trg Dositeja Obradovica 4,
21000 Novi Sad, Serbia, djurovic@uns.ns.ac.yu
[2]Departamento de Fisica Teorica Atomica y Optica, Facultad de Ciencias, Universitad de Valladolid, P. Prado de la Magdalena s/n,47071Valladolid, Spain

Stark broadening measurements are important for plasma diagnostics as well as for theory testing and astrophysical applications. This paper is a part of our comprehensive investigations on Xe II spectral lines broadening.

Helium (95%) – xenon (5%) plasma at a pressure of 3 kPa was generated by discharging 20 μF capacitors, charged up to 9 kV, through the cylindrical tube. Under these conditions, plasma emission lasted for about 300 μs. Spectroscopic measurements were performed end-on, 2 mm from the tube axis. Complete experimental set-up was described in details in [1]. Intereferometric method was used for electron density determination. Two laser beams (543.0 nm and 632.8 nm) were used. They were passing through the discharge tube in the axial direction 2 mm from the tube axis, symmetricaly to the spectroscopic channel. Electron density was in the range ($0.2 – 1.6 \times 10^{23}$ m^{-3}). Electron temperature was determined by a Boltzmann-plot of 24 Xe II lines and it was in the range 18300 – 25500 K.

During the analysis of the Xe II spectrum we found an interesting case. Two spectral lines of double ionized xenon 327.29 nm and 395.47 nm are classified in literature as lines from the same multiplet $5p^4$ ($^3P_1$) 5d [3] - $5p^4$ ($^3P_2$) 4f [4]^o [2, 3]. Measured Stark full halfwidth of the Xe II 327.29 nm line is 42.54 pm with estimated error of ± 12% and for Xe II 395.47 nm line is 99.88 pm with estimated error of ± 16%. These results correspond to electron density of 1×10^{23} m^{-3} and temperature of 22000 K. It is well known from [4] that the halfwidths of the lines belonging to the same multiplet should agree within several percents. Our results show the difference between halfwidths of the lines for more than two times. Theoretical calculations were not performed because of lack of the perturbing energy levels data in the literature [2, 3]. Mistakes due to the selfabsorption effect or wrong identification of the lines are excluded.

The conclusion is that appertainance of these two lines to the same multiplet should be rechecked.

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Th2-8

IONIZATION OF ALKALI-METAL RYDBERG ATOMS BY BLACKBODY RADIATION

I.I.Beterov[1], D.B.Tretyakov[1],I.I.Ryabtsev[1], A.Ekers[2], N.N.Bezuglov[3]
[1]Institute of Semiconductor Physics, Pr. Lavrentyeva 13, 630090, Novosibirsk, Russia
[2]University of Latvia, Institute of Atomic Physics and Spectroscopy, Riga, Latvia
[3]St.Petersburg State University, Fock Institute of Physics, St. Petersburg, Russia
E-mail: beterov@isp.nsc.ru

Results of theoretical calculations of ionization rates of Rb and Na Rydberg atoms by blackbody radiation are presented. Calculations have been performed for nS, nP and nD states of Na and Rb, which are commonly used in a variety of experiments, at principal quantum numbers $n = 8 - 65$ and at three ambient temperatures of 77, 300 and 600 K. In the calculations we have taken into account the contributions of BBR-induced redistribution of population between Rydberg states prior to photoionization and field ionization by extraction electric field pulses.

A semi-classical model [1] was used to calculate the bound-bound and bound-free matrix elements. The obtained results show that these phenomena affect both the magnitude of total ionization rates and shapes of their dependencies on the principal quantum number n. The theoretical ionization rates are compared with the results of our earlier measurements of BBR-induced ionization rates of Na nS and nD Rydberg states with $n = 8 - 20$ at 300 K [2], and good agreement for all states except nS with $n > 15$ is obtained. Useful analytical formulae allowing quick estimates of ionization rates are also presented.

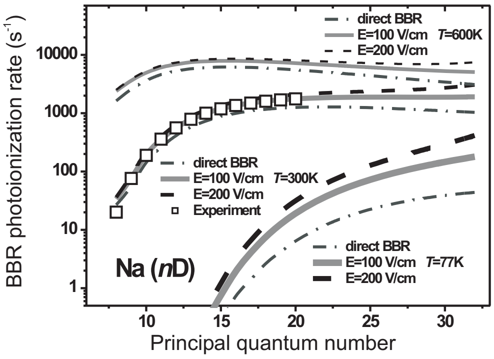

Figure 1: Theoretical and experimental BBR-induced photoionization rates of Na(nD) states at various temperatures and two different amplitudes of extraction electric field pulses.

Acknowledgements

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Th2-9

Readout of Delayline Detectors using Transient Recorder Technique

Lutz Foucar[1], Achim Czasch[1,2], Ottmar Jagutzki[1,2], Sven Schoessler[1], Till Jahnke[1],
Horst Schmidt-Boecking[1,2], and Reinhard Doerner[1]

[1]Johann Wolfgang Goethe-Universitaet Frankfurt am Main, Institut fuer Kernphysik
[2]RoentDek GmbH, Im Vogelshaag 8, Kelkheim

In order to study high correlated systems, it is necessary to detect and measure the position of all participating fragments with high precision. One can use the COLTRIMS (Cold Target Recoil Ion Momentum Spectrometer) Technique to obtain all particles. With this Technique one measure the Momentum of all particles using a time of flight and Position Measuring Detector. To detect the position of the impact on an MCP Detecor a Delayline Anode is used. Usually the readout of the Delayline Anode is done via a Constant Fraction Discriminator (CFD) and a Time to Digital Converter (TDC). We are studying the advanced of using a Transient Recorder Readout of Delayline Anode Detectors over Hardware Constant Fraction Discriminators. Using the Transient Recorder Readout Technique, one is able to detect many particles with a very small dead time.

Th2-10

L_3M_x–$M_xN_{4,5}$ X-ray satellites spectra in the Lβ_2 region of 5d transition elements

Surendra Poonia

Division of Natural Resources and Environment,
Central Arid Zone Research Institute, Jodhpur - 342 003, Rajasthan, India
E-mail: surendra_1975@yahoo.com, poonia.surendra@gmail.com

Abstract:

The X-ray satellite spectra arising due to L_3M_x–$M_xN_{4,5}$ (x ≡ 1-5) transition array, in elements with Z = 74 to 90, have been calculated. While the energies of various transitions of the array have been determined by using available Hartree-Fock-Slater (HFS) data on K–LM and L–MN Auger transition energies and their relative intensities of all the possible transitions have been estimated by considering cross - sections for the Auger transitions simultaneous to a hole creation and then distributing statistically the total cross sections for initial two hole states L_3M_x amongst various allowed transitions from these initial states to $M_xN_{4,5}$ final states by Coster-Kronig (CK) and shake off processes. In both these processes initial single hole creation is the prime phenomenon and electron bombardment has been the primary source of energy. The calculated spectra have been compared with the measured satellite energies in Lβ_2 spectra. Their intense peaks have been identified as the observed satellite lines. The one to one correspondence between the peaks in calculated spectra and the satellites in measured spectra has been established on the basis of the agreement between the separations in the peak energies and those in the measured satellite energies. It has been established that two satellites observed in the Lβ_2 region of the X-ray spectra of various elements and named β_2^{I} and β_2^{II} in order of increasing energy are mainly emitted by $L_3M_{4,5}$–$M_{4,5}N_{4,5}$ transitions. It is observed that the satellites, β_2^{I} in the spectra of elements with Z = 74 to 77 has been assigned to superposition of $^3F_4$-$^3G_5$ and $^3F_4$-$^3D_3$ transitions and that this must be the most intense of all these satellites. The same transitions have been proved to be the main origin of the satellite, β_2^{II}, reported in the elements $_{78}$Pt to $_{90}$Th. Further, the satellite β_2^{I}, reported in the spectra of elements with Z = 78 to 90, has been associated with the transitions $^3D_3$–$^3F_4$ and $^1D_2$-$^1F_3$. Finally, the line β_2^{II}, reported in the spectra of elements Z = 74-77, has been assigned to $^1F_3$-$^1G_4$ transition. Unfortunately, no experimental data are available on the intensities of these satellites. This suggests a need of detailed investigation, both theoretical and experimental, of these spectra.

LITHIUM HYPERFINE SPLITTING AND THE NUCLEAR VECTOR POLARIZABILITY

M. Puchalski and K. Pachucki
Institute of Theoretical Physics, Warsaw University
Hoża 69, 00-681 Warsaw, Poland.

The value of the hyperfine splitting depends to large extend on the distribution of the magnetic moment within the nucleus. By the comparison of experimental values with theoretical predictions for energy levels and hyperfine splitting [1] one can obtain the size of charge and magnetic distributions of unstable nuclei, which enhance our knowledge of basic nuclear properties [4]. Lithium and Be^+ are of interest because hyperfine splitting can be accurately calculated and there is a variety of lithium and beryllium isotopes, some of them with large neutron hallo [4, 5]. We will present a new and accurate values for the hyperfine splitting in Li and Be^+, possibly including higher order relativistic effects and the nuclear vector polarizability. Our computational approach is based on explicitly correlated Hylleraas functions, which provide the best convergence for energy levels including relativistic corrections [1, 2, 3].

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Th2-12

PROBABILITIES OF MULTIPLE SHAKE PROCESSES IN SUDDEN APPROXIMATION

A.G.Kochur, V.A.Popov

Rostov State University of Transport Communication, Rostov-na-Donu, 344038
Russia, agk@rgups.ru

Creation of an inner-shell n_0l_0-vacancy in an atom may lead to additional monopole excitation or ejection of its outer-shell nl-electrons into the states with the same orbital quantum number l. Those processes are called shake up (SU) and shake off (SO) processes. Sudden perturbation approximation allows easy calculation of the SU+SO probabilities [1].

It is often supposed [2] that the n_0l_0nl shake processes (nl electron is excited/ejected upon n_0l_0 inner-shell ionization) are exclusively single shake processes, *i.e.* only one nl electron is excited or ejected. However, our estimates of double shake processes [3] showed that they may be noticeable.

In this work, within the sudden approximation, we calculate separately the probabilities of single, double, triple and quadruple shake processes in atoms with $3 \leq Z \leq 55$ due to K-, L-, M-, and N-inner-shell ionization [4].

Our calculations showed that multiple shake processes have considerable probabilities making up to 30% of total shake probabilities depending on the initial vacancy n_0l_0 and on the subshell nl being additionally excited/ionized.

Double shake processes dominate making about 90% of all the multiple shake processes probabilities, triple processes are small, and quadruple shakes are negligible. With the beginning of a new subshell occupation, both single and multiple shake probabilities increase sharply. Relative contribution of multiple shake processes also increases upon crossing the borders of the periodic table rows.. Along the row of the periodic, table the relative role of multiple shake processes decreases gradually until a new subshell is opened.

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Th2-13

Interaction between Rydberg series of doubly excited states in Kr and Xe after excitation with narrow bandwidth synchrotron radiation observed by photon induced fluorescence spectroscopy (PIFS)

S. Klumpp, W. Kielich, L. Werner, A. Ehresmann
H. Schmoranzer
K.-H. Schartner
V.L Sukhorukov, I.D. Petrov, and Ph.V. Demekhin

Institute of Physics and CINSaT , University of Kassel, Germany
Department of Physics, TU Kaiserslautern, Germany
I. Institute of Physics, University of Giessen, Germany
Rostov State University of Transport Communications, Russia

Synchrotron radiation was produced by the quasiperiodic undulator U125/2 of BESSY II, Berlin, and dispersed by a 10m normal-incidence monochromator equipped with a 1200 lines/mm grating. This synchrotron radiation with a narrow bandwidth (1.8meV at 21.6eV) was used to excite gaseous Xe at pressures of 35mTorr in a target cell at room temperature. The emitted fluorescence radiation was dispersed by a 1m normal-incidence monochromator equipped with a 2400 lines/mm grating and recorded by a position-sensitive detector within a fluorescence wavelength range between 90nm and 100nm. The presented measurement concentrates on the exciting-photon energy range between 25.25eV and 25.50eV where according to Codling and Madden [1] the absorption spectrum of XeI is structured by a number of resonances which they connected to doubly excited states in XeI. It was possible to resolve in the dispersed fluorescence emission spectra of excited XeII states more resonances as in earlier measurements [1, 2]. These states are mainly populated by autoionization of the doubly excited XeI states. An analysis of the assignments of these states is currently in work. Calculations for a similar case in Kr will be shown taking into account core relaxation and interaction between many resonances and many continua explaining the Rydberg series 5s*n*p $^4P_{1/2}$ and 5s*n*p $^2P_{3/2}$ of doubly excited states in KrI in the fluorescence emission spectra of KrII [3].

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Th2-14

THEORETICAL MODELS FOR THE CASCADE DECAYS

A.G.Kochur

Rostov State University of Transport Communication, Rostov-na-Donu, 344038
Russia, agk@rgups.ru

Creation of one or several inner-shell vacancies in an atom produces a highly excited short-lived state giving rise to a multi-step de-excitation cascade. To calculate various characteristics of the cascades, we proposed an approach based on the straightforward construction of the cascade de-excitation trees in one-electron configuration-average approximation [1,2].

Within this scheme, the final ion charge spectra of singly ionized, resonantly excited and hollow atoms are calculated, the cascade affected Auger and X-ray emission spectra are investigated ([3] and references therein). A new phenomenon of the increase of the X-ray emission from an atomic outer shell upon resonant excitation of the same atom's inner shell is explained [4].

Combination of the approach [1,2] with thorough multiplet structure calculations for the principal cascade-produced states has made it possible:

- to develop a new spin-sensitive coincidence technique in photoelectron spectroscopy [5],
- to explain the recent Auger electron–photoion coincidence experiment [6] with narrow energy window for Auger electrons [7],
- to study the role of the inter-multiplet Auger transitions in the decay of resonantly excited Ar$1s^{-1}4p$ state [8],
- to calculate the probabilities of photon emission from cascade-produced ionic states of some cosmic atoms [9,10].

Consideration of monopole and non-monopole double Auger processes allowed to explain the production of highly charged ions upon the decay of less-hollow vacancies [11,12].

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Th2-15

OSCILLATOR STRENGTHS FOR SINGLY IONIZED SILICON USING NON-ORTHOGONAL WAVE FUNCTIONS

S. S. Tayal
Department of Physics, Clark Atlanta University, Atlanta, USA

The importance of core-valence correlation and core correlation corrections and interactions between the $3s^2nl$ (nl=0,2) Rydberg series and the $3s3p^2$ perturber states in singly ionized silicon have been examined using term-dependent non-orthogonal orbitals in the multiconfiguration Hartree-Fock approach [1] and B-spline box-based multi-channel method [2]. Large sets of spectroscopic and correlation non-orthogonal functions have been chosen to describe adequately term dependence of wave functions, various correlation corrections and strong interactions in the $3s^2nd\ ^2D$ Rydberg series. The mean radii of the correlation orbitals are comparable to spectroscopic orbitals and thus the correlation corrections are very well represented. The relativistic corrections are included through the Breit-Pauli Hamiltonian. The spin-orbit, spin-other-orbit, spin-spin, mass and Darwin Breit-Pauli operators are included in the calculations.

Extensive configuration-interaction wave functions have been used in the representation of target levels to calculate oscillator strengths and transition probabilities. The accuracy of our calculated oscillator strengths is evaluated by the agreement between the length and velocity formulations combined with the agreement between the calculated and measured transition energies. Our results are compared with experimental measurements, previous calculations and astronomical observations. The oscillator strengths for fine-structure transitions between levels up to n=12 have been calculated. The length and velocity forms of oscillator strengths show very good agreement for most transitions.

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Th2-16

STARK REDISTRIBUTION OF RADIATION TRANSITION PROBABILITIES IN ATOMIC MULTIPLET LINES

A. A. Kamenski and V. D. Ovsiannikov

Department of Theoretical Physics, Voronezh State University,
394006, Voronezh, Russia, E-mail: San40@bk.ru

The behavior of multiplet sublevels in a dc field depends on the value of the tensor polarizability of multiplet state. We have calculated numerical data for this quantity in P- and D- states of alkali atoms and helium, starting from the first excited to arbitrary high Rydberg levels, using the Green function in the Fues' model potential approximation for the valence-electron states. The asymptotic polynomials of the effective principal quantum number ν extrapolating the polarizabilities to the states with $\nu = 10 \div 1000$ were derived [1].

Together with the field-induced variation of energy, the reconstruction of wavefunctions in atomic multiplet causes essential changes in radiation matrix elements and transition probabilities. An important feature of the Stark effect on multiplet states of many-electron atoms is the anticrossing of two (doublet) sublevels with equal principal and angular quantum numbers *nL*. The "doublet" levels interacting in pairs may exist among states with arbitrary spin and specific magnetic quantum number, for example, those with $|M| = L + S + 1$. Our calculations are based on the integral Schrödinger equation for close levels, including the completely reduced Green function with the mean energy of multiplet [2]:

$$\Psi(\mathbf{r}) = \sum_{i=1}^{k} a_{J_iM} \left[1 + G^{(nL)}(\mathbf{r},\mathbf{r}')\left(\hat{V}(\mathbf{r}') - \Delta E\right)\right]^{-1} \left|\phi_{nLJ_iM}(\mathbf{r}')\right\rangle .$$

We have derived analytical expressions for the dipole transition probability between arbitrary atomic doublet states in the electric field F_0. E.g., for the π-transition from the state $|n\,L\,M,\pm\rangle$ to the isolated state $|n'\,L' = L-1\,M\rangle$ the probability ratio to the total probability of the doublet transitions in a field-free atom is:

$$R_{\pm}^{\pi}(f) = \frac{1}{2}\left\{ 1 \pm \frac{\zeta\left(f^2-1\right) sign\left(\alpha_{nL}^{t}\right)}{\sqrt{1+f^2\left(f^2-2\right)\zeta^2}} \right\},$$

where $f = F_0 / F_A$, the "+"("–") sign corresponds to the substate with greater (smaller) energy, and ζ is a dimensionless parameter which depends on the quantum numbers of the doublet atomic states. Near anticrossing, $F_0 \approx F_A$, the both probabilities become equal to one another, $R_+(1) = R_-(1)$. The strong field, $f \to \infty$, breaks down the spin-orbit structure of atomic states so as to transform transition probabilities into those of a spin-less atom, with only one of the two values $R_{\pm}(\infty)$ remaining nonzero.

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Th2-17

Rovibrational Spectroscopy of Para-H_3^+ Enriched Populations in a Cryogenic 22-Pole Ion Trap

Annemieke Petrignani, Holger Kreckel, Max Berg, Dennis Bing, Sascha Reinhardt, Andreas Wolf

Max-Planck Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany

We present the manipulation of the nuclear spin of cold H_3^+ ions and the infrared action spectroscopy on para-H_3^+ enriched populations. This research is motivated by providing new data on the dynamics and the rate coefficients of dissociative recombination (DR) of cold para- and ortho-H_3^+ ions. The DR experiments are performed at the ion storage ring TSR, using H_3^+ ions that are buffer-gas cooled in a cryogenic RF ion trap before their injection into the storage ring. The first experimental runs of this type showed an increase in the DR cross section when para-H_2 was used as parent gas for the H_3^+ ion beam [1]. Theory, however, mainly predicts a decreased cross section for para-H_3^+ ions [2]. Although the para-H_3^+ contribution was not measured, an increase in its population is expected when using para-H_2 as the parent gas.

To improve the knowledge on the H_3^+ nuclear-spin states in these experiments, we utilise rovibrational laser spectroscopy in the cold H_3^+ ion trap [3]. In addition, this will reveal information on the ortho-para conversion rates in collisions of para/ortho-H_3^+ with para/ortho-H_2. The H_3^+ ions are produced in a RF ion source through electron-impact ionisation of para-H_2 gas. These ions are subsequently stored in a cryogenic 22-pole RF ion trap of 55 K and buffer-gas cooled with Helium. The three lowest rotational states of the vibrational ground-state H_3^+ ions are excited using an infrared diode laser. Argon gas is then used as a chemical probe, as it can only react with these laser-excited H_3^+ ions, forming ArH^+ which is detected as the spectroscopic signal. The para-to-ortho ratio is determined from the relative intensities between the respective ortho- and para-transitions. First results indicate an increase in the para-H_3^+ spectral-line intensities when using para-H_2 gas in the ion source as compared to using normal-H_2 parent gas. Dependencies on the ion-source parameters and the ion-trap temperature are currently under investigation. In future, the 22-pole setup will be used in ion storage ring experiments on H_3^+ DR in the lowest ortho- and para-levels.

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Th2-18

MODIFIED FUES POTENTIAL FOR GROUND-STATE WAVEFUNCTIONS OF MULTIVALENT ATOMS

E.Yu. Il'inova and V.D. Ovsiannikov

Department of Physics, Voronezh State University, Russia
E-mail addresses: ovd@phys.vsu.ru

In this paper we propose a generalization of the Fues' model potential approach [1] to the ground-state wavefunctions of the multivalent atoms.

Generation of the analytical presentation for the wave functions and Green functions of atoms with several valence electrons is an important problem of atomic spectroscopy [2,3]. Successful applications of the Fues' model potential to the single valence-electron atoms were based on the convenient analytical expressions for the relevant quantities [4]. However, some discrepancies remained against the well approved numerical data for the ground-state susceptibilities of atoms with two or more valence electrons.

Of all the one-electron states, the ground-state wavefunction in the model potential approximation is the least accurate, since it overlaps significantly with the core states. Therefore, in numerical calculations more accurate results (starting from the dipole oscillator strengths and polarizabilities) were obtained with the use of the wave function from the quantum defect theory [1] or simply with an empirical renormalization factor [4].

Our proposal consists in the substitution of a modified potential $\hat{V}_F^m$ for the Fues model potential [1]

$$\hat{V}_F(\mathbf{r}) = -\frac{Z_i}{r} + \sum_{\gamma=0}^{\infty} \frac{B_\gamma}{r^2}\hat{P}_\gamma$$

by adding a supplementary Coulomb term $-(Z_\gamma - Z_i)/r$, thus replacing the residual ion charge $Z_i = 1$ by an energy-dependent (together with B_γ) noninteger number Z_γ ($\gamma = l$ is the angular momentum in a spin-less single-electron case), determined on the basis of:
1) the coincidence of the $\hat{V}_F^m$ eigenspectrum with the energy spectrum $E_{n\gamma}$ of atom;
2) the mutual orthogonality of the radial wave functions within a given spin-orbital series γ of atomic states ($\hat{P}_\gamma$ is the projection operator onto the subspace γ);
3) Z_γ tends to Z_i for $\gamma \rightarrow \infty$ or $E_{n\gamma} \rightarrow 0$.

These requirements have resulted in significant corrections to the ground-state wavefunctions of the multivalent atoms. So, for atoms with two valence electrons, the influence of the long-range polarization potential has resulted in the decrease of the nuclear potential shielding, therefore here $Z_0 > 1$ with increasing Z_0 from beryllium (Z_0=1.13) to mercury (Z_0=1.3). On the contrary, for the inert-gas atoms (neon, argon, krypton, xenon) with six valence electrons the repulsive interactions between electrons in the valence p^6 shell may result in the increase of the nuclear charge shielding, so here $Z_0 < 1$, with increasing Z_0 from neon (Z_0=0.56) to xenon (Z_0=1.0). The variation of the residual charge together with the centrifugal potential has resulted in significant increase of accuracy of the numerical results. The most spectacular of them is the numerical value for the static dipole polarizability of neon, which in the $\hat{V}_F$ approximation was 0.785 $\mathring{A}^3$, whereas in the $\hat{V}_F^m$ approach it is 0.403 $\mathring{A}^3$ (the experimental value is 0.396 $\mathring{A}^3$).

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Th2-19

ON DETERMINATION OF ABSOLUTE ATOMIC DENSITIES FROM MEASURED RELATIVE INTENSITIES WITHIN RESONANCE MULTIPLETS DISTORTED BY SELF-ABSORPTION

B.P. Lavrov, A. S. Mikhailov

Faculty of Physics, St.-Petersburg State University, 198904, Russia.
E-mail: lavrov@pobox.spbu.ru

The opportunities of the application of the recently proposed approach [1] in optical emission spectroscopy of non-equilibrium plasmas have been studied. The approach consists of several methods of the determination of *absolute* particle densities of atoms from measured *relative* intensities within resonance multiplets distorted by self-absorption. The main idea of the approach is that in the case of sufficient self-absorption for a pair of resonance lines having common upper level the ratio of intensities doesn't depend on the population density of upper level, but depends on the length of homogeneous plasma column along optical axis L, the gas temperature T, and populations of the sublevels of multiplet structure of the ground state. In the case of Boltzmann distribution over the sublevels with the temperature T, the intensity ratio depends on the temperature T and the product NL, where N is the total population of the ground state, usually close to the atomic particle density.

All available spectroscopic data concerning resonance spectral lines of atoms having multiplet ground states from Boron up to Gallium were analyzed. It is found that in the case of the C, O, F, S and Cl atoms an application of the methods needs VUV technique, while densities of the B, Al, Si, Sc, Ti, V, Co, Ni and Ga atoms may be obtained by means of the intensity measurements in UV and visible parts of emission spectrum suitable for ordinary middle class spectrometers used for optical diagnostics and monitoring of non-equilibrium plasmas including industrial plasma technologies. The intensity ratios for 104 prospective pairs of resonance lines of the Al, Si, Sc, Ti and V atoms were calculated for gas temperatures T = 500÷4500 K and the values of the product NL = $10^8 \div 10^{15}$ $cm^{-3} \cdot m$. The results show that the temperature dependence of the intensity ratio is much smaller than its dependence on the optical length NL. Sometimes the uncertainty in the temperature may be even neglected. For every pair of lines the range of sensitivity of the relative intensity to NL is about one-two orders of magnitude, mainly $10^{10} \div 10^{12}$ $cm^{-3} \cdot m$.

Experimental studies of hollow cathode discharge in Ne-Ga mixture have shown that joint use of two resonance doublets of Ga (the 417,2/403,3 nm and the 294,4/287,4 nm) gives plausible values of the density of Gallium atoms even in the case of non-equilibrium distribution of population density among sublevels of multiplet structure of the ground state.

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Th2-20

EFFECTS OF ELECTRIC FIELD ON THE DECAY BRANCHING RATIO OF $^1P^e$ DOUBLY EXCITED STATES IN HELIUM

M. Žitnik[1], F. Penent[2], P. Lablanquie[2], A. Mihelič[1], K. Bučar[1], R. Richter[3], M. Alagia[4]
and S. Stranges[5]

[1]Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia (matjaz.zitnik@ijs.si)
[2]LCP-MR, Univ. Pierre et Marie Curie 6, CNRS (UMR 7614), 11 rue Pierre et Marie Curie, 75231 Paris Cedex 05, France
[3]Sincrotrone Trieste, I-340 12, Trieste, Italy
[4]INFM-TASC, Padriciano 99, I-340 12 Trieste, Italy
[5]Dipartimento di Chimica, Universita di Roma La Sapienza and INFM Unit, 00185 Rome, Italy

We have measured the lifetimes of $^1P^e$ (n=9-12) doubly excited states in static electric fields (1-6 kV/cm) by observing the decay of the fluorescence signal as a function of time [1]. The effects of the field on these helium states below the second ionization threshold are twofold: their excitation becomes possible due to the Stark mixing with the optically allowed $^1P^o$ series, and their lifetime is strongly modified by the opening of the autoionization channel, not accessible in the zero field. Although the electric field represents only a tiny perturbation of the atomic potential, a substantial shortening of the lifetimes below 100 ps is observed. This is the simplest quantum system where the ratio of autoionization to fluorescence decay probability can be effectively controlled by an electric field of moderate strength.

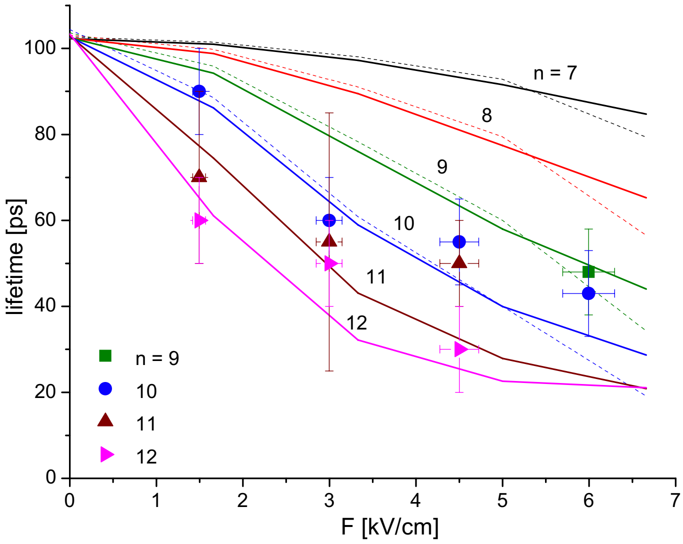

Figure: $^1P^e$ lifetime dependence on n and the electric field strength F and comparison with the first order (dotted line) and complex rotation calculations [2]. (full line).

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Th2-21

High-resolution study of the doubly excited states of Helium – excitation of $^{1/3}$S metastable Helium atoms.

M. Alagia[1,2], M. Coreno[3,4], H. Farrokhpour[5,6], P. Franceschi[7], K. C. Prince[8,2], R. Richter[8], J. Söderström[9], S. Stranges[10, 1, 2]

[1]CNR-ISMN Sez.Roma, P.le A. Moro 5, I-00185 Roma, Italy
[2]Laboratorio Nazionale TASC, INFM-CNR, 34012 Trieste, Italy,
[3] CNR-IMIP, Montelibretti (Rome), I-00016 Italy,
[4]INSTM, Trieste, Italy,
[5]Chemistry Department, Isfahan University of Technology, Isfahan 84154, Iran
[6]The Abdus Salam International Centre for Theoretical Physics, I-34014 Trieste, Italy
[7]Dipartimento di Fisica, Universita´ di Trento, 38050 Povo (TN), Italy
[8]Sincrotrone Trieste, Area Science Park, I-34012 Basovizza,Trieste, Italy
[9]Department of Physics, Uppsala University, Box 530, S-75121 Uppsala, Sweden
[10]Dipartimento di Chimica and Unità INSTM, Università di Roma "La Sapienza", I-00185 Roma, Italy

Doubly excited states of helium are a prototype system to study electron correlation in atoms. Since their discovery by Madden and Codling [1] they have been subject to various experimental and theoretical studies [2]. In all of the experimental work the doubly exited states were investigated using one photon excitation from the helium ground state, but theoretical studies have also investigated the ionization and excitation of metastable atoms [3] revealing different relative absorption cross sections and a nearly Lorentzian line shape. Here we present the first experimental study of doubly exited states following excitation of triplet and singlet metastable helium atoms. Since the target is extremely dilute, this is a very demanding measurement. First members of the series have been observed and their relative absorption cross sections are compared with theoretical predictions. In the triplet manifold we have observed transition from the 1s2s $^3S^e$ state of helium to the first members ($^3P^o$) of the $_2(1, 0)^+_n$ and $_2(1, 0)^-_n$ series (the notation follows ref [3]). Although the transitions have not been measured before, the energies of the excited states are known from emission and theoretical studies. In the singlet manifold we have observed transitions from the 1s2s $^1S^e$ state to the ($^1P^o$) $_2(1, 0)^+_2$ and $_2(1, 0)^-_3$ states, which are accessible in absorption from the ground state. The transitions from metastable states show a drastically different intensity ratio with respect to transitions from the ground state.

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Th2-22

STARK SHIFTS OF SOME Xe II BLUE LINES

M. Ćirišan[1], R. J. Pelaez[2], S. Djurović[1], J. A. Apparicio[2] and S. Mar[2]

[1]Faculty of Sciences, Department of Physics, Trg Dositeja Obradovica 4,
21000 Novi Sad, Serbia, mihaela@uns.ns.ac.yu
[2]Departamento de Fisica Teorica Atomica y Optica, Facultad de Ciencias, Universitad
de Valladolid, P. Prado de la Magdalena s/n,47071Valladolid, Spain

This work reports Stark shift measurements of 10 ionized xenon spectral lines from blue region (410 nm – 470 nm). These data are important for plasma diagnostics purposes, theory testing and applications.

Pulsed arc helium (95%) – xenon (5%) plasma at a pressure of 3 kPa, generated by discharging 20 μF capacitors, charged up to 9000 V, through the cylindrical tube, was analysed here. Complete experimental set-up was described in details in [1]. Two wavelength intereferometric method was used for electron density determination Electron density was in the range ($0.2 - 1.6 \times 10^{23}$ m^{-3}). Electron temperature, determined by a Boltzmann-plot was in the range 18300 – 25500 K.

Shift results are given in Table 1. Depending on the experimental error, data are classified as A (15%), B (<25%) and C (<40%).

Table 1. Experimental Stark shifts for $N_e = 1 \times 10^{23}$ m^{-3}, $T_e = 22000$ K

No.	Configurations	Terms	Wavelength (nm)	d_m (pm)
1	$5s5p^6$ - $5p^4$ ($^3P_2$) 6p	$^2S_{1/2}$ - $[2]°_{3/2}$	477.918 A	6.7
2		$^2S_{1/2}$ - $[1]°_{1/2}$	438.493 A	7.2
3	$5p^4$ ($^3P_2$) 5d - $5p^4$ ($^3P_2$) 6p	$[2]_{5/2}$ - $[1]°_{3/2}$ $[2]_{3/2}$ - $[1]°_{3/2}$	467.456 B 481.802 B	5.8 7.9
4	$5p^4$ ($^3P_2$) 5d - $5p^4$ ($^3P_0$) 6p	$[2]_{3/2}$ - $[1]°_{1/2}$	410.034 C	-1.0
5	$5p^4$ ($^3P_2$) 5d – $5p^4$ ($^1D_2$) 6p	$[1]_{3/2}$ - $[3]°_{5/2}$	424.441 C	-7.1
6		$[1]_{3/2}$ - $[1]°_{3/2}$	410.495 C	-0.9
7	$5p^4$ ($^3P_1$) 5d – $5p^4$ ($^1D_2$) 6p	$[1]_{3/2}$ - $[1]°_{1/2}$	402.519 C	3.9
8		$[1]_{3/2}$ - $[2]°_{3/2}$	416.216 B	7.1
9	$5p^4$ ($^3P_0$) 5d – $5p^4$ ($^1D_2$) 6p	$[2]_{5/2}$ - $[3]°_{7/2}$	453.249 B	-2.8

Multiplets were ordered as in [2]. For obtaining the Stark shifts, special attention was paid to experimental procedure, data treatment and deconvolution procedure to exclude other broadening mechanisms. Theoretical calculations were not performed because of the lack of perturbing energy levels data in [2, 3].

These results are quite new in the literature and they can increase the present database of Xe II shift measurements.

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Th2-23

LANDE g- FACTORS OF ROVIBRONIC LEVELS OF THE $(4d)^{1,3}\Pi_g^-$ AND $(4d)^{1,3}\Delta_g^-$ STATES OF HYDROGEN AND DEUTERIUM MOLECULES

S.A. Astashkevich

Physics Department, St.-Petersburg State University, 198504, Russia.
E-mail: astashkevich@mail.ru

The values of the Lande g- factors of rovibrational levels of the $(4d)r^3\Pi_g^-$, $(4d)s^3\Delta_g^-$ [1], $(4d)S^1\Delta_g^-$ [2] electronic states of H_2 and D_2 and $(4d)R^1\Pi_g^-$ state of D_2 [2] have been founded at the first time. The data for vibrational (v=0-3 for triplet states of H_2 and v=0 for singlet states of H_2 and singlet and triplet states of D_2) and rotational (N=1-4 for H_2 and N=1-5 for D_2) levels are received semi-empirically in the framework of the non-adiabatic model taking into account the electronic-rotational interaction (L-uncoupling) of $4d^{1,3}\Pi_g^-$ and $4d^{1,3}\Delta_g^-$ states in the pure precession approximation.. It is used coefficients of expansion of the wave functions of rovibrational levels of the $r^3\Pi_g^-$, $s^3\Delta_g^-$, $R^1\Pi_g^-$ and $S^1\Delta_g^-$ states over adiabatic wave functions. These coefficients are calculated semi-empirically by us used experimental data about rovibrational term energies and the results of the numerical calculation of the overlap integrals of the vibrational wave functions of these states used *ab initio* data about adiabatic potential curves of these states.

It is founded that the perturbed values of g- factors are much closer to ones appropriate to Hund's case d for coupling of angular momenta than Hund's case b. It have been established that interference effects of interaction of the $4d\pi\Pi_g$ и $4d\delta\Delta_g$ states result to significant regular (up to 9 times for the $(4d)^{1,3}\Pi_g^-$ states) and irregular (up to 70 times for $(4d)^{1,3}\Delta_g^-$ states) differences non-adiabatic values of g- factors from adiabatic ones. Also it is obtained that the effects lead to significant differences (up to 1.5 times for the $(4d)^{1,3}\Pi_g^-$ states and almost 3.5 times for the $(4d)^{1,3}\Delta_g^-$ states) between the nonadiabatic values of the g- factors of the same rotational levels of lowest vibrational levels of the same electronic states of the different isotopomers H_2 and D_2 whereas the values should be the same in the adiabatic approximation. It is established that perturbations of g- factors of rovibrational levels of electronic states of 4d- term complex is essentially more significant than ones for 3d- term complex with the same values of vibrational and rotational quantum numbers.

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Th2-24

DISTRIBUTION OF VIBRATIONAL EXCITATIONS ACCOMPANIED INNER-SHELL IONIZATION IN MOLECULES

A. A. Pavlychev and D. A. Mistrov

Institute of Physics, St. Petersburg State University, St. Petersburg, Petrodvoretz,
198504, Russia

Distribution $f_{v'}$ of vibrational 0 -> v’ excitations that accompany K-shell ionization in free molecules is investigated. The deviations of $f_{v'}$ from the Franck-Condon distribution attract our main attention. Considering R-dependence of the amplitude of electronic dipole transition we express $f_{v'}$ as a product of the Franck-Condon factor $F_{v'}$ and an interferential factor $J_{v'}(k)$ dependent on photoelectron wave number k

$$f_{v'} = F_{v'} J_{v'}(k) \, .$$

Within the vibrationally-dependent-fixed-nuclei approximation [1] the analytical relations connecting $J_{v'}(k)$ with parameters of intramolecular interference of scattered photoelectron waves and potential functions of initial and final molecular states are obtained. In particular, for linear diatomic molecules this factor is

$$J_{v'}(k) = 1 - 4k \frac{\sigma^{+}_{v'\Sigma}}{\sigma^{+}_{v'}} \frac{l^2}{d} (v' - \frac{d^2}{2l^2}) \operatorname{Im}(1 - BS)^{-1}_{11\Sigma}$$

Here $d \equiv R_e - R^+$ and $l^2 = \hbar^2 / \mu\omega$ where μ is the reduced mass, ω is the vibrational spacing in the ground state, R_e and R^+ are equilibrium internuclear distances in the ground and ionic states. $\sigma^{+}_{v'\Sigma} / \sigma^{+}_{v'}$ is the ratio of the single-hole ionization cross section for 1s(Σ) ->Σ transition to the cross section for both 1s(Σ) ->Σ and Π transitions. B and S are the reflection and scattering matices (see, e.g.[1]). The interferential factor results in essential deviations in $f_{v'}$ from the Franck-Condon distribution in the shape resonance vicinity and oscillates smoothly far from the core-ionization threshold.

The distributions $f_{v'}$ in linear molecules are computed and compared with the experimental data. The influence of electron density redistribution due to core-hole ionization, anharmonicity of molecular frame motion and multielectron excitations on vibrational excitations is discussed. Site-selective properties of $f_{v'}$ are also discussed.

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Theoretical study of resonant states of H_3^+ and D_2H^+ molecular ions.

Bruno C. Silva, Paolo Barletta, James J. Munro and Jonathan Tennyson
Department of Physics and Astronomy,
University College London,
Gower St., London WC1E 6BT, UK

H_3^+ is an interesting molecule, both experimentally, as it plays an important role in astrophysics, and theoretically, as it is the simplest triatomic molecule. More than two decades ago Carrington and co-workers observed a remarkably rich dissociative photo-excitation spectrum in H_3^+ which attracted a wealth of theoretical attention. In a later, more sophisticated investigation [1], they studied in more detail the isotopologues of H_3^+, which showed spectra as complex as H_3^+. As to date their findings remain largely unexplained.

One aspect of this photo-dissociative process is that it involves excitations from the highest bound states to the lowest resonant states just above dissociation. We calculated the energies and lifetimes of these resonant states for J=0 and J=3 in H_3^+ and J=0 for D_2H^+ using a Complex Absorbing Potential (CAP) method [2]. The resonance search was performed with a newly developed automated algorithm, the results of which are presented here.

These studies were made possible by previous calculations of vibrational wavefunctions converged to a sub-wavenumber level of accuracy [3,4], as well as the first calculation of J=3 states of H_3^+ up to the dissociation limit [5]. These detailed *ab initio* calculations of vibrational-rotational states up to and beyond dissociation required powerful numerical techniques and large scale calculations on super-computer class machines. For this purpose we implemented an experimental parallel version of UCL's nuclear motion computational suite for triatomics (DVR3D) [6] on a national super computer (HPCx).

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Th2-26

RELATIVISTIC CI OSCILLATOR STRENGTHS FOR LOWEST TRANSITIONS IN SILVER AND GOLD ISOELECTRONIC SEQUENCES

L Glowacki and J Migdalek

Chair of Computer Science and Computer Methods
Pedagogical University of Cracow, 30-084, Krakow, Poland

As it had been demonstrated almost 30 years ago, the inclusion of core-valence electron correlation is important in calculating accurate oscillator strengths for ns –np transitions not only for alkalis but also for noble metals. However in those days the only way to include this effect within the Dirac-Fock scheme was to treat it in the semiclassical core polarization picture using an appropriate model potential. Such approach turned out to be very successful for many systems, among them silver and gold isoelectronic sequences [1]. Even now the accurate representation of valence-core electron correlation influence on oscillator strengths within the relativistic CI or MCDF scheme poses a very difficult task, particularly, if numerous transitions have to be studied. Ion this paper we present oscillator strength calculations performed for silver and gold isoelectronic sequences using modified version of relativistic CI method proposed by us earlier [2]. This method employs numerical Dirac-Fock wavefunctions generated in the field of ab initio model potential with non-integer outermost core shell occupation number to improve the efficiency of the CI representation of core- valence electron correlation. The results of this approach are compared with our earlier data obtained in the semiclassical core-polarization picture [1] as well as with available experimental data.

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Th2-27

MEASUREMENT OF PRESSURE DEPENDENT DISPERSION OF INERT GASES

A. Börzsönyi[1], K. Osvay[1,2], A. P. Kovács[1], Zs. Heiner[1,3], M.P. Kalashnikov[2]

[1] Department of Optics, University of Szeged, P.O.Box 406, Szeged 6701, Hungary
[2] Max Born Institute, Max-Born-Str. 2A, D 12489 Berlin, Germany
[3] Institute of Biophysics, Biological Research Center, Szeged, Hungary
osvay@mbi-berlin.de

Generation of high harmonics and white continuum are among the direct applications of interactions of high intensity ultrashort pulses with various gases. Recently it has been also demonstrated that filament generation in inert gases at certain pressure can lead to not only spectral broadening but also to self-compression. These processes are explained by a combination of linear and nonlinear propagation effects. Surprisingly enough, almost no experimental data are available even for linear dispersion of such gases in the near infrared, where few cycle laser pulses are typically generated.

In this paper we report on what we believe the first measurement of pressure dependent dispersion of femtosecond laser pulses in Ar, He, Kr, N_2, Ne, Xe, and air.

The technique of spectrally and spatially resolved interferometry was used to establish the spectral phase shift of 800 nm femtosecond laser pulses propagating back and forth in a vacuum tube with a length of 4.5 m. Inserting the tube into a Mach-Zehnder interferometer, the dispersion coefficients as group delay (GD), group delay dispersion (GDD) and third order dispersion (TOD) can be to high accuracy determined from the spectral shape of the fringes. From the knowledge of the exact propagation length within the vacuum tube, the specific dispersion coefficients (dispersion for a unit length of gas) are determined.

The measurement carried out within the pressure range of 40µbar to 1bar revealed that GD (Fig. 1a) and GDD (Fig. 1b) of each gas are proportional to pressure, in agreement with the Lorentz-Lorenz dispersion theory. Xenon and helium exhibit the largest and smallest dispersion, respectively, while air, argon, and nitrogen are very similar to each other. Note, that the accuracy of the measurement of specific GD and GDD is as high as 1 fs/m and 0.2 fs^2/m, respectively, due to the long propagation length in the vacuum tube, and the careful control of the experimental conditions.

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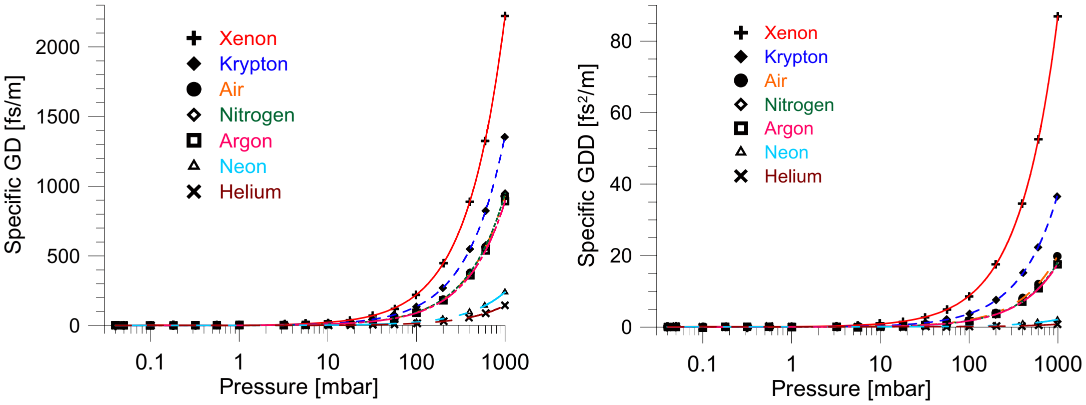

Figure 1. Pressure dependent specific GD (a) and GDD (b) of inert gases at 800 nm.

Th2-28

USE OF MAPPED GRIDS AND ABSORBING POTENTIALS IN MULTICHANNEL SCATTERING CALCULATIONS

T.P. Grozdanov * and R. McCarroll**

*Institute of Physics, P.O. Box 57, 11001 Belgrade, Serbia
**Laboratoire de Chimie Physique - Matière et Rayonnement, (UMR 7614 du CNRS)
Université Pierre et Marie Curie, 75231-Paris Cedex 05, France

We investigate the use of discrete variable representation (DVR) grid methods and absorbing potentials in multichannel time-independent scattering calculations. An exactly solvable, coupled-two-channel problem involving square-well potentials [1] is used to asses the quality of numerical results.

The S-matrix is calculated by using absorbing-boundary-condition Green's function [2] defined with the help of a transmission-free absorbing potential [3]. Numerical results show that the regions of high and intermediate scattering energies can be satisfactory treated by using standard equidistant DVR–grids [4]. This includes the precise description of Feshbach resonances, where the special care must be devoted to positioning of the absorbing potential and adjustment of the density of grid points.

The most difficult are numerical treatments of close vicinities of thresholds, where the Wigner threshold laws are applicable. The extremely long de Broglie wavelengths involved require extremely extended grids and extremely long absorption lengths, which makes the use of equidistant DVR-grids impractical. The solution [7] is the introduction of non-equidistant grids through mapping procedures of the scattering coordinate, similarly to those used previously [5, 6] in calculations of extremely loosely bound states.

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Th2-29

$2p_{3/2}^{-1}3x^{-1}$-$3x^{-1}4d^{-1}$ X-Ray satellites spectra in the $L\beta_2$ region

Surendra Poonia

Division of Natural Resources and Environment,
Central Arid Zone Research Institute, Jodhpur - 342 003, Rajasthan, India
E-mail: surendra_1975@yahoo.com, poonia.surendra@gmail.com

The X-ray satellite spectra arising due to $2p_{3/2}^{-1}3x^{-1}$-$3x^{-1}4d^{-1}$ (x ≡ s, p, d) transition array, in elements with Z = 42 to 90, have been calculated. While the energies of various transitions of the array have been determined by using available Hartree-Fock-Slater data on $1s^{-1}$-$2p^{-1}3x^{-1}$ and $2p_{3/2}^{-1}$-$3x^{-1}$,$3x'^{-1}$ Auger transition energies and their relative intensities of all the possible transitions have been estimated by considering cross - sections for the Auger transitions simultaneous to a hole creation and then distributing statistically the total cross sections for initial two hole states $2p_{3/2}^{-1}3x^{-1}$ amongst various allowed transitions from these initial states to $3x^{-1}4d^{-1}$ final states by Coster-Kronig (CK) and shake off processes. In both these processes initial single hole creation is the prime phenomenon and electron bombardment has been the primary source of energy. The calculated spectra have been compared with the measured satellite energies in $L\beta_2$ spectra. Their intense peaks have been identified as the observed satellite lines. The one to one correspondence between the peaks in calculated spectra and the satellites in measured spectra has been established on the basis of the agreement between the separations in the peak energies and those in the measured satellite energies. It has been established that four satellites observed in the $L\beta_2$ region of the X-ray spectra of various elements and named β_2^{I}, $\beta_2^{(b)}$, β_2^{II} and $\beta_2^{(c)}$ in order of increasing energy are mainly emitted by $2p_{3/2}^{-1}3d^{-1}$-$4d^{-2}$ transitions. In the present study, we report the transition assignments to the satellites β_2^{I}, $\beta_2^{(b)}$, β_2^{II} and $\beta_2^{(c)}$ reported in the spectra of elements with Z = 42 to 52 and the satellites named β_2^{I} and β_2^{II} in the L - emission spectra of the elements of $_{74}$W to $_{90}$Th. It is observed that out of these four satellites, $\beta_2^{(b)}$ can be assigned to superposition of $^3F_4$-$^3G_5$ and $^3F_4$-$^3D_3$ transitions and that this must be the most intense of all these satellites in the elements Z = 42-50. In the range of elements Z = 52 to 77, the satellite β_2^{I} is emitted by these transitions. The same transitions have been proved to be the main origin of the satellite β_2^{II}, reported in the elements $_{79}$Pt to $_{90}$Th. It has been well established that the transitions $^1F_3$-$^1G_4$ and $^3D_3$-$^3D_3$ is the main source of the emission of the satellite β_2^{II} in the elements $_{42}$Mo to $_{77}$Ir. Coming to the other two satellites in this region of the spectra, the line $\beta_2^{(c)}$, observed in the spectra $_{42}$Mo to $_{50}$Sn, is mainly assigned to the transition $^3P_1$-$^3D_2$. Lastly, the line β_2^{I}, observed in the spectra of elements Z = 42 to 46, is assigned to the transitions $^3D_3$–$^3F_4$ and $^1D_2$-$^1F_3$, while in the range of elements with Z = 78 to 90, β_2^{I} has been assigned to these transitions. In the elements $_{48}$Cd and $_{50}$Sn, the line β_2^{I} has been associated with transition $^3F_4$-$^3F_4$. Unfortunately, no experimental data are available on the intensities of these satellites. This suggests a need of detailed investigation, both theoretical and experimental, of these spectra.

Th2-30

PRODUCTION OF NEGATIVE IONS AFTER S 2p SUBSHELL PHOTOIONIZATION IN SF_6 IN THE SHAPE RESONANCES VICINITY

A. A. Pavlychev and X. O. Brykalova

Institute of Physics, St. Petersburg State University, St. Petersburg, 198504, Russia

Formation of negative fragments after X-ray excitation of neutral molecular species has received high attention recently (see, e.g. [1-3]). When photon energy approaches to core ionization thresholds the distributions of positively and negatively charged photoions demonstrate complex and different spectral dependences. In the present work relationships between shape resonances and anion yield after inner-shell ionization are examined. The two-step mechanism of anion production is applied. For the shape resonances observed in anion yield [3] above S 2p thresholds in SF_6 we write

$h\nu + SF_6 \rightarrow SF_6(2p^{-1}) \rightarrow SF_6^{+*} + e^-$

followed by

$SF_6^{+*} \rightarrow SF_5^{2+} + F^-$

Dynamic properties of the transient singly ionized and valence excited SF_6^{+*} states play an important role in spectral dependence of anion yield. To describe the T_{2g} and E_g shape resonances in the cross section Q^- of anion yield we take into account coupling of elastic and inelastic channels in 2p-photoelectron transmission through the molecular region. The elastic channel describes the single-hole ionization cross section σ^+ that reproduces the shape resonances. The inelastic channels describe the satellite excitations [4] as well as the attachment of the photoelectron to the residual cation. In the framework of the optical potential concept (see, e.g. [4]) the cross section Q^- is :

$$Q^- = \sigma^+ \alpha\gamma K(1-K)^{-1}.$$

This equation links the cross section Q^- with spectral variations of the cross section σ^+. Q^- is proportional to σ^+ where α and γ are respectively probabilities of anion formation from the parent SF_6^{+*} state and S 2p-hole Auger decay. The constant K describes coupling of the elastic and inelastic channels.

This approach allows us to rationalize both the appearance of the shape resonances in anion yield above S 2p threshold in SF_6 [3] and the lineshape of the shape resonances in σ^+. Suppression of the shape resonance above 1s ionization thresholds in diatomics [1] and important role of molecular vibrations in anion yield is also discussed.

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Th2-31

STARK EFFECT ON THE PROBABILITY OF THE RADIATION TRANSITIONS BETWEEN SINGLET STATES IN ATOMS

Ovsiannikov V. D., Kamenski A. A. and Tarusin A. A.

Department of Physics, Voronezh State University, 394006, Voronezh, Russia
E-mail address: ovd@phys.vsu.ru

The basic spectroscopic properties of atoms — the frequencies and intensity of emitted and absorbed lines — provide the principal information to pave the way for understanding, handling and control of the atomic ensembles, of the interaction between atoms and of the internal atomic structure. The variation of frequency in a dc electric field $\mathbf{F}_0 = F_0\mathbf{e}_0$ is determined by the shift and splitting of atomic energy levels, commonly called the Stark effect. The variation of the line intensity and transition probability involves, together with the Stark effect, an additional information on the variation of the matrix elements, and finally, of the initial- and final-state wave functions.

On the analogy with the usual Stark effect, the field dependence of the line intensity and transition probability may be quantitatively described in terms of the series in powers of F_0. The corresponding series for the wavefunctions, matrix elements, probabilities and intensities of the hydrogen Stark lines were first derived in [1], starting from the first-order term up to an arbitrary order in F_0. The derivation of these series has become possible due to a simple analytical expression for the Coulomb Green function in parabolic coordinates.

In many-electron atoms the breakdown of the spin-orbit coupling in the multiplet structure of levels is observed, which may be accompanied by the so-called anticrossing of the fine-structure sublevels. In the anticrossing field the intensities of the fine-structure components may equalize and with the field growth the number of multiplet lines will reduce since the intensity of one part of them will vanish to zero, whereas the intensity of the remaining lines will increase [2]. The further redistribution of probabilities will continue similar to those of a spin-less atom.

In this paper we consider the Stark effect on the probabilities of the dipole transitions between singlet states of atom. Here the first non-vanishing dipole correction both to the frequency and to the matrix element is quadratic in F_0. Hence, the probability of the dipole transition between an initial (i) and final (f) state in the field may be presented as

$$W_{fi} = W_{fi}^{(0)} \left\{1 + F_0^2 \left[w_\perp + \left(w_\parallel - w_\perp\right) |\mathbf{e}_0 \cdot \mathbf{e}|^2\right]\right\}, \tag{1}$$

where $W_{fi}^{(0)}$ is the field-free (F_0=0) probability, $\mathbf{e}$ is the unit polarization vector of the emitted (absorbed) photon. The coefficients $w_{\parallel,\perp}$ are the combinations of the third-order dipole transition matrix elements, static dipole polarizabilities of the upper and lower levels and the factors of the normalization corrections to the upper- and lower-level wavefunctions. The numerical calculations with the use of the single-electron Green function in the Fues model potential approximation has revealed a strong dependence of $w_{\parallel,\perp}$ on the principal quantum number $\nu{=}1/\sqrt{-2E_f}$ of the upper level with the energy E_f. This dependence may be presented in terms of the polynomial in powers of ν. E.g. for the transitions to highly excited $n_f\,{}^1P_1$ states from the lower $n_i\,{}^1S_0$ states in parahelium,

$$w_\parallel = -3126.26\nu^{10} + 996.7\nu^9 - 549\nu^8; \quad w_\perp = -2313.32\nu^{10} + 530.7\nu^9 + 1521\nu^8. \tag{2}$$

The coefficients of these polynomials for $n_i{=}1 \div 5$ and $n_f{\geq}n_i{+}5$ are almost independent of the lower-state energy. Computations demonstrate a 1% accuracy of (2) up to $\nu{=}1000$.

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Th2-32

ROTATIONAL EXCITATION OF DEUTERATED ISOTOPOLOGUES OF NH_3 By He and H_2

Machin, L.^(1), Roueff E.^(1), Valiron P.^(2)

(1) LUTh and UMR 8102, Observatoire de Paris, 5 Place J. Janssen, 92190 Meudon, France
(2) LAOG and UMR 8102, Observatoire de Grenoble, 38 Saint martin d'Hères

All deuterated isotopologues of ammonia have been recently detected in cold interstellar clouds [1, 2, 3]. The interpretation of the observed millimeter and submillimeter transitions of NH_3 and its isotopologues requires the detailed knowledge of the possible excitation mechanisms. The study of rotational excitation of deuterated isotopologues of ammonia by a structureless atom or molecule involves several modifications compared to the corresponding mechanism relative to the pure hydrogenated component:
Whereas the intermolecular electronic potential surface is not modified by the presence of additional neutrons, the center of mass of the system : molecule + perturber is changed. In addition, the symmetry properties are also modified except in the case of ND_3. However, in this latter case, the exchange properties of deuterons, which are bosonic particles, lead to a significant increase of the nuclear degeneracy and the occurrence of a new symmetry type level (A1). We have investigated this problem in the frame of a quantal close-coupled treatment of the collision with the most recent intermolecular potential surfaces available ([4] for collisions with He and [5] for molecular Hydrogen). Corresponding results involving NH_3, NH_2D and ND_2H in collisions with He have been presented in [6, 7, 8, 9]. We will present at the conference the most recent implementations concerning ND_3-He and discuss corresponding results involving H_2 in its ground rotational level.

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Th2-33

THE BINOMIAL POTENTIAL OF ELECTRON-PROTON INTERACTION ALTERNATIVE TO THE COULOMB LAW

V.K. Gudym[1] and E.V. Andreeva[2]

[1]Space National Agency of Ukraine, Kyiv, Ukraine
[2]Institute of Physics of Semiconductors of the NASU, Kyiv, Ukraine
vgudym@mail.ru

On the basis of only classical assumptions, we have shown earlier [1,2] that an electron and a proton interact by the binomial law

$$V = -\frac{e^2}{r} + \frac{\Gamma}{r^2} \qquad (1).$$

and have determined the value of the constant Γ as $6.10276 \cdot 10^{-28}$ *CGSE units.*

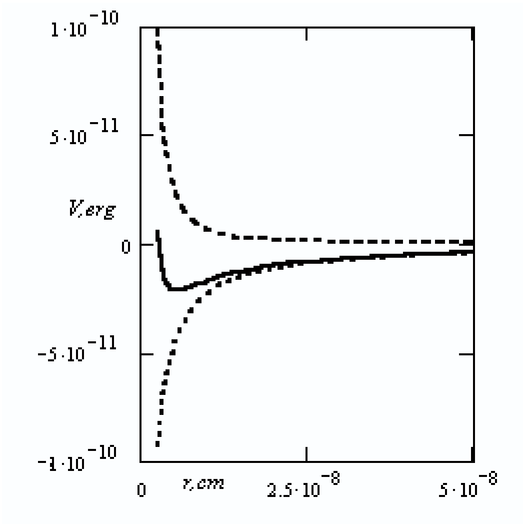
In the figure, we present the plot of potential (1) by a solid line together with the separate contributions of the first negative (Coulomb law) and second positive terms.

Potential (1) has been verified by us in the analysis of both the Kepler task of a hydrogen atom where the energy takes the form

$$E = \frac{m\dot{r}^2}{2} + \frac{M^2}{2mr^2} - \frac{e^2}{r} + \frac{\Gamma}{r^2} \qquad (2)$$

and the Schrödinger equation

$$\Delta\Psi + \frac{2m}{\hbar^2}\left(E + \frac{e^2}{r} - \frac{\Gamma}{r^2}\right)\Psi = 0 . \qquad (3)$$



We have also analyzed the scattering of an electron by a proton, as a special case of the Kepler task[3]. Below, we give the formula for the deflection angle φ_{ob} as a function of the impact parameter ρ :

$$\varphi_{0b} = \sqrt{\frac{E\rho^2}{E\rho^2 + \Gamma}} \cdot \arccos\left[\frac{1}{\sqrt{1 + \frac{4E(E\rho^2 + \Gamma)}{e^4}}}\right] . \qquad (4)$$

The calculations have shown that the formula describing the scattering of electrons in the binomial potential well represents the process within the range of impact parameters down to 10^{-13} cm for the energies of an electron from several *eV* up to hundreds of *MeV*. Further, on the basis of potential (1), we have shown the basic opportunity for the solution of the classical task concerning the movement of an electron in the field of a proton for a hydrogen atom. On this way, we were succesful to clarify the nature of the Bohr postulates, the Planck constant, and some other constants which were not treated earlier within the framework of classical mechanics. For the theory of Schrödinger, we have demonstrated, with the use of potential (1), the opportunity to understand and to resolve a number of its internal contradictions. In particular, it turns out to be possible to derive, for the first time, a wave package being stable in time in the problem concerning a hydrogen atom and to explain the mechanism of birth of a quantum in the classical interpretation.

Generally, potential (1) can be considered as a link between the classical and quantum theories.

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Th2-34

PHASE-SHIFTED MULTICHANNEL QUANTUM DEFECT THEORY ANALYSIS OF THE OBSERVED 5dnd J = 11/2 AUTOIONIZING RYDBERG SERIES OF EUROPIUM ATOM

S. Bhattacharyya[1], M. A. N. Razvi[1], S. Cohen[2] and S. G. Nakhate[1]

[1]Spectroscopy Division, Bhabha Atomic Research Centre, Mumbai 400 085, India
[2] Atomic & Molecular Physics Laboratory, Physics Department, University of Ioannina, GR–45110 Ioannina, Greece

Among lanthanides, europium is an experimentally convenient two electron system. Its spectrum is more complex than other two electron systems like helium and alkaline earth atoms because the coupling between the two outer electrons and the spin 7/2 half-filled 4f core results in multiple closely spaced ionic limits. The Rydberg series converging to those multiple limits exhibit significant inter-series interactions. Multichannel Quantum Defect Theory (MQDT) has been one of the most successful theoretical methods for interpreting perturbed bound and autoionizing spectra. Up to now MQDT has been mostly applied in closed inner-shell systems but not extensively tested in lanthanides, where there are semi-empirical eigen-channel MQDT analyses for ytterbium [1] and, more recently, for the J = 3/2 autoionizing Rydberg series of europium below the $4f^7 5d\ ^9D_4$ threshold [2].

Here we present the spectroscopy and MQDT analysis of the J = 11/2 odd-parity autoionizing Rydberg series of europium up to $5d\ ^9D_4$ threshold. The experiment was performed in a heat-pipe-oven. The autoionizing states under consideration were populated via a two-color stepwise laser excitation scheme through the $4f^7 5d6p\ ^{10}F_{7/2,\,9/2}$ intermediate levels and detected by a thermionic diode. Wavelength calibration was achieved by recording simultaneously the known optogalvanic signal of a uranium hollow cathode lamp and the interference fringes of a Fabry-Perot etalon (both illuminated by small fractions of the second scanning dye laser beam). All signals were processed by independent boxcar integrators and stored to a personal computer. The europium spectra are classified in two 5dnd (n=15-55) autoionizing Rydberg series converging to the ionic level $5d\ ^9D_4$ and eight 5dnd members (n=13-20) converging to the higher $5d\ ^9D_5$ ionic level. Energy levels spacings point the jj-coupling scheme as the most appropriate for describing the above states. The observed inter-series interactions are successfully interpreted by an empirical phase-shifted MQDT model. Energy levels positions and spectral profiles are reproduced within the experimental uncertainties. It is also shown that the interaction between discrete levels and degenerate continua is weak, resulting in narrow and almost symmetric autoionization line shapes.

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Th2-35

MANY-PARTICLE QUANTUM THEORY OF RESONANCE INELASTIC SCATTERING OF AN X-RAY PHOTON BY ATOM AND ION

A.N.Hopersky, A.M.Nadolinsky, V.A.Yavna

Rostov State University of Transport Communication, Rostov-na-Donu, 344038
Russia, hopersky_vm_1@rgups.ru

We developed a non-relativistic version of many-particle quantum theory of inelastic scattering of photon (incident photon energy $\hbar\omega_1$ and scattered photon energy $\hbar\omega_2$ from 300 eV to 1.5 MeV) near the inner shells ionization thresholds of free atoms and multiply charged atomic ions.

The effect of the wide hierarchy of many-electron phenomena on the absolute values and the shape of doubly-differential cross section of resonant inelastic scattering is studied for the light (Ne [1,2], Ar [3]) and a heavy (Xe [4]) atoms, and for the neon-like ions (Si^{4+},Ar^{8+} [5]). The energy regions of K- and KL_{23} (Ne), KM_{23} (Ar), KO_{23} (Xe)–ionization thresholds are studied. Demonstrated is the development of the spatially extended scattering cross section structure into the main (Ne $K\alpha_{1,2}$; Ar $K\beta_{1,3}$; Xe $K\alpha_{1,2}$, $\beta_{1,3}$, $\beta_2^{I,II}$) and the satellite (Ne $K\alpha_{3,4}$; Ar $K\beta^V$) structures of the photon-impact-induced X-ray emission spectra of these elements.

The calculation results are predictions, while at the fixed incident photon energies they compare well with the experiment ($\hbar\omega_1$ = 5.41 keV [6] (Ne); 3.199 keV, 3.246 keV [7] (Ar); 34.42 keV [8] (Xe)).

In [9] we extend the results of [1-5] to the X-ray vacuum ultra-violet region ($\hbar\omega_1$ from 10 to 80 eV).

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Th2-36

OBSERVATION OF PERTURBATIONS IN TRANSITION PROBABILITIES FOR ROVIBRONIC LINES OF THE (4pσ) $f^3\Sigma_u^+$, (4pπ) $k^3\Pi_u^+ \rightarrow$ (2sσ) $a^3\Sigma_g^+$ BANDS OF H_2

B.P. Lavrov, A. V. Modin, and I. S. Umrikhin

Faculty of Physics, St.-Petersburg State University, 198904, Russia.
E-mail: lavrov@pobox.spbu.ru

The ratios of the transition probabilities for pairs of P- and R-branch lines, having common upper rovibronic level, of the (0-0), (1-1) and (1-0) bands of the $f^3\Sigma_u^+ \rightarrow a^3\Sigma_g^+$ and (0-0) band of the $k^3\Pi_u^+ \rightarrow a^3\Sigma_g^+$ band systems of H_2 were measured. Previously transition probabilities of hydrogen were studied only for emission of bands coming from electronic states with the united atom principle quantum number n=3 [1]. Together with our recent work [2] devoted to the studies of 4d → 2p electronic transitions the present one reports the results of first experimental studies of radiative characteristics of high-lying n=4 electronic states of hydrogen molecule.

The emission of optically thin plasma sheath in the constriction of d. c. capillary-arc discharge in pure hydrogen under the pressure P=6 Torr and the current density j=0,015-0,1 A/mm^2 was used as a light source. The image of the focal plane of 2,65 m Ebert-Fastie spectrograph was recorded by blue pixels of 8.0 MPix CMOS-matrix (22,5x14,8 mm^2) of the Canon EOS 350D digital camera connected to PC. For experimental determination of the spectral distribution of relative sensitivity of the spectrometer we used two different calibrated tungsten ribbon lamps. It is important to note, that we observed the 1-2% intensity modulation of the image by the interference picture similar to Newton rings caused, apparently, by nonideality of projective optics and existence of thin film MgF_2 coverings on mirrors and the grating. The effect should be taken into account in intensity measurements of high precision.

The 17 ratios of the line strengths for pairs of P and R lines, having common upper rovibronic level have been measured. Significant deviations (up to two orders of magnitude) of the experimental data and predictions of adiabatic theory (ratios of Honl-London factors) are observed. It is established, that the deviations are increasing with growth of the rotational quantum number N of upper level that specifies essential role of the electronic-rotational interaction (L-decoupling) of corresponding 4pσ and 4pπ adiabatic states. Pronounced correlation between N-dependencies of relative transition probabilities for lines coming from the pair of mixed electronic-vibrational states ($f^3\Sigma_u^+, v=0$ and $k^3\Pi_u^+$, $v=0$; the v is vibrational quantum number) was observed. It shows that the perturbations are mainly determined by the interaction between pairs of rovibronic adiabatic states. We hope our experimental results could be considered as a challenge for an *ab initio* and multichannel quantum-defect calculations of the transition probabilities for high Rydberg states of simplest neutral molecule.

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RELATIVISTIC CORRECTIONS TO ISOTOPE SHIFT IN LIGHT MANY-ELECTRON IONS

V. A. Korol[1,2] and M. G. Kozlov[1]

[1] Petersburg Nuclear Physics Institute, Gatchina, Russia
[2] St. Petersburg State Polytechnic University, St. Petersburg, Russia

We calculated isotope mass shift for several light ions using Dirac wave functions and mass shift operator with relativistic corrections of the order of $(\alpha Z)^2$ found in [1]. Electronic correlations are accounted for with the help of the CI+MBPT method [2]. In this method valence correlations are included by means of configuration interaction (CI) and core-valence correlations are treated within second order many-body perturbation theory (MBPT), which is used to form an effective Hamiltonian for valence electrons.

Calculated relativistic corrections to the specific mass shift varied from a fraction of a percent for carbon ions, to 2% for magnesium. Relativistic corrections to the normal mass shift were typically smaller. Interestingly, the final relativistic mass shifts for the levels of one multiplet appeared to be even closer, than for non-relativistic operator and about one order of magnitude smaller, than typical relativistic correction. That can be important for the astrophysical search for possible variation of the fine structure constant α. It was shown in [3], that in such studies the isotope shift is a source of important systematic error. Our calculations show, that for levels of the same multiplet this systematics is negligible, and they can be used as probes for α-variation. More generally, an accurate knowledge of the mass shift can be used to separate isotope effects from the effect of α-variation. That allows on the one hand to look for the possible α-variation, and on the other hand to study isotope abundances in the early universe [4].

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Th2-38

ON THE S-WAVE MODEL OF TWO-ELECTRON ATOMS

L. U. Ancarani

Laboratoire de Physique Moléculaire et des Collisions,
Université Paul Verlaine - Metz, 57078 Metz, France

s-wave models of two-electron systems can be useful as a benchmark to study the corresponding physical problem. In this contribution, the focus is on one of the simplest *s*-wave models of two-electron atoms [1-3], in which the electron-electron repulsion ($1/r_{12}$) is replaced by the lowest order term ($1/r_>$, where $r_>=\max(r_1,r_2)$) in a one-centre expansion about the nucleus (r_1,r_2 are the two radial electron coordinates, and r_{12} the electron-electron distance).

Recently Howard and March [3] have claimed to have found the exact ground-state solution of this model. The electron density is then calculated and seen to satisfy a second-order differential equation. In a subsequent publication [4] the momentum density is studied in great detail, with particular emphasis on the asymptotic behaviour.

By comparing the *s*-wave model with the corresponding real two-electron atom for S-states, a simple analytical property has been found [5]: the mean ground-state energy obtained with a trial wave-function depending on r_1 and r_2 only (*i.e.* including radial correlation only) is the same for the two problems. Simple, well-known, trial wave-function for two-electron atoms yield a mean energy lower than the "exact" ground-state energy given by Howard and March [3], in clear contradiction with the variational principle. The solution proposed in [3] is actually not acceptable on physical/mathematical grounds, the reason being that, while the function is continuous, its derivative is not.

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Th2-39

RELATIVISTIC NUCLEAR RECOIL, ELECTRON CORRELATION AND QUANTUM ELECTRODYNAMIC EFFECTS IN BE- AND B-LIKE ARGON IONS

Z. Harman[1], R. Soria Orts[1], A. Lapierre[1], J.R. Crespo López-Urrutia[1],
A.N. Artemyev[1,2], U.D. Jentschura[1], C.H. Keitel[1], V.M. Shabaev[2], H. Tawara[1],
I.I. Tupitsyn[1,2], J. Ullrich[1], A.V. Volotka[2]

[1]Max Planck Institute for Nuclear Physics, Saupfercheckweg 1, 69117 Heidelberg,
Germany; [2]Department of Physics, St. Petersburg State University,
Oulianovskaya 1, Petrodvorets, 198504 St. Petersburg, Russia

We have performed extensive theoretical studies of the $1s^22s^22p\ ^2P_{3/2} - {}^2P_{1/2}$ forbidden M1 transition in B-like argon ions. The radiative lifetime [1] and mass isotope shift [2] associated with this line have been determined with high accuracy using the Heidelberg electron beam ion trap (EBIT).

Accurate radiative lifetimes are sensitive to quantum electrodynamic corrections like the electron anomalous magnetic moment and to relativistic electron-electron correlation effects. The lifetime of the Ar^{13+} $1s^22s^22p\ ^2P_{3/2}$ metastable state was determined to be 9.573(4)(5) ms (stat)(syst) [1]. Theoretical predictions cluster around a value that is approximately 3σ shorter than the high-precision experimental result. This presently unexplained discrepancy highlights the need for further investigations of radiative lifetimes with highly charged ions in the region of intermediate nuclear charge numbers.

The wavelengths of the above transition in Ar^{13+} and the $1s^22s2p\ ^3P_1 - {}^3P_2$ M1 transition in Ar^{14+} were compared for the isotopes ^{36}Ar and ^{40}Ar [2]. The observed isotope shift effect has confirmed the relativistic theory of nuclear recoil effects in many-body systems [3]. Our calculations, based on the fully relativistic recoil operator, are in excellent agreement with the measured results. A calculation applying the nonrelativistic part of the operator only would yield values for the isotope shift which are smaller than the experimental result by a factor of roughly three. To our best knowledge, the relativistic recoil effect has not been observed experimentally so far.

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Th2-40

Blackbody Induced Ionization of Rydberg States in Helium.

Glukhov I. L. Ovsiannikov V.D.

Voronezh State University: 394006, Russian Federation,
Voronezh, Universitetskaya sq. 1, Department of Physics

The production and control of atoms in Rydberg states is one of the current problems of the atomic spectroscopy [1]. To provide necessary conditions for their correct treating the finest effects, in particular those of the blackbody radiation, on the atomic level structure should be taken into account. We consider the general regularities of the blackbody ionization, which may significantly affect the lifetime of Rydberg states.

Matrix elements for transitions to continuum were calculated numerically on the basis of the Fues' model potential approach [2, 3]. They were used for determining ionization rates of singlet and triplet S-, P- and D-states with $n = 8 \ldots 45$.

Obtained results are in a good agreement with the approximation formula:

$$P_n = \left(a_1 x^2 + a_2 x^3 + a_3 x^4\right) \frac{1}{\exp[x] - 1} \quad \text{with} \quad x = \frac{W_n}{kT}, \tag{1}$$

where T is the absolute temperature; W_n is the ionization energy of the respective level. The coefficients a_i in (1) are temperature-dependent. Good results for $T \geqslant 200$ K are given by the third-order polynomial approximation:

$$a_i = \sum_{k=0}^{3} b_{ik} \left(\frac{T}{100}\right)^k, \tag{2}$$

where b_{ik} are constant coefficients, independent of state and temperature. They were calculated for the Rydberg singlet and triplet S-, P- and D-states. For example, the $B = \{b_{ik}\}$ - matrices for singlet and triplet S-states of helium respectively are:

$$B_{^1S} = \begin{pmatrix} 394 & -415.1 & 250.5 & 5.354 \\ -81.50 & 77.73 & -53.87 & -4.754 \\ -15.02 & 17.31 & -3.316 & 1.703 \end{pmatrix}, \tag{3}$$

$$B_{^3S} = \begin{pmatrix} 195 & -203 & 111.6 & 2.781 \\ -48.74 & 46.99 & -26.57 & -1.478 \\ 7.90 & -5.533 & -2.073 & 0.3553 \end{pmatrix}. \tag{4}$$

At the fixed temperature T formula (1) gives accurate ionization rate values not only for far Rydberg states, but also for the maximum area. Relation (1) determines correctly both the position and the height of the ionization rate maximum, as a function of the principal quantum number.

Formulae (1) and (2) accompanied with b_{ik} coefficients like (3) and (4) make possible to quickly calculate ionization rates with a correct temperature extrapolation, the deviation of which from the results of the direct computations doesn't exceed 2% at $T = 1500$ K and 6% at $T = 2000$ K.

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Th2-41

INNER SHELL IONISATION AND RELAXATION OF CO MOLECULE STUDIED BY COINCIDENCE SPECTROSCOPIES

P. Bolognesi [1], V. Feyer [1,2], L. Avaldi [1,3], A. Lahmam-Bennani[4], E. M. Staicu Casagrande[4], S. Semenov[5], V.V. Kuznetsov[5] and N. Cherepkov[5]

[1] CNR-IMIP, Area della Ricerca di Roma 1,CP 10, 00016 Monterotondo Scalo, Italy
[2] Institute of Electron Physics, National Academy of Sciences, Uzhgorod, Ukraine
[3]CNR-INFM-TASC, Gasphase beamline@Elettra, Trieste, Italy
[4] LCAM, Bât 351 Université Paris-Sud XI,F-91405 Orsay Cedex, France
[5] State University of Aerospace Instrumentation, St. Petersburg – Russia

In photoionization experiments the particular charge distribution of molecular orbitals gives rise to rather different angular distributions of the ejected electrons compared to atoms due to the loss of spherical symmetry. In order to characterize completely the inner shell molecular photoionization we have combined a series of coincidence experiments. The experiments were performed at the Gas Phase beamline of Elettra using the multicoincidence end station [1]. In a first set of measurements in CO the Auger–photoelectron coincidence angular distribution has been measured on and off the C 1s shape resonance region for both the X and B CO^{2+} states. Then photoelectron-ion coincidence angular distributions have been measured at the same photon energies used in the previous experiment. The results are compared with calculations based on the Hartree-Fock approximation and the statistical tensor formalism [2]. Both experiment and theory show that the Auger electron – photoelectron angular correlations are not sufficiently sensitive to the details of the Auger electron wave function to allow a "complete" Auger experiment in molecules. On the other hand, our calculations demonstrate that the Auger electron angular distribution measured in the molecular frame is very sensitive to the individual contributions of different partial waves of the Auger electron.

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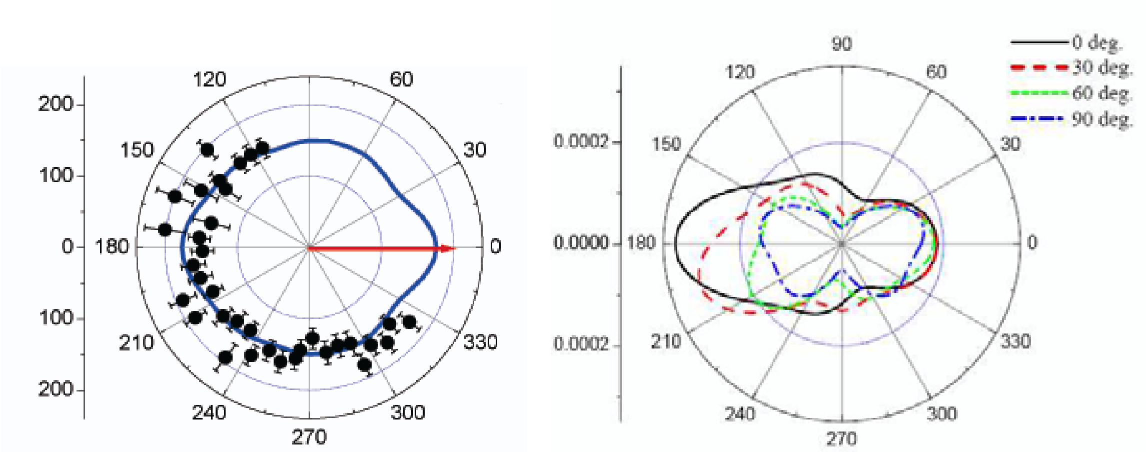

Figure 1: Left: Angular distributions of the C 1s photoelectron in coincidence with the Auger electron ejected in the decay to the CO^{2+} B state. The measurements have been done at hν=305 eV, i.e. on the σ* shape resonance, and the photoelectron is detected at 0° with respect to the direction of the polarization of the incident radiation. The full lines correspond to the predictions of the calculations. Right: The Auger electron–photoelectron angular correlations for the CO^{2+} B final state at hν = 305 eV and different angles of the photoelectron emission relative to the light polarization vector.

Th2-42

SUB-DOPPLER SPECTROSCOPY OF Tm I VAPOUR IN THE SPECTRAL REGION 410-420 nm

N. Kolachevsky, A. Akimov, K. Chebakov, I. Tolstikhina, P. Rodionov, S. Kanorsky, and V. Sorokin

P.N. Lebedev Physics Institute, Leninsky prosp. 53, Moscow, 119991 Russia

It has been experimentally shown that some rare-earth atoms can be efficiently laser-cooled using strong transitions near 400 nm [1, 2]. The use of cold rare-earth atoms enable detailed study of ultracold collisions, development of deterministic single-atom sources and is useful for some other applications. Among rare-earth elements, tulium possesses relatively simple level structure. The single stable isotope ^{169}Tm has a nuclear spin of $I = 1/2$. Cold thulium is a favorable candidate for optical clocks applications, since the forbidden transition at 1.14 μm between the fine structure sublevels $(J_g = 5/2) - (J_g{}' = 7/2)$ of the ground state $4f^{13}6s^2$ has a spectral line width of only 1 Hz. It has been shown [3] that the collisional shift and broadening of such transitions in the rare-earth atoms are suppressed due to the closed $6s^2$ shell, which open possibility for precision spectroscopy in a dense atomic sample.

In this work have we studied two candidates for cooling transitions from the ground state $(J_g = 7/2)$ to the states $4f^{12}5d_{3/2}6s^2(J_e = 9/2)$ at 410.6 nm ($A = 6\times10^7$ s^{-1}) and $4f^{12}5d_{5/2}6s^2(J_e = 9/2)$ at 420.4 nm ($A = 2.5\times10^7$ s^{-1}). Using the second harmonic of a Ti:Sa laser we have measured the saturation absorption spectra with resolution of 1 MHz and determined the hyperfine splitting of the upper levels. Similarly, we determined the hyperfine structure of two other neighbouring upper levels which correspond to the transitions at 409.4 nm $(J_e = 5/2)$ and 418.9 nm $(J_e = 7/2)$. This can be useful if the repumper laser from $(J_g = 5/2)$ is necessary.

Both transitions at 410.6 nm and 420.4 nm are not completely closed and small decay probability to the neighbouring odd parity levels exist which can prevent efficient cooling. Since there are only few dipole-allowed transitions from the upper levels, one can roughly evaluate the branching ratio using the COWAN code package [4]. The fraction of atoms which do not return to the ground state is about 10^{-5} and 10^{-4} for the 410.6 nm and 420.4 nm transitions respectively. We conclude that the transition at 410.6 nm can be used for the efficient cooling of Tm I (see also considerations given in [2]). Lower temperatures can be achieved by the subsequent switching to the completely closed cooling transition at 530.7 nm ($A = 2.3\times10^6$ s^{-1}) which can be excited by the second harmonics of Nd:GSGG laser.

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Th2-43

LASER OPTOGALVANIC SPECTROSCOPY OF NEON AND MONTE CARLO LEAST-SQUARES FITTING OF ASSOCIATED WAVEFORMS

Prabhakar Misra [a] and Xianming L. Han [b]

[a] Department of Physics & Astronomy, Howard University, Washington D.C. 20059
pmisra@howard.edu, Tel: 202-806-4913
[b] Department of Physics & Astronomy, Butler University, Indianapolis, IN 46208
xhan@butler.edu, Tel: 317-940-9873

Optogalvanic transitions in neon have been excited using a tunable dye laser impinging on a DC discharge lamp. The laser excites neon atoms from a lower level L_1 to a higher level L_2. Frequent collisions transfer the atoms from L_2 to a neighboring state L_2'. Subsequently, the neon atoms radiatively decay down to several lower levels, L_3, L_4 and L_5, and thereby acquire a different population distribution in the discharge plasma [1]. As a result of the re-distribution of energetic neon atoms, the total ionization rate will generate a different discharge current. The time-dependent optogalvanic signal waveforms were recorded with a digital oscilloscope and fitted using the following equation:

$$s(t) = \sum_{j=1}^{j_{max}} \frac{a_j}{1 - b_j\tau}[exp(-b_j t) - exp(-t/\tau)]$$

where the amplitudes a_j and rates b_j are related to the various collision/radiation parameters associated with the plasma, and τ is an instrumental time constant. In order to determine the parameters $\{a_j, b_j\}$, a sum of exponential functions was used to model the observed optogalvanic waveforms. However, as these functions are highly correlated, conventional least-squares fitting algorithms did not work very well, especially if more than three terms in the above sum were used. For this reason, we employed the Monte Carlo technique, using both the search and random walk, to develop a stable least-squares fitting algorithm that converges rapidly at a rate $1/N^{1/2}$, where N was the number of computations performed. The algorithm was stable regardless of the number of parameters used in fitting the waveforms. The Monte Carlo least-squares fitting of the experimental optogalvanic signal waveforms will be illustrated using the 630.2 nm neon transition.

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Th2-44

GROUND STATE POTENTIAL OF KCs MOLECULE

Ruvin Ferber[1], Ilze Klincare[1], Olga Nikolayeva[1], Maris Tamanis[1], Asen Pashov[2],
Horst Knöckel[3], Eberhard Tiemann[3]

[1]Institute of Atomic Physics and Spectroscopy and Department of Physics, University of Latvia, *19Rainis blvd., LV-1586, Riga, Latvia, E-mail:* onikolay@latnet.lv
[2] Department of Physics, Sofia University, 5 *J Bourchier blvd, 1164 Sofia, Bulgaria*
[3] Inst.f. Quantenoptik, Leibniz Universität Hannover, *Welfengarten 1, 30167 Hannover, Germany*

Despite of great interest in alkali heteronuclear diatomic molecules, i.e. as an object to get BEC, there are still no experimental spectroscopic data on the KCs molecule. Existing information consists of *ab initio* calculations of KCs potentials [1,2] and of long-range coefficients [3], and of experimental measurements of the dc electric dipole polarizabilities [4]. The only experimental observation of KCs laser induced fluorescence was of very low resolution and does not provide any spectroscopic constants [5].

We present the first experimental ground state potential of KCs molecule. KCs molecules were formed in a heat-pipe oven at a temperature of about 280^{o} C under ca. 2 mbar of Ar buffer gas pressure. Laser light from either an Ar^{+} laser or a dye laser with R6G dye or a diode laser (11600-11900 cm^{-1} tuning range) was used for excitation. The resulting fluorescence to the ground state was observed and recorded using a Bruker IFS125HR Fourier transform spectrometer with ca. 0.03 cm^{-1} spectral resolution. Totally about 100 fluorescence progressions (i.e. each from a single excited rovibronic level to a number of vibrational levels in the ground state) have been recorded and assigned, providing ca. 3000 lines used in the fit of the potential. A preliminary quantum number assignment was based on the potential from [1]. In the fitting process the v-numbering was decreased by one vibrational quantum to get the best fit. Currently the assigned transitions span the range from v=0 to 96 and from J=15 to 156 which covers more than 95% of the potential well depth. IPA procedure [6] was used to fit the ground state potential. Up to now the best potential fit provides a standard deviation of 0.01 cm^{-1} and describes the assigned progressions (including one for the ^{41}K^{133}Cs isotopomer) with a precision of 0.005 cm^{-1} for most of the lines, giving however in some cases unexplained deviations up to 0.03 cm^{-1}. The experimental work is under way and we believe that by increasing the body of data we can improve the situation.

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Th2-45

SPECTROSCOPIC STUDIES OF THE HIGHLY EXCITED VIBRATIONAL LEVELS OF THE $A^1\Pi$ AND $X^1\Sigma^+$ STATES IN $^{14}C^{16}O$

U. Domin, R. Kępa*, M. Ostrowska-Kopeć

Atomic and Molecular Physics Laboratory, Institute of Physics University of
Rzeszów, 35-959 Rzeszów, Poland
*rkepa@univ.rzeszow.pl

In the electronic, emission spectrum of the $^{14}C^{16}O$ isotopic molecule eight bands of the Fourth-Positive ($A^1\Pi$ - $X^1\Sigma^+$) system have been recorded and analyzed for the first time. Under high resolution and by using the Th standard lines as a calibration spectrum [1] the bands: 7-19, 8-20, 9-21, 10-21, 11-22, 12-23, 12-24, and 13-24, involved highly excited vibrational levels of the $A^1\Pi$ and $X^1\Sigma^+$ states have been recorded by conventional photographic spectroscopy. Estimated precision of the single molecular lines is considered to be in the range of 0.020-0.030 cm^{-1}. The reduction of the spectra and the calculation of the rovibronic structure parameters were performed separately for the excited and comprehensively perturbed $A^1\Pi$ state levels, and for the ground and regular $X^1\Sigma^+$ state. Considering the precision of the wavenumbers of observed spectral lines and the highest observed J-values only the B_υ and D_υ rotational as well as the ν_0-band origins were statistically significant and calculated. Numerous rotational perturbations were observed and identified in the highly excited (υ=7-13) vibrational levels of the $A^1\Pi$ state in $^{14}C^{16}O$, for the first time. All perturbations of the $A^1\Pi$ levels observed in this work as well as those observed in our laboratory earlier for the υ=0-6 levels [2-4] were confronted with perturbations predicted from theoretical calculations [5].

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Th2-46

SERIES OF DOUBLY-EXCITED STATES $^1S^e$ AND $^3S^e$ OF He*

T. T. Gien

Department of Physics and Physical Oceanography, Memorial University of
Newfoundland, St John's, NL, Canada A1B 3X7

The Harris-Nesbet variational method [1] which has been known to provide very accurate results of phase shift and cross section in electron-hydrogenlike-ion collisions at low energy [2], is considered for the determination of the series of singlet and triplet resonances $^1S^e$ and $^3S^e$ below the N=2 excitation threshold of He^+. These resonances are also known as doubly-excited autoionization states of He in this range of energy. We considered the extended four-state (E4S) scheme [2] which is supplemented by a great number of correlation terms for our calculation of both singlet and triplet S-wave scattering phase shifts.

In a similar fashion as in our work on singlet and triple P-wave resonances [3], we have tediously swept through the energy range of the resonance region below the N=2 excitation threshold of He^+ to detect these resonances. The accurate S-wave phase shifts obtained in a fairly great number around a resonance position are then fit to the Breit-Wigner formula

$$\delta(E) = \delta_0 + \tan^{-1}\left[\frac{\Gamma/2}{E - E_r}\right] \qquad (1)$$

in order to determine the position and width of the resonance.

A significantly great number of these S-wave singlet and triplet doubly-excited states belonging to the two series a and b were located by us with their positions and widths accurately determined. Many of them were located by us for the first time, to our knowledge. A comparison has been made between our results of position and width and those determined also by other research groups or individuals but with the use of different numerical methods and especially those determined by Burgers et al [4] who, by the way, has been known to locate a greatest number of these resonances so far.

Complete results of this work will be reported at the conference with discussion.

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Th2-47

PHOTODOUBLE IONIZATION OF HE WITH CIRCULARLY POLARIZED RADIATION

P. Bolognesi[1], V. Feyer[1,2], A. Kheifets[3], S. Turchini[4], N. Zema[4] and L. Avaldi[1,5]

[1]CNR-IMIP, Area della Ricerca di Roma1, 00016 Monterotondo Scalo,Italy
[2] Institute of Electron Physics, National Academy of Sciences, Uzhgorod, Ukraine
[3] Research School of Physical Sciences and Engineering, ANU, Canberra, Australia
[4]CNR-ISM, Area della Ricerca di Roma 2, Via del Fosso Cavaliere, Roma,Italy
[5]CNR-INFM-TASC, Gas Phase Photoemission Beamline@Elettra, Trieste, Italy

Photodouble ionization, PDI, of He represents the simplest process where the role of the electron correlations can be studied in detail and a lot of experimental and theoretical interest has been paid to this process [1 and references therein]. The most direct way to study PDI is an experiment where the two photoelectrons are detected in coincidence after energy and angle selection, i.e. the measurement of the triple differential cross section, $d^3\sigma/d\Omega_1 d\Omega_2 dE_1$ (TDCS), where Ω_1 and Ω_2 are the angles of emission of the two electrons and E_1 is the energy of one of them. When the incident radiation is circularly polarized it has been predicted and then experimentally observed [1] that the He TDCS displays an helicity dependence, i.e. a non vanishing circular dichroism can be measured.

In this work we have performed a set of experiments with both linearly and circularly polarized radiation at 128 eV in unequal energy sharing conditions (E_1=3.5 eV and E_2=44.5 eV) at the GAPH [2] and CIPO[3] beamlines of Elettra storage ring. Then using the method proposed by Bolognesi et al.[4] we have extracted from the experiment the gerade and ungerade amplitudes and their relative phase. Moreover in a second set of measurements we have checked one of the most interesting predictions of theories: the existence of 'dynamic nodes' in the CD, occurring whenever the ungerade and gerade amplitudes of the TDCS have a phase difference $\delta = 0$ or π. The experimental results compare well (Fig.1) with the predictions of the CCC theory [5].

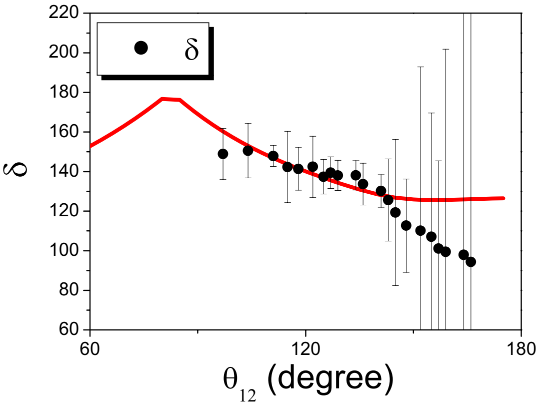

Fig. 1: Relative phase between the gerade and ungerade amplitudes . The full curve is the prediction by CCC

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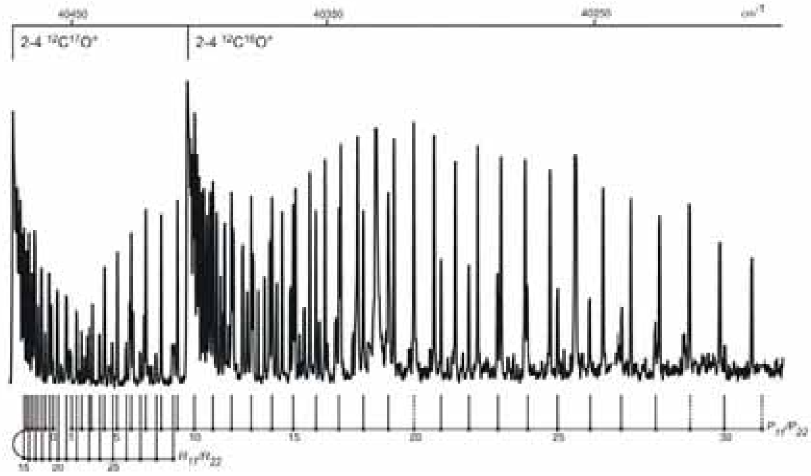
Th2-48

THE $B^2\Sigma^+$ - $X^2\Sigma^+$ TRANSITION OF $^{12}C^{17}O^+$: 2-υ” PROGRESSION

W. Szajna[a], R. Hakalla, R. Kępa[b], M. Zachwieja

Atomic and Molecular Physics Laboratory, Institute of Physics University of
Rzeszów, 35-959 Rzeszów, Poland
[a]szajna@univ.rzeszow.pl, [b]rkepa@univ.rzeszow.pl

The $B^2\Sigma^+$ - $X^2\Sigma^+$ electronic transition in the emission spectrum of $^{12}C^{17}O^+$ was first observed in our laboratory [1-2]. In this paper, we present the observation three new bands (2-4, 2-5, and 2-6) of this system in the region 36000-41000 cm^{-1}. The $^{12}C^{17}O^+$ was excited in a hollow-cathode lamp, equipped with a graphite cathode and filed with molecular oxygen (enriched ~45% of the $^{17}O_2$ isotope) under 1.0 Torr pressure.



A compressed portion of the low resolution spectrum of the $B^2\Sigma^+$ - $X^2\Sigma^+$ system of CO^+ shows the isotopic shift between $^{12}C^{17}O^+$ and $^{12}C^{16}O^+$.

The rotational analysis of the bands was performed with effective Hamiltonian of Brown [3]. Molecular constants were derived from a merge calculations, including both the present wavenumbers and the spectroscopic data published by us previously. The principal equilibrium constants for the ground $X^2\Sigma^+$ state are $\omega_e = 2185.9658(84)$, $\omega_e x_e = 14.7674(11)$, $B_e = 1.927001(38)$, $\alpha_e = 1.8236(22)\times10^{-2}$, $\gamma_e = -0.331(28)\times10^{-4}$, $D_e = 6.041(12)\times10^{-6}$, $\beta_e = 0.100(31)\times10^{-7}$ cm^{-1}, while the equilibrium constants for the excited $B^2\Sigma^+$ state are $\sigma_e = 45876.499(15)$, $\omega_e = 1712.201(12)$, $\omega_e x_e = 27.3528(39)$, $B_e = 1.754109(35)$, $\alpha_e = 2.8706(57)\times10^{-2}$, $\gamma_e = -1.15(19)\times10^{-4}$, $D_e = 7.491(20)\times10^{-6}$, $\beta_e = 2.13(12)\times10^{-7}$, $\gamma_e = 2.0953(97)\times10^{-2}$ and $\alpha_{\gamma e} = -9.46(59)\times10^{-4}$ cm^{-1}, respectively. The RKR potential energy curves were constructed for the $B^2\Sigma^+$ and $X^2\Sigma^+$ states, and Franck-Condon factors were calculated for the vibrational bands of the *B*-*X* system.

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Th2-49

PHOTOIONIZATION OF N_2 VALENCE SHELL BETWEEN 200 AND 400 EV: DIPOLE AND NON-DIPOLE PARAMETERS

P. Bolognesi[1], V. Feyer[1,2], R. Flammini[1], L. Avaldi[1,3]
D. Toffoli[4,5], P. Decleva[4]

[1] CNR-IMIP, Area della Ricerca di Roma1, CP10, 0016 Monterotondo Scalo, Italy
[2] Institute of Electron Physics, 21, Universitetska St., 88017 Uzhgorod, Ukraine
[3] CNR-INFM-TASC, Gasphase beamline@Elettra, Trieste, Italy
[4] Dipartimento di Chimica, Università di Trieste, Trieste, Italy
[5]Chemistry Department, University of Aahrus, Denmark

A cornerstone in the application of angle-resolved photoelectron spectroscopy is the dipole approximation (DA) for the description of the interaction of radiation with matter. This has provided useful information on the photoionization process itself and the orbital structure of the molecular targets [1]. Recent measurements in noble gases provided evidences of the breakdown of the DA already in the VUV region of the spectrum, for photon energies as low as few tens of eV [2 and references there in]. For the valence shells of molecules, ()both experimental and theoreticalal works have been very sparse so far [2,3,4]. Significant nondipolar effects with an oscillatory behaviour have been recently predicted in the region from threshold to 2000 eV in N_2 by a theory which uses a single-channel approach to the scattering problem, based on a single center expansion of both bound and continuum orbitals and a Kohn-Sham hamiltonian (SCE-DFT)[5]. Here we present the results of a set of measurements performed at the GAPH beamline at Elettra using the option offered by the multicoincidence end-station [6] to set a group of analyzers in the plane containing both the direction and polarizion vector of the incident radiation.

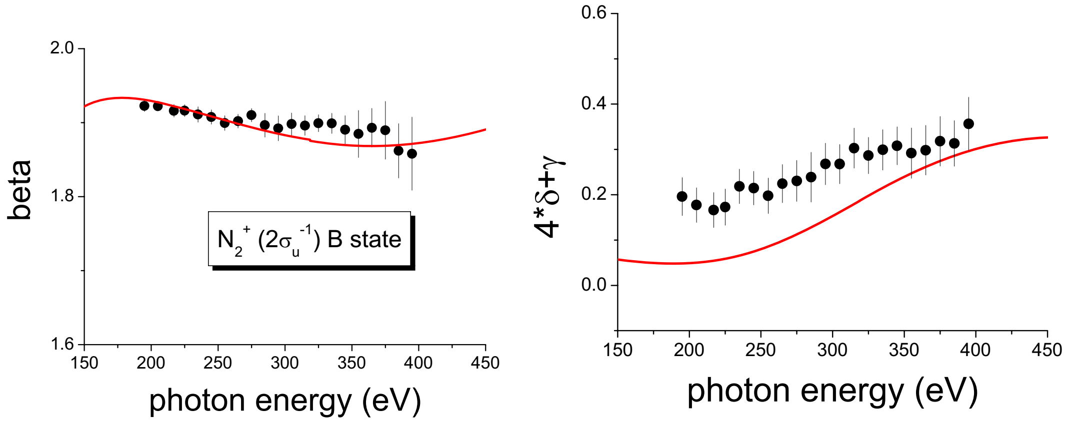

Figure 1: The dipole and non-dipole asymmetry parameters for the N_2^+ B state.

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Th2-50

Ab initio calculation of high angular momentum states for H_3^+ near dissociation.

P Barletta, B C Silva and J Tennyson
Department of Physics and Astronomy,
University College London,
Gower St., London WC1E 6BT, UK

The spectroscopy of H_3^+ and its isotopes has attracted considerable attention following the series of experiments of Carrington and co-workers [1]. They have studied the dissociative photo-excitation of the molecule in a kinetic energy window of 3000 cm^{-1}. The spectrum associated with this process was very dense, and its main features are still unexplained by the theory. One of the characteristics is that an important role was played by states with very high angular momentum (or J) which are associated with the high kinetic energy release.

Due to the centrifugal barrier, there is maximum value allowed for J depending on the molecule and the isotope considered. For higher J there are not bound molecular states, while for J just below threshold there is a very limited number of bound states. In this work we have studied the vibrational-rotational states of H_3^+ and its main isotopomer D_2H^+ for high values of the angular momentum, near the dissociation limit. As a computationl tool we have used the DVR3D computer suite [2]. Results will be presented at the meeting.

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Th2-51

ROVIBRONIC TRANSITION PROBABILITES FOR THE $(3d)^{1,3}\Lambda'_g{}^- \rightarrow (2p)^{1,3}\Lambda''_u$ BAND SYSTEMS OF H_2, HD AND D_2

S.A. Astashkevich, B.P. Lavrov

Faculty of Physics, St.-Petersburg State University, 198904, Russia.
E-mail: lavrov@pobox.spbu.ru

Absolute values of the spontaneous emission transition probabilities for electronic-vibro-rotational (rovibronic) spectral lines of the $I^1\Pi_g{}^-$, $J^1\Delta_g{}^- \rightarrow B^1\Sigma_u{}^+$ and $i^3\Pi_g{}^-$, $j^3\Delta_g{}^- \rightarrow b^3\Sigma_u{}^+$ band systems of H_2, $I^1\Pi_g{}^-$, $J^1\Delta_g{}^- \rightarrow C^1\Pi_u{}^\pm$ band systems of H_2 and D_2 and $i^3\Pi_g{}^-$, $j^3\Delta_g{}^- \rightarrow c^3\Pi_u{}^\pm$ band systems of H_2, HD and D_2 have been obtained semi-empirically in the framework of simple non-adiabatic model taking into account the electronic-rotational interaction (L-uncoupling) of the $3d^{1,3}\Pi_g{}^-$ and $3d^{1,3}\Delta_g{}^-$ states in the Van Fleck "pure precession" approximation [1,2]. We used: 1) coefficients of the Born-Oppenheimer (BO) basis-set expansion of the perturbed wave functions of upper rovibronic levels obtained semi-empirically from observed term values; 2) absolute values of electronic transition moments obtained from semi-empirical analysis of branching ratios for spontaneous emission in rotational structure of the bands and experimental lifetimes of rovibronic levels; 3) experimental data the wavenumbers of rovibronic transitions; 4) vibronic matrix elements calculated numerically with *ab initio* Born-Oppenheimer potential curves.

Most of the data for transitions to the $B^1\Sigma_u{}^+$ and the $b^3\Sigma_u{}^+$ states are obtained for the first time. The data for transitions to the $C^1\Pi_u{}^\pm$ and the $c^3\Pi_u{}^\pm$ states are amplified with regard to ones received earlier. It is shown that electronic-rotational interactions of the $3d^{1,3}\Pi_g$ and $3d^{1,3}\Delta_g$ states lead to rather high absolute values (more than 10^7 c^{-1}) of the transition probabilities for the $J^1\Delta_g{}^- \rightarrow B^1\Sigma_u{}^+$ and $j^3\Delta_g{}^- \rightarrow b^3\Sigma_u{}^+$ band systems forbidden for electric dipole transitions in BO approximation. Dependences of the transition probabilities on rotational quantum number are similar for similar bands of singlet and triplet $\Delta_g{}^- \rightarrow \Pi_u{}^-$ electronic transitions. However absolute values of transition probabilities for triplet bands are 2÷2.5 times higher than those for analogous singlet bands except for Q-branches of $I^1\Pi_g{}^- \rightarrow C^1\Pi_u{}^+$ and $i^3\Pi_g{}^- \rightarrow c^3\Pi_u{}^+$ band systems of H_2 and D_2. For these branches the specified distinction may reach two orders of magnitude. Such peculiarities of the perturbations (L-uncoupling) in the transition probabilities may be considered as some kind of interference effects.

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LASER PROBING MEASUREMENTS AND CALCULATIONS OF LIFETIMES OF THE $^2D_{3/2}$ AND $^2D_{5/2}$ METASTABLE STATES IN Ba II

Gurell J.[1], Biémont E.[2, 3], Blagoev K.[4], Fivet V.[2], Lundin P.[1], Mannervik S.[1], Norlin L.-O.[5], Quinet P.[2, 3], Rostohar D.[3], Royen P.[1] and Schef P.[1]

[1]Department of Physics, Stockholm University, Albanova, SE-10691 Stockholm, Sweden
[2]Service d'Astrophysique et de Spectroscopie Université de Mons-Hainaut, 20 Place du Parc B-7000 Mons, Belgium
[3]Institut de Physique Nucléaire, Atomique et de Spectroscopie (IPNAS) Université de Liège, Sart Tilman, Bât. B15 B-4000 Liège, Belgium
[4]Institute of Solid State Physics, 72 Tzarigradsko Chaussee, BG-1784 Sofia, Bulgaria
[5]Physics Department, Royal Institute of Technology, Albanova, SE-10691 Stockholm, Sweden

The lifetimes of the $^2D_{3/2,5/2}$ states in Ba II have been measured with a Laser Probing Technique (LPT) [1,2] at the ion storage ring facility CRYRING [3], MSL, Sweden. The lifetime of the $^2D_{3/2}$ state proved to be the longest lifetime ever measured with this technique utilizing fast ion beams, τ = 89,4±15,6 s. Also the $^2D_{5/2}$ state has a lifetime of the order of tens of seconds which was determined to be τ = 32,0±4,6 s. These new measurements are also supported by two new pseudo-relativistic Hartree-Fock calculations [4] resulting in τ = 82,0 s and τ = 31,6 s respectively.

These lifetimes have been measured previously by several groups but the experimental lifetimes of the $^2D_{3/2}$ state from the different studies are inconsistent. The value presented in this study shows good agreement with both the experimental result of Yu et al. [5] and also with several calculated values [6-8]. The measured lifetime of the $^2D_{5/2}$ state is also in agreement with several previous measurements and calculations [6-10].

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Th2-53

ANOMALOUS MAGNETO-OPTICAL RESONANCES ON THE $2p^53s$ STATES IN A Ne DISCHARGE

P. Todorov1), A. Gorbenko2), V. Polischuk2), D. Slavov1), L. Petrov1), G. Todorov1)
1)Institute of Electronics, BAS, boul. Tzarigradsko Shosse 72, 1784 Sofia, Bulgaria
2)SRI of Physics University of St Petrburg, 198903,Ulyanovskaya 1, St. Peterburg, Russia

In a series of works [1 and ref. therein], magneto-optical resonances (MOR) have been experimentally observed, resulting from destruction of the self-alignment of the resonant-$^3P_1$ ($1s_4$), (Pashen notation) and the metastable $^3P_2$ ($1s_5$) levels of NeI. Narrow MOR have been observed also irradiating Ne discharge at the transition $3s_2 - 2p_4$ ($\lambda = 632.8$ nm), where as a possible explanation of their origin the hypothesis for the metastable $^3P_2$ level self-alignment has been used [2]. The possibility to directly observe the alignment of the metastable states originates from the fact that the optical properties (absorption, refraction) of the glow discharge plasma are influenced by applied magnetic field, resulting in a destruction of self-alignment created by the plasma. The experimental set-up and geometry are the same as the used in [1]. As a probe radiation source, a dye laser has been utilized. The discharge gas cell has dimensions: 30 cm length and 0.7 cm diameter. The main part of the measurements was carried out for Ne pressure range from 0.13 to 0.3 Torr. The discharge current was not higher than 40 mA. The dependence of the transmitted dye-laser radiation intensity has been recorded as a function of the axial magnetic field applied (Faraday geometry). In the Table below are given the widths of the MORs observed at different Ne lines, compared to the Hanle signal widths observed in fluorescence.

λ, nm	Lower level J	Lande -g-factor	MOR (this work) $\Delta H_{1/2}$, Gauss	Upper level J	Lande g-factor	(Hanle effect) $\Delta H_{1/2}$,Gauss
585.2	$1s_2$ 1	1.034		$2p_1$ 0		
616.3	$1s_3$ 0		~5	$2p_2$ 1	1.34	2.32
626.6	$1s_3$ 0		~4.5	$2p_5$ 1	0.999	3.8
603.0	$1s_4$ 1	1.464	~2.3	$2p_2$ 1	1.34	2.32
607.4	÷ ÷	÷ ÷	1.67	$2p_3$ 0	-	-
609.6	÷ ÷	÷ ÷	~2	$2p_4$ 2	1.301	2.57
594.4	$1s_5$ 2	1.503	~0.3 ; 2.9	$2p_5$ 1	0.999	3.8
614.3	÷ ÷	÷ ÷	~ 0.28:;2.7	$2p_6$ 2	1.229	2.39
588.2	÷ ÷	÷ ÷	0.33	$2p_2$ 1	1.34	2.32

The most surprising results have been observed at the lines 616.3 and 626.6 nm. The absorbing level $^3P_0$ ($1s_3$) has a g-factor $J = 0$; thus no MO Faraday signal from this level should be expected. Besides, MO signals for the 585.2 nm line have not been observed. From the level $1s_5$, two-component signals have been registered. A model describing the behavior of the MOR observed at the $2p^53s$ Ne level will be discussed.

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Th2-54

AB INITIO CALCULATIONS OF THE SULFUR ELECTRON AFFINITY IN THE MCHF APPROACH

Thomas CARETTE[1], Oliver SCHARF[1], Michel R. GODEFROID[1]
and Charlotte FROESE FISCHER[2]

[1]Chimie quantique et Photophysique, Université Libre de Bruxelles, B 1050 Brussels, Belgium
[2]National Institute of Standards and Technology, Gaithersburg, MD 20899-8422, USA

The fine structure of ^{32}S and ^{32}S^{-} have been measured recently using the photodetachment microscope [1]. This technique combines an accuracy and a sensitivity high enough to allow the electron images to be recorded, even for the rarest isotopes [2]. Such experiments have been performed by the same group on a beam of ^{34}S^{-} opening the possibility of measuring the isotope shift ^{32,34}S on the electron affinity [3]. The theoretical calculation of the latter requires elaborate wave functions for estimating the expectation values of the mass polarization term [4]. The quality of the wave functions should be first assessed by monitoring the electron affinity itself.

Ab initio calculations of this property from the total energies of the infinite-mass systems S-/S are performed, adopting the numerical multiconfiguration Hartree-Fock (MCHF) approach using the ATSP-2K package [5]. It is well known that the differential correlation effects between the negative ion and the neutral atom are crucial for estimating the electron-affinity. Various correlation models including in a systematic way valence, core-valence and core correlation, limiting the core to the n=2 shell are attempted to describe this delicate balance. The one-electron orbitals are optimized using a single- and double multi-reference expansion. The valence correlation results converge to the non relativistic experimental value within 0.17 eV. Different computational strategies for including additional core-valence and core correlation in an all-electron approach are presented. Getting a better and reliable agreement with observation is definitely a hard task, the models being limited by our available computer facilities for approaching the total energy difference.

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Th2-55

LONG-LIVED ^{3}c(ν′) STATES OF THE HgAr, HgKr AND HgXe VAN DER WAALS MOLECULES.

O.S. Alekseeva*, A.Z. Devdariany**, M.G. Lednev*, A.L. Zagrebin**

o.alek@rambler.ru

*Dept. of Physics, Baltic State Technical University, 198005, St. Petersburg, Russia
**Institute of Physics, St. Petersburg University, 198904, St. Petersburg, Russia

Numerous spectroscopic experiments have been performed for the study of the optical transitions in the Hg-rare-gas (RG) Van der Waals molecules. Majority of these studies are devoted to the transitions between molecular states which are correlated with atomic states, coupled by allowed optical transitions, such as ground Hg(6^1S_0) and excited Hg(6^3P_1) states.

In the present report the first results concerning the dependencies of the radiative lifetimes $\tau_{\nu'}$ of the long-lived states $c^3 1(^3P_2)$ of the HgAr, HgKr and HgXe molecules on the vibrational quantum numbers ν′ are presented. The probabilities A (ν′, ν′′) of the ^{3}c(ν′) – ^{1}X(ν′′) transitions are calculated also. The bases of the calculations are the potential curves *U(R)* for the $c^3 1$ states [1] and dipole momentum *D(R)* [2] of the molecular radiative transitions $c^3 1 – X^1\Sigma$ determined by making use of the semiempirical method of quasimolecular term analysis and available experimental data. The results of the calculations are presented in Tables.

Table 1. Radiative lifetimes $\tau_{\nu'}$ (in 10^{-6} s) of the $c^3 1$ states of the HgRG Van der Waals molecules.

ν′	HgXe	HgKr	HgAr
0	150	206	790
1	95	154	520
2	67	129	440
3	56	116	430
4	49	109	
5	44	106	

Table 2. The probabilities A(ν′, ν′′) (in s^{-1}) of the ^{3}c(ν′)-^{1}X(ν′′) transitions

RG	Xe						Kr					
ν′ / ν′′	0	1	2	3	4	5	0	1	2	3	4	5
0	140	669	1765	3418	5545	7577	16	77	210	410	660	940
1	910	3090	5690	7520	7920	6970	190	700	1470	2320	3040	3520
2	2190	4500	4400	2410	530	23	820	2140	3150	3400	3010	2290
3	2380	1950	190	440	2130	3240	1670	2460	1780	700	80	44
4	1040	18	920	1850	1040	73	1560	670	0	433	1080	1290
5	75	270	690	30	480	1440	540	44	730	770	280	4

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Th2-56

THE Cd (5 ^3P_J)-Kr INTERACTION POTENTIALS.

O.S. Alekseeva*, A.Z. Devdariany**, M.G. Lednev*, A.L. Zagrebin**

o.alek@rambler.ru

*Dept. of Physics, Baltic State Technical University, 198005, St. Petersburg, Russia
**Institute of Physics, St. Petersburg University, 198904, St. Petersburg, Russia

In the present study the interaction potentials for the Cd (5 ^3P_J)-Kr system are determined with the use of the semiempirical method of the quasimolecular term analysis [1], [2] and experimental data for the Cd (5 $^3P_1$)-Kr interaction [3]. The potential curves are presented (Fig. 1).

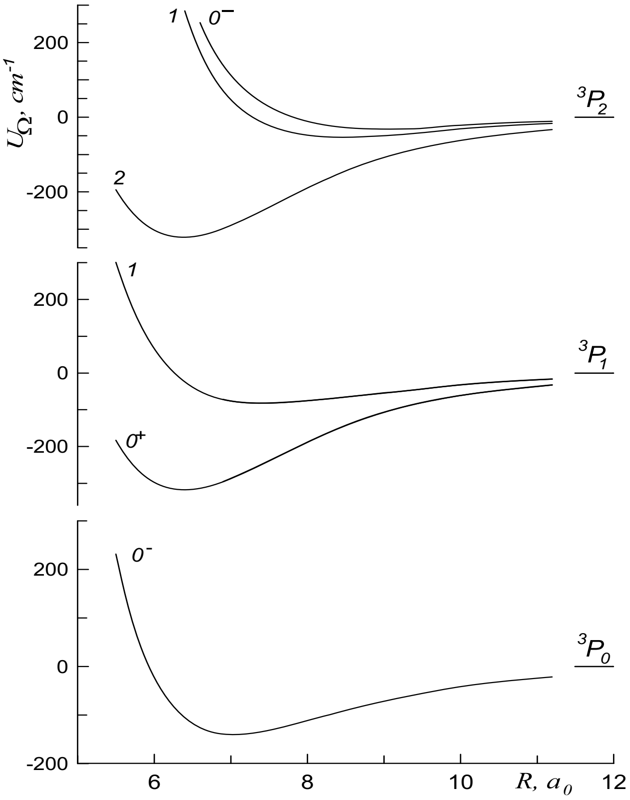

Fig. 1 Experimental potentials for the Cd ($^3P_1$)-Kr [3] interaction and determined semiempirical potentials for the Cd ($^3P_{0,2}$)-Kr system.

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Th2-57

SOFTWARE FOR MAGNETIC FLUX DENSITY CALIBRATION

A. Buczek, G. Szawioła, W. Koczorowski, A. Walaszyk, E. Stachowska

Poznan University of Technology, Chair of Quantum Engineering and Metrology
ul. Nieszawska 13B, 60-965 Poznań, Poland

E-Mail: adam.buczek@put.poznan.pl

The preliminary report presented at the ICAP Conference [1] shows the possibility of magnetic flux density measurement based on the observation of the Zeeman splittings of the two isotopes Eu^{151} and Eu^{153}. The isotopes have the same nuclear spin, similar natural abundances but the nuclear g_I-factor is nearly equal to 2. This property allows to subtract the contribution to the Zeeman splitting originating from the electronic magnetic moment keeping the smaller nuclear terms.

The present report describes a computer program appropriate for Zeeman structure analysis needed to determine the magnetic flux density. It allows to simulate and examine a pattern of M1 transitions between the Zeeman states of the hyperfine sublevels as a function of the flux density, taking into account simultaneously both isotopes.

The key part of the algorithm is coded with the very popular LabVIEW graphical programming language from National Instruments [2]. Our program related to our software for the simulation of hyperfine structures [3] can easily be integrated with the existing system based on LabVIEW. It could also easily be adopted to any optical-microwave double resonance spectroscopic experiment.

An open source beta-version of this program is available from the authors on request [4].

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[4] *adam.buczek@phys.put.poznan.pl*

Th2-58

ATOMIC STRUCTURE CALCULATION FOR Zn-like W ION

A. Mihailescu, V. Stancalie
National Institute for Laser, Plasma and Radiation Physics, Laser Dept., P.O.Box
MG-36, Bucharest, 077125 ROMANIA, Association EURATOM/MEdC

Experimental and theoretical data for highly ionized atoms are needed for diagnostics of astrophysical and laboratory plasmas. Highly ionized atoms appear in magnetically confined high-temperature fusion plasmas, such as those created with Tokamaks, stellarators, magnetic mirrors, etc, as well as in inertially confined plasmas, produced with powerful lasers or particle beams. The presence of heavy, ionized atoms results in energy losses and plasma cooling. However, since the radiation emitted from the impurities provides detailed information about the physical processes, the understanding how the inhomogeneities combine to produce an observed mean emission measure is important for testing proposal for possible heating mechanisms.

Highly ionized atoms have several properties that differ from those of neutral and few times ionized atoms. For example, there are large magnetic effects which cause the ‘fine structure’ splitting to exceed the electrostatic structure separation. The allowed electric dipole transitions encounter strong competition from forbidden transitions. The transition rates for the forbidden decays scale with higher powers of Z than those of dipole transitions. The effects of quantum electrodynamics also scale with high powers of Z. Theoretical description of such effects involves the use of relativistic quantum mechanics and an accurate treatment of electron-electron correlation effects

The primary purpose of the present work is to provide atomic structure calculation results for Zn-like W ion. The atomic structure problem is concerned with the computation of energy levels and rates of spontaneous transition among levels of the same ion (*A*-value) and from autoionizing levels of one ion to levels of the next ionisation species (autoionization rates). The calculation reported here is part of a general investigation which started with collision data for transitions of type [Ar]$3d^{10}$ $4s\, nl \rightarrow$ [Ar]$4s\, n'l'$ with n, n'=4,5 and l, l'=0,1, 2, 3 where ΔJ=0,1 [1]. To compute the atomic structure of W ions we performed similar detailed calculation using the same computer series programs[2].
This paper presents oscillator strengths, weighted Einstein transition probabilities and wavelengths along with preliminary results for selected autoionizing levels. Results have been compared to those availabele in the literature [3, 4] and a good agreement has been observed.

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LIFETIME DETERMINATIONS IN Xe VII- Xe IX

E. Biémont[1,2], M. Clar[1], V. Fivet[2], H.-P. Garnir[1],
P. Palmeri[2], P. Quinet[1,2], D. Rostohar[1]
[1]Institut de Physique Nucléaire, Atomique et de Spectroscopie,
Université de Liége, Sart Tilman (Bât. B15), B-4000 Liége, Belgium
[2]Astrophysique et Spectroscopie,
Université de Mons-Hainaut, B-7000 Mons, Belgium

A recent compilation by E.B. Saloman (NIST) [1] of all xenon lines and levels (from XeI to Xe LIV) has triggered a new interest for that atom. However, concerning lifetimes and radiative transition probabilities, our knowledge of ionized Xe is still very poor. Such data however are strongly needed in different fields of physics including astrophysics and plasma physics.

We will present recent results [2,3] concerning radiative lifetimes that have been calculated by a relativistic Hartree-Fock approach including core-polarization effects and a purely relativistic multiconfiguration Dirac-Fock method. The accuracy of our of results has been assessed through comparisons with radiative lifetime measurements obtained by beam-foil spectroscopy, one of the rare methods able to provide experimental data in these multicharged ions. An overall good agreement between theory and experiment has been observed allowing to assess the reliability of the new data.

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Contact : hpgarnir@ulg.ac.be

Th2-60

ON THE FINE STRUCTURE BRANCHING RATIOS OF PHOTODETACHMENT INTENSITIES THROUGH THE IRREDUCIBLE TENSORIAL EXPRESSION OF SECOND QUANTIZATION OPERATORS

Oliver SCHARF and Michel R. GODEFROID

Chimie quantique et Photophysique, Université Libre de Bruxelles, Brussels, Belgium

The fine structure of S and S^- have been measured recently using the photodetachment microscope technique [1]. In the appendix of their work, branching ratios of the fine structure components for s-wave photodetachment of $^{32}S^-$ were calculated using a "standard" approach and compared with the results deduced from the "fractional parentage" formula of Engelking and Lineberger [2]. The two formalisms yield to the same numerical results. A similar agreement between the two approaches, that appears as a "surprise" at first sight of the rather different expressions, was found in the study of the relative intensities of the hyperfine components of photodetachment from $^{17}O^-$ [3]. The authors of both publications [1,3] do not refer in their analysis to the work of Pan and Starace [4]. Yet, the latter does integrate the "standard" approach formula when limiting the partial waves summation to the lowest value (l=0 for the present case) according to Wigner's law, resulting in a complete separation of dynamical and geometric factors. Although the link between their general expression of the partial photoionization cross section and the previously published results [2,5,6] is established in [4], it is limited to a detailed footnote and remains somewhat obscure for a non-specialist.

The present approach based on the irreducible tensorial expression of the second quantization form of the electric dipole transition operator reproduces Pan and Starace's cross section expression and sheds some light on the fundamental relation between the various formalisms and results.

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Th2-61

Spectroscopic manifestation of radiation trapping in a supersonic beam

E. Saks[1], A. Janovs[1], P. Špels[1], I. Sydoryk[1], N. N. Bezuglov[2], I. I. Beterov[3],
I. I. Ryabtsev[3], K. Miculis[1], A. Ekers[1],
[1] Institute of Atomic Physics and Spectroscopy, LU, LV-1586 Riga, LATVIA
[2] V.A.Fock Institute of Physics, 198904 St. Petersburg, RUSSIA
[3] Institute of Semiconductor Physics SB RAS, 630090, Novosibirsk, RUSSIA

Alkali resonance lines are long known to be affected by radiation trapping in dense vapour media. In this report we demonstrate effects of radiation trapping in a collimated supersonic beam of Na atoms. The atomic beam was crossed by a laser at right angles, while laser excitation spectrum of sodium D_2-line was measured at the angles of 45° and 90° with respect to the atomic beam axis. The following unexpected features were observed in the excitation spectrum. Firstly, it was found that the spectral lines are broader or narrower than the expected Doppler width for observation at 45° and 90°, respectively. Secondly, the spectral components corresponding to excitation of different hyperfine levels exhibited intensity ratios different from those expected from the theoretical line strengths. Both findings are explained by a combination of effects of optical pumping and radiation trapping (RT). At low laser intensities, when nonlinear optical effects can be neglected, RT can strongly affect lineshapes of the HFS components. Comparison of the excitation spectrum measured at 45° with the calculation for different atom densities in the beam is shown in Fig.1. The simulation is based on the approach described in [1], and it takes into account anisotropy of the velocity distribution of atoms in the beam. The best agreement between the theory and the experiment was observed for $n_{3S}=3.6\times10^{10}$ cm^{-3}, which is close to the density calculated from the saturated vapor pressure and geometry of the beam. Sensitivity of RT to the density of atoms in the beam can be exploited as a tool to measure atom densities in atomic beams.

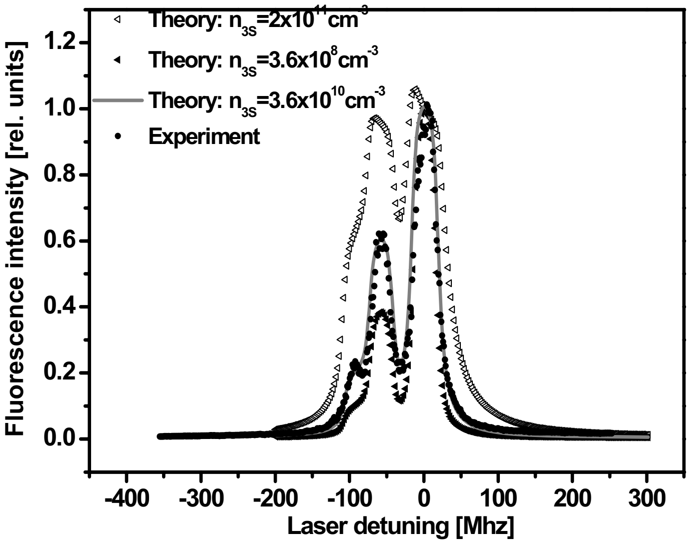

Fig.1. Laser excitation spectrum of Na($3p_{3/2}$) F' = 1, 2, 3 levels from the $3s_{1/2}$ F"=2 level observed under 45°.

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Th2-62

FLUORESCENCE OF HELIUM DOUBLY EXCITED STATES BELOW $N = 2$ IN HOMOGENEOUS ELECTRIC FIELD

Andrej Mihelič* and Matjaž Žitnik

Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

We study the Stark effect on doubly excited states of the helium atom below the $N = 2$ ionization threshold in high electric fields. The *ab initio* photoionization and total inelastic photon scattering cross sections for field strengths up to 100 kV/cm are calculated and compared to the ion yield [1] and the recent VUV fluorescence yield measurements [2,3]. The method of complex scaling is used, for incident photons with the polarization vector **P** both parallel and perpendicular to the externally applied electric field **F**. Radiation damping due to coupling of the atom to the radiation field is taken into account [4], which may be seen to be crucial for those states that decay predominantly by fluorescence. The present results are the first *ab initio* calculations of the photoionization cross sections that explain in detail the measured signal for the parallel experimental setup ($\mathbf{P} \parallel \mathbf{F}$), and the first predictions for the perpendicular experimental geometry ($\mathbf{P} \perp \mathbf{F}$). Furthermore, the total inelastic scattering cross sections in strong fields are calculated for the first time for both linearly independent polarizations.

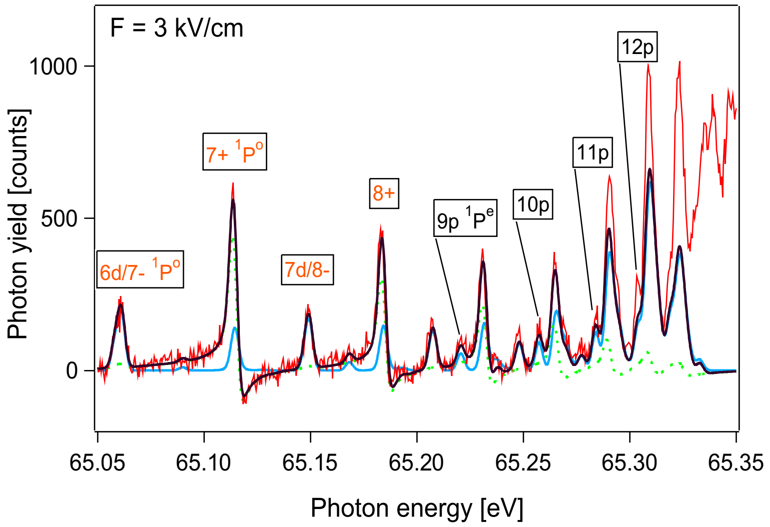

Figure: The calculated and measured [3] fluorescence yield. The dashed line is the admixture of the (calculated) photoionization signal due to the fluorescence generated by collisions of charged particles with the experimental equipment.

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* Electronic address: andrej.mihelic@ijs.si

Th2-63

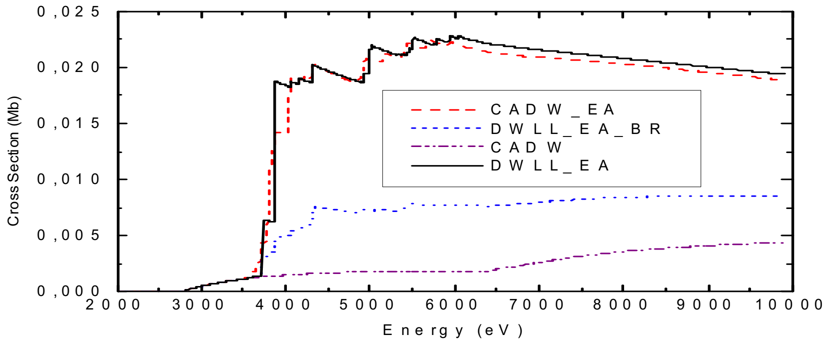
EXCITATION-IONIZATION CROSS-SECTION Na-LIKE TIN

A. Yumak, U. Golcek, I. Yavuz and Z. Altun

Marmara University, Department of Physics, 34722, Ziverbey, Istanbul, Turkey.

The electron impact ionization cross section for Na- like Sn has been calculated in both configuration-average [1] and level-resolved distorted-wave [2] methods. The ground configuration of Sn^{39+} is $1s^2 2s^2 2p^6 3s$. The direct ionization cross sections have been calculated for the 2s, 2p, and 3s sub-shells in both methods. The contributions from the $1s^2 2s^2 2p^5 3snl$ and $1s^2 2s 2p^6 3snl$ excited configurations with n=3, 4, 5, 6 and l=0, 1,2,3,4 as excitation-autoionization channels are also included. We present result with and without branching ratios allowing radiative stabilization before the autoionization. The effects of level splitting on the excitation-autoionization contribution are studied. The threshold energies and the bound radial orbitals are calculated using the Cowan relativistic Hartree-Fock atomic structure code which includes mass-velocity and Darwin terms. Such corrections are also included in the calculations of radial continuum orbitals.

The curve labeled CADW represent the total direct ionization cross section calculated with the configuration-average distorted-wave method associated with the direct ionization of 2s, 2p and 3s subshells. The curve labeled CADW_EA includes contributions from the excitation-autoionization channels. The DWLL_EA curve represents the total cross section calculated using distorted wave method which is the sum of the direct and indirect cross sections of excitation-autoionization channels. The same calculation including the branching ratios are presented in the curve labeled CADW_EA_BR.



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Th2-64

SPECTROSCOPY OF HEAVY MULTI-CHARGED IONS AND EXOTIC ATOMIC SYSTEMS: QED PERTURBATION THEORY APPROACH

A.V.Glushkov, E.P.Gurnitskaya, O.Yu.Khetselius and L.A.Vitavetskaya

Odessa University, P.O.Box 24a, Odessa-9, 65009, Ukraine-Russia

A consistent theoretical approach, based on the relativistic density functional (DF) approach and quantum electrodynamics perturbation theory (QED PT) [1,2], is used for the calculation of the exotic atomic and nuclear systems. One of the main purposes is establishment of a quantitative link between quality of the nucleus structure modelling and accuracy of calculating energy and spectral properties. Another one is application of our atomic-nuclear numerical code to calculation of spectra of the hadronic (pion, kaon, hyperon) atoms. Ab initio approach to relativistic calculation of the spectra for multi-electron super heavy ions with an account of relativistic, correlation, nuclear, radiative effects on the basis of gauge-invariant quantum electrodynamics perturbation theory is used. Zeroth approximation is generated by the effective functional, constructed on the basis of the comprehensive gauge invariance procedure [2]). The wave functions zeroth basis is found from the Klein-Gordon (pion atom) or Dirac (kaon, hyperon) equation. The potential includes the effective core potential, the electric and polarization potentials of a nucleus (the Fermi model, the gaussian form of charge distribution in the nucleus and the uniformly charged sphere are considered) [2]. For low orbits there are important effects due to the strong hadron-nuclear interaction (pion atom). The energy shift is connected with length of the hadron-nuclear scattering (scattering amplitude under zeroth energy). There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams (particles screening, particle-hole interaction, mass operator iterations). The magnetic inter-electron interaction is accounted in the lowest (on α constant of hyperfine structure), the Lamb shift polarization part- in the Uhling-Serber approximation, self-energy part of the Lamb shift is accounted effectively with the use of the Green functions method. We carried out calculations: Shifts and widths of transitions (2p-1s,3d-2p, 4f-3d) in some pionic and kaonic atoms.

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ISOBAR SELECTIVE LASER PHOTODETACHMENT IN TRACE ELEMENT ANALYSIS

P. Andersson[1], A. Lindahl[1], O. Forstner[2], D. Hanstorp[1]

[1]Department of Physics, Gothenburg University, SE-412 96 Gothenburg, Sweden
[2] Institut fuer Isotopenforschung und Kernphysik, VERA-Laboratory,
University of Vienna, Kavalierstrakt A-1090 Wien
E-mail: `anton.lindahl@physics.gu.se`

We are investigating the possibility to use laser photodetachment of negative ions as an isobaric selective filter in accelerator based mass spectrometry (AMS). If successful, this method can be used to obtain higher sensitivity in radiodating experiments or, alternatively, construct smaller and hence cheaper AMS facilities.
The radionuclide of particular interest in this work is ^{182}Hf, which is produced in supernova explosions. The half-life of this isotope is 9 million years. Hence, any ^{182}Hf produced at the time of the formation of our solar system will now have decayed. Detection of this isotope in terrestrial samples would therefore indicate reminiscences from a recent supernova explosion in the vicinity of our solar system.
A major problem when detecting the heavy trace element ^{182}Hf in machines available today is to separate it from the stable isobar ^{182}W, which results in an interfering background. Currently, this background is suppressed by using suitable molecular ions in the injection stage of the accelerator [1].
In this work we are presenting a study where we investigate the possibility to achieve an additional suppression of the interfering ^{182}W isobar using the photodetachment process. Test experiments have been carried out in a small ion beam apparatus where pulsed tunable laser radiation is used to measure the photodetachment cross section of different molecular ions. We will present studies of the photodetachment process for various tungsten and hafnium molecules with the aim to identify a possible scheme to obtain an isobaric suppression.

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Th2-66

Determination of the hyperfine structure constants of high-lying even parity electronic levels of lanthanum atom

B. Furmann

Chair of Quantum Engineering and Metrology
Faculty of Technical Physics, Poznań University of Technology
Poznań Poland
Boguslaw.Furmann@put.poznan.pl

The results of the measurements of the hyperfine structure constants for over 60 electronic levels belonging to the even configurations in lanthanum atom with energy values within the range 16000-40000 cm^{1} [1] are presented. The investigations have been performed with the method of laser induced fluorescence in a hollow cathode [2]. Since the spectral lines involving the levels studied are very weak, their hyperfine structure was not extensively investigated before. Very precise results, obtained with resonance methods, were available only for low-lying levels [3]. In the energy range investigated within this work previously available literature date concern only less than twenty levels [4, 5]. In most cases the hyperfine structure constants presented within this work have been obtained for the first time. Moreover, several new levels in lanthanum atom with energies above 30000 cm^{-1} have been found. A modified method of determination of the energies of new electronic levels is presented, based on the experimental analysis of the relation between the population changes of the levels and the laser induced fluorescence signal.

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Th2-67

THEORY OF THE STARK EFFECT: INFLUENCE OF DIMENSION

V.V. Bondarchuk, I.M. Shvab

Uzhgorod National University, 54 Voloshin str., Uzhgorod 88000, Ukraine
igor_shvab@yahoo.com

The results of theory of Stark effect [1] are generalized in case of space of arbitrary dimension D. By means of perturbation theory and comparison equations method the asymptotic expansion of solution of Schrödinger equation are built for a D-dimensional hydrogenlike atom in a uniform electric field F [2]:

$$\left[-\frac{1}{2}\Delta-\frac{Z}{r}+Fx_1\right]\Psi(\vec{r})=E\Psi(\vec{r})\,.$$

Here $r=\left(\sum_{i=1}^{D}x_i\right)^{1/2}$ is the hiperradius, F is the field strength directed along an axis x_1, $\hbar=m_e=e=1$. The Schrödinger equation can further be separated in hyperparabolic coordinates $\Psi(\vec{r})=f_1(\xi)f_2(\eta)\Upsilon(\Omega_{D-2})$ yielding for $f_1(\xi)$ and $f_2(\eta)$:

$$\frac{\partial^2 f_1(\xi)}{\partial\xi^2}+\frac{D-1}{2\xi}\frac{\partial f_1(\xi)}{\partial\xi}+\left[\frac{E}{2}+\frac{\beta_1}{\xi}-\frac{F}{4}\xi-\frac{m_{D-2}(m_{D-2}+D-3)}{4\xi^2}\right]f_1(\xi)=0\,,$$

$$\frac{\partial^2 f_2(\eta)}{\partial\eta^2}+\frac{D-1}{2\eta}\frac{\partial f_2(\eta)}{\partial\eta}+\left[\frac{E}{2}+\frac{\beta_2}{\eta}+\frac{F}{4}\eta-\frac{m_{D-2}(m_{D-2}+D-3)}{4\eta^2}\right]f_2(\eta)=0\,,$$

$$f_1(\xi)\underset{\xi\to 0}{\approx}\xi^{\frac{m_{D-2}}{2}}\,,\quad f_2(\eta)\underset{\eta\to 0}{\approx}\eta^{\frac{m_{D-2}}{2}}\,,$$

$$f_1(\xi)\underset{\xi\to\infty}{\approx}\frac{A}{\xi^{D/4}}\exp\left(-\frac{F^{1/2}}{3}\xi^{3/2}+\frac{E}{F^{1/2}}\xi^{1/2}\right),$$

$$f_2(\eta)\underset{\eta\to\infty}{\approx}\frac{B}{\eta^{D/4}}\sin\left(\frac{F^{1/2}}{3}\eta^{3/2}+\frac{E}{F^{1/2}}\eta^{1/2}+\Phi\right).$$

Using the comparison equations method the asymptotic expansion in a power series of F for the energy level $E(F)$ which is valid for small F within members $O(F^5)$ is obtained. Asymptotic expression is obtained for imaginary addition ΔE to energy of the system which determines the width of level on which a discrete atomic level runs back at overlay of the external electric field. Found out enough strong dependence ΔE on the size of charge Z of nuclei, and also space dimension D. For large value D width of level practically does not depend on a value of principal quantum number and asymptotically tend to zero.

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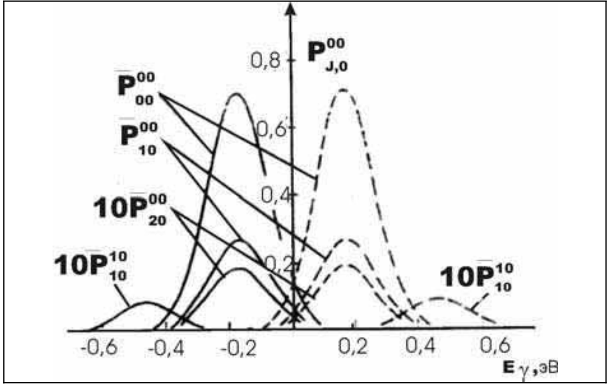
Th2-68

NEW LASER-ELECTRON NUCLEAR EFFECTS IN THE NUCLEAR γ TRANSITION SPECTRA IN ATOMIC AND MOLECULAR SYSTEMS

A.V.Glushkov and S.V.Malinovskaya

Odessa University, P.O.Box 24a, Odessa-9, 65009, Ukraine-Russia

A new class of problems has been arisen in the modern quantum optics and spectroscopy and connected with modelling of the co-operative laser-electron-nuclear phenomena in the atomic and molecular systems [1]. It includes a calculation of the probabilities and energies of the mixed γ-optical quantum transitions in atoms and molecules, intensities of the complicated γ-transitions due to the changing of the molecular excited states population under action of laser radiation, quantum chemical calculation of the complex “laser-nuclear-molecule” systems. Due to the emission or adsorption of the nuclear γ-quantum in molecular system there is changing the electron vibration-rotation molecular states. As result, general energetic and structural properties of system are changed. We at first develop a new, consistent, quantum-mechanical approach to calculation of the electron-nuclear γ transition spectra (set of vibration satellites in molecule) of nucleus in atom and molecule, based on the relativistic density functional (DF) formalism and energy approach (S-matrix formalism of Gell-Mann and Low) [1,2]. Decay and excitation probability are linked with imaginary part of the atom (molecule) - field system. For radiate decays it is manifested as effect of retarding in interaction and self-action and calculated within QED DFT theory. Calculation results of the electron-nuclear γ -transition spectra of the nucleus in some atomic and multiatomic systems are given. As illustration in fig. 1 a spectrum of emission and adsorption of nucleus ^{127}I (E_γ=203keV) in molecule of H^{127}I; is presented (fig.1 is corresponding to the initial state of molecule: $v_a=0$, $J_a=0$). Estimates are made for vibration-nuclear transition probabilities for number of molecules: diatomics, three-atomic XY_2 ($D_{\propto h}$), four-atomic $XY_3(D_{3h})$, five-atomic $XY_4(T_d)$, six-atomic XY_3Y_2 (D_{3h}), seven-atomic $XY_6(O_h)$ ones.



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Th2-69

Direct diagonalization of the hyperfine structure matrix – example of the even configurations of lanthanum atom

J. Ruczkowski, J. Dembczyński, M. Elantkowska

Chair of Quantum Engineering and Metrology, Faculty of Technical Physics,
Poznan University of Technology,
Nieszawska 13B, 60-965 Poznan, Poland
Jerzy.Dembczynski@put.poznan.pl

High precision measurements of the hyperfine structure (hfs) splittings of electronic levels, especially by rf-spectroscopic methods make it possible to study even fairly complicated aspects of the interaction between electron shells and the nucleus, which can result in determination of the nuclear moments with high accuracy.
We report the parametrization method of the hyperfine structure which takes into account simultaneously one and two-body effects appearing in the second order perturbation theory.
In order to include the J-off-diagonal effects in the hyperfine structure, direct diagonalization of the matrix containing J-diagonal as well as J-off-diagonal elements has to be performed in the basis of Ψ(configuration,vSLJF) states, in the many configurations approximation. Usually, the "repulsion" effects of the neighbouring levels with the same quantum number F are considered. It requires the precision up to 16 significant digits. The diagonal part of this matrix consists of coefficients corresponding to particular components of the energy of a hyperfine structure E_F : center of gravity of hfs energy W_J and the experimental hfs constants A, B, C and D. These parameters are treated as free in the fitting procedure of the experimental and the calculated hfs energies E_F. The differences between E_F and $E_{F\pm1}$ values are equal to experimentally determined hyperfine structure intervals. Values of J-off-diagonal matrix elements are fixed.
As a result, we obtain final values of the hyperfine structure constants, which can be used again to determine the radial hfs parameters.

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Th2-70

RESONANT DOUBLE PHOTO-IONISATION SPECTROSCOPY OF STRONTIUM

Dr E. Sokell, Dr M. Grimm, P. Sheridan*
Atomic and Molecular Physics Group, School of Physics, UCD Dublin, Ireland

Double photo-ionisation (DPI), though forbidden by the one electron model of ionisation, provides insight into electron correlation inside the atom. Triple differential cross-section (TDCS) measurements indicate the DPI cross-section with respect to the energy of one electron along with the angle of ejection of the two electrons. TDCS measurements for the resonant DPI process in strontium were performed at the Synchrotron Radiation Source (SRS), Daresbury Laboratory, (UK). The TDCS was measured on the $4p \rightarrow 4d$ resonance due to the extremely low cross-section for the direct process. The two ejected electrons were detected in coincidence in the plane perpendicular to the propagation vector of the incident light, one at -90^o to the photon $\vec{E}$ vector and the second in a range approximately from 90^o to 270^o from the first electron. The atomic strontium was produced in a cylindrical oven heated to 570^oC and directed to the interaction region by 6 converging atomic beams. Experimental data is presented for unequal energy sharing of the excess energy by the two electrons. These results are compared to the selection rules outlined by Maulbetsch *et al.* [1] and to the parametrisation of the TDCS by Malegat *et al.* [2], although they are not intended for the resonance case. Agreement between experiment and theory is not obtained when the $4p \rightarrow 4d$ resonance is assumed to have pure $^1P^o$ symmetry. Possible reasons for this discrepancy are discussed with reference to previous data by West *et al.* [3].

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* email: paul.sheridan@ucd.ie

TRANSITION PROBABILITIES IN SINGLY IONIZED PROMETHIUM (Pm II)

V. Fivet[1], P. Quinet[1,2] and É. Biémont[1,2]
[1] Astrophysique et Spectroscopie, Université de Mons-Hainaut,
B-7000 Mons, Belgium
[2] IPNAS, Université de Liège, Sart Tilman (Bât. B15),
B-4000 Liège, Belgium
Vanessa.fivet@umh.ac.be,pascal.quinet@umh.ac.be,E.Biemont@ulg.ac.be

Recently, Cowley *et al.* [1] reported the possible identification of Pm in the spectra of the stars HD 101065 and HR 465, an identification which raises questions about the possible sources of this short-lived radioactive element. As conventional theories of nucleosynthesis are not able to provide plausible mechanisms for the production of a measurable amount of Pm in the atmospheres of unevolved stars, this requires the consideration of nuclear reactions as a possible explanation for generating this element. A confirmation of this suggestion would definitely establish that spallation processes can affect in a significant way the chemical composition of stellar envelopes.

The analysis of the available astrophysical observations however is hindered by the large uncertainties resulting from the lack of transition probabilities for Pm II. In this perspective, a detailed investigation of the atomic transitions of this radioelement is strongly needed and particularly interesting not only for confirming the presence of this element in some stars but also for a quantitative reliable determination of its abundance.

In the present work, we report on the first determination of theoretical transition probabilities for a set of 46 Pm II transitions of astrophysical interest. These results have been obtained within the framework of a relativistic Hartree-Fock approach taking core-polarization effects into account. Configuration interaction effects, which are expected to play a major role in this complex spectrum, have been included in the calculations within the limits imposed by the available computers. The present results extend the content of DREAM, a database of astrophysical interest for lanthanides, which is available and regularly updated on a web site of Mons University [2].

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ATOMIC STRUCTURE CALCULATIONS IN THE ACTINIDES: THE CASES OF PLUTONIUM (Pu II) AND OF AMERICIUM (Am I)

V. Fivet[1], P. Quinet[1,2] and É. Biémont[1,2]
[1] Astrophysique et Spectroscopie, Université de Mons-Hainaut,
B-7000 Mons, Belgium
[2] IPNAS, Université de Liège, Sart Tilman (Bât. B15),
B-4000 Liège, Belgium
Vanessa.fivet@umh.ac.be,pascal.quinet@umh.ac.be,E.Biemont@ulg.ac.be

Recently Gopka *et al.* [1] claimed that they had identified some lines of radioactive elements with Z = 84-99 (with the exception of At and Fr) in the spectrum of the CP star HD 101065 (Przybylski star) and explained their presence as a result of radioactive decay of Th and U nuclei and neutron capture processes producing some transuranium isotopes.

In relation with their radioactivity, the actinides have been rather little investigated up to now. On the theoretical side, the complications result from the extreme complexity of the spectra of these elements and ions and, on the experimental side, from the difficulty to have access to sufficient samples of transuranians for laboratory investigations.

In the present work, we report on the first determination of transition probabilities for Am I and Pu II transitions of astrophysical interest. In Am I, they extend and improve some preliminary results recently published [2]. The reliability of a relativistic Hartree-Fock model of atomic structure, taking configuration interaction and core-polarization effects into account, is assessed through comparisons with the few experimental radiative lifetimes reported in the literature [3].

It is expected that these sets of new data will help the astrophysicists for establishing on a firmer basis the eventual presence of some lines of radioactive elements in the spectra of CP stars like the Przybylski star.

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Th2-73

Vibrational analysis of the N_2^+(C-X) fluorescence after inner-shell excitation of N_2

A Ehresmann[1],
L Werner[1], S Klumpp[1], Ph V Demekhin[1,2], V L Sukhorukov[2,3], H Schmoranzer[3] and
K-H Schartner[4]

[1]Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology, University of Kassel, D-34109 Kassel, Germany
[2]Rostov State University of Transport Communications, 344038 Rostov-on-Don, Russia
[3]Department of Physics, Kaiserslautern University of Technology, D-67653 Kaiserslautern, Germany
[4]I. Institute of Physics, Justus-Liebig University Giessen, D-35392 Giessen, Germany

The fluorescence emission after photoexcitation of the N_2 $1s^{-1}\pi^*$ (v) inner-shell resonances were studied experimentally and theoretically in the fluorescence spectral range between 165 nm and 205 nm. This range is dominated by the strong N_2^+(C $^2\Sigma_u^+ \rightarrow$X $^2\Sigma_g^+$) vibronic band sequences with constant $\Delta v = v' - v''$. Individual bands are hardly resolvable due to almost parallel potential curves of the C and X state of N_2^+. Calculations performed in the present work show that the broad unresolved background in the fluorescence spectra corresponds to the D $^2\Pi_g \rightarrow$ A $^2\Pi_u$ and (2) $^2\Pi_g \rightarrow$ A $^2\Pi_u$ band systems in the N_2^+ ion, extending the analysis performed in [1]. With new experiments using photon-induced fluorescence spectrometry (PIFS) [2] with very high fluorescence resolution of about 0.1nm FWHM individual N_2^+ C(v') → X(v'') vibronic bands could be resolved within the $\Delta v = -6$ and -7 sequences. Calculations of the observed fluorescence spectra, taking into account predissociation of the N_2^+ C vibronic states with $v' \geq 3$ and molecular rotation describe very well the determined fluorescence emission cross sections for the individual vibronic bands of the N_2^+(C-X) system completing the analysis of the N_2 $1s^{-1}\pi^*$ (v) inner-shell resonances decay into the N_2^+ C state carried out in [3, 4].

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Th2-74

AUGER EFFECT IN ATOMS AND SOLIDS: CALCULATION OF THE AUGER DECAY CHARACTERISTICS IN ATOMS AND SOLIDS

S.V.Ambrosov, A.V.Glushkov, L.V.Nikola and T.A.Florko

Odessa University, P.O.Box 24a, Odessa-9, 65009, Ukraine-Russia

Paper is devoted to calculation of characteristics of the Auger decay in the complicated atomic systems and solids. S-matrix Gell-Mann and Low formalism, quantum-electrodynamical perturbation theory and density functional theory are used in calculation scheme [1,2] The cross-sections of ionization of the internal shells for a number of atoms (*Na,Si, Au*) and energies of Auger electron transitions in solids (*Na,Si,Ge,Ag*) are calculated with account of the correlation effects.

As example in table 1 we present the experimental and theoretical data on the Auger electrons energies for solids. Theoretical data in the column B are corresponding to results of present calculation. For comparison in the column A we present the well known data of Larkins [3], obtained with using the equivalent core approximation. The last method gives an accuracy ~ 2 eV. Our approach gives significantly more exact results, first of all, because of more correct accounting for inter electron correlation effects and using more comprehensive relativistic electron functions basises [1].

Table 1

Experimental and theoretical data on the Auger electrons energies for solids: semiempirical calculation data of Larkins [3]; B – present data;

Element	Auger line	Experiment	Theory A	Theory B
Na	$KL_{2,3}L_{2,3}\ ^1D_2$	994,2	993,3	994,2
Si	$KL_{2,3}L_{2,3}\ ^1D_2$	1616,4	1614,0	1616,2
Ge	$L_3M_{4,5}M_{4,5}\ ^1G_4$	1146,2	1147,2	1146,1
Ag	$M_5N_{4,5}N_{4,5}\ ^1G_4$	353,4	358,8	353,4

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Th2-75

RESOLUTION ENHANCEMENT BY DECONVOLUTION IN ELECTRON ENERGY LOSS SPECTROSCOPY

S. Aksela, A. Mäkinen, and S. Urpelainen

Department of Physical Sciences, P.O.B. 3000, FIN-90014 University of Oulu, Finland

Numerical deconvolution method recovery[1] has been applied to high resolution electron energy loss spectra of Kr and Xe rare gases. It is demonstrated that the method can be used successfully both to improve the resolution and to remove the asymmetry of original peaks.

Electron energy loss spectra are ideal for deconvolution applications because the instrument function is easily and reliably obtained from the elastically scattered primary peak. The fundamental conditions for the successful application of deconvolution procedure is the reliable information of the broadening function which will be deconvoluted from the measured spectrum and good statistics in the original spectra because deconvolution always increases the statistical noise. Our results show that the numerical deconvolution is a powerful and helpful tool under these conditions. Its power has not yet fully utilized in electron spectroscopy.

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Th2-76

HYPERFINE INTERACTION-AFFECTED METASTABLE LEVEL LIFETIMES IN NI-LIKE IONS OF XENON

E. Träbert [1,2], P. Beiersdorfer [2], G. V. Brown [2]

1 Ruhr-Universität Bochum (Germany), 2 UC LLNL, Livermore, CA (USA)

Electron beam ion trap experiments with a time-resolving cryogenic microcalorimeter have shown a metastable level, $3d^9$ 4s $^3D_3$, in Ni-like ions of Xe. The level is long lived, because its only decay path is via a magnetic octupole (M3) transition [1]. Such metastable levels play a role in plasma dynamics and are important for density diagnostics. The experimental lifetime value of about 11.5 ms, however, fell short of the theoretical predictions that range from 14 ms to almost 19 ms.

Yao et al. [2] conjectured that the experimental result, in fact, agreed with theory, but that it was necessary to recognize that the experiment had used natural Xe and thus a mixture of isotopes, and that in the two odd isotopes ^{129,131}Xe (which make up about 49% of the natural isotope abundance) the hyperfine interaction mixes the $3d^9$ 4s $^3D_3$ level with the $3d^9$ 4s $^3D_2$ level. The latter has a faster E2 decay channel, and therefore the magnetic sublevels that mix should have a lifetime that is shorter than in the absence of nuclear spin.

We have since remeasured the metastable level lifetime at the Livermore electron beam ion trap SuperEBIT, employing a much more efficient, but much less energy-resolving, proportional counter. The new data [3] have vastly better statistics; with the natural isotope mix, the multi-exponential shape of the decay curve is now clearly demonstrated. Using an even isotope, ^{132}Xe (without nuclear spin and therefore without hyperfine structure), we find a single decay component of about 15 ms, in agreement with the prediction by Yao et al. [2]. In the odd isotope ^{129}Xe, a second decay component of about 3 ms arises from the single hyperfine mixed sublevel. (^{131}Xe is predicted to have several mixed sublevels with different lifetimes, which would be difficult to disentangle in the decay curve analysis.) Yao et al. claim the existence of an interference effect in the hyperfine mixing that would give the magnetic sublevels of ^{129}Xe individual lifetimes within a 10% band around the 3 ms lifetime seen. Our experiment is not sensitive to this scatter, and the purported interference effect itself has since been put in doubt on the basis of fundamental symmetry arguments [4]. The basic hyperfine effect, however, has been confirmed by our measurements and needs to be taken into account in any applications.

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Th2-77

Lifetime vibrational interference effects during the NO $1s^{-1}\pi^*$ (v_R) resonance Auger decay into the NO^+ A $^1\Pi$ state investigated through NO^+ (A $^1\Pi \longrightarrow$ X $^1\Sigma^+$) dispersed fluorescence

A Ehresmann[1], W. Kielich[1], L Werner[1], S Klumpp[1], Ph V Demekhin[1,2], V L Sukhorukov[2,3], H Schmoranzer[3] and K-H Schartner[4]

[1]Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology, University of Kassel, D-34109 Kassel, Germany
[2]Rostov State University of Transport Communications, 344038 Rostov-on-Don, Russia
[3]Department of Physics, Kaiserslautern University of Technology, D-67653 Kaiserslautern, Germany
[4]I. Institute of Physics, Justus-Liebig University Giessen, D-35392 Giessen, Germany

Experiments using photon-induced fluorescence spectrometry (PIFS) on simple molecules were in the past mainly devoted (with some exceptions) to the investigation of valence shell electron excitations and the corresponding decay processes of the photoexcited states. Only a few fluorescence investigations were carried out on decay mechanisms of inner shell excitations (see e.g. [1]). Such an excitation of an inner-shell electron in a molecule induces very complex relaxation processes, which are governed by the competition between Auger transitions and fragmentation (predissociation) of the molecule. In the present work we investigated a particular aspect of the Auger decay of the $1s^{-1}\pi^*$ (v_R) resonances of NO excited by monochromatized synchrotron radiation and observed by photon-induced dispersed fluorescence spectrometry (PIFS) [2], measuring VUV-fluorescence emission cross sections in the wavelength range between 118 nm and 143 nm: the influence of lifetime vibrational interference (LVI) on the individual decay probabilities.

In recent studies [3,4] it was shown by investigating the dispersed C(v') → X(v'') fluorescence in the N_2^+ ion hat LVI effects in the Auger decay of the N_2 $1s^{-1}\pi^*$ resonance are negligibly small. This is understandable since the energetic difference between individual N_2 $1s^{-1}\pi^*$ (v_R) states of about 230 meV is about twice as large than their natural linewidths. Since this difference (195 meV) for the N*O $1s^{-1}\pi^*$ (v_R) states is only about 1.5 times larger than their natural widths and for the NO* $1s^{-1}\pi^*$ (v_R) states this difference is already smaller than their natural widths pronounced LVI effects are expected. These LVI effects have been observed for the latter case.

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Th2-78

SOLVENT EFFECT ON THE 0-0 PHOSPHORESCENCE BAND AND CHANGE OF POLARIZABILITY UNDER THE $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ TRANSITION IN MOLECULAR OXYGEN

Vladimir S. Pavlovich

Institute of Molecular and Atomic Physics, 70 Prospect Nezalejnasty, Minsk, 220072, Belarus

In presented work the experimental data from Wessels and Rodgers [1] on solvent effect on the peak position of the 0-0 band $\nu_{\max}$ of the $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ phosphorescence of molecular oxygen are described through a new relation for solvatochromic shift due to dispersion and induction interactions [2], obtained with help the continuum Onsager's cavity model. Thus

$$\nu_{\max} = 7882.4 + \Delta\nu_{\text{rep}} + \Delta\nu_{\Sigma} - \frac{\Delta\alpha_{\text{eg}}}{a_O^3} P(n,\varepsilon,I_s)\,,\quad P(n,\varepsilon,I_s) = \frac{3E_{00}^2 I_s}{I_s^2 - E_{00}^2} P_n + k_B T\, P_\varepsilon$$

where $\Delta\nu_{\text{rep}}$ and $\Delta\nu_{\Sigma}$ denote the effect of repulsive and multipole interactions, $\Delta\alpha_{\text{eg}}$ is the change of polarizability under $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ transition, a_O is Onsager radius, E_{00}=7882.4 cm^{-1} (energy gap of solute in the gas phase taken from Herzberg), I_s is the ionization potential of solvent molecule, $P_n = \frac{n^2-1}{n^2+2}$, $P_\varepsilon = \frac{\varepsilon-1}{2\varepsilon+1}$ with n and ε being the reflective index and the dielectric constant of solvent. The induction effect arises from the interaction of an induced dipole moment in oxygen molecule with chance electric field produced by the random motion of the solvent dipoles.

The used 35 solvents with known I_s are divisible into three principle groups with virtually alike linear correlation between $\nu_{\max}$ and the $P(n,\varepsilon,I_s)$ with slope −0.073 ±0.004. Say the first group includes *n*-alkanes, *n*-alcohols (but methanol), benzene and its halogen derivatives, acetone, tetrahydrofuran, C_2Cl_4, toluene and benzonitrile (20 solvents). The second group includes methanol, CCl_4, $CHCl_3$, dioxane and CS_2. The one exception to all solvents is represented by water and acetonitrile. After detail analysis we came to the conclusion that the red shift results in the dipole-dipole, dispersion and induction, interactions as well as from the interactions of multipoles, among which quadrupole-quadrupole interactions play a dominant role. Water, acetonitrile, dioxane, methanol, $CHCl_3$, CS_2 and CCl_4 was shown to have the highest guadrupolarity. The repulsion makes a blue shift of the 0-0 band, which is a more or less alike for all solvents that early pointed by Schmidt [3]. Since $\Delta\alpha_{\text{eg}} = 0.073 a_O^3$, it has been found with a_O=1.37 Å that the polarizability in the $a^1\Delta_g$ state is 0.19 ±0.03 Å^3 above than that in the $X^3\Sigma_g^-$ state. There is a need to point that our result for $\Delta\alpha_{\text{eg}}$ do not support that of −0.08 Å^3 early obtained by quantum mechanical calculations from Ogilby and co-workers [4].

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Th2-79

UNRAVELLING THE STRUCTURE OF THE METASTABLE DIHYDROGEN ANION

F. Mezdari[1], N. de Ruette[2], X. Urbain[2]

[1]LCAM, Université Paris-Sud, Bât. 351, F-91405 Orsay, France
[2]Département de physique/PAMO, Université catholique de Louvain, chemin du cyclotron 2, B-1348 Louvain-la-Neuve, Belgium

Among the simplest molecular anions, H_2^- in its ground electronic state decays within femtoseconds due to the location of its potential well above that of H_2. On the other hand, weak beams of H_2^- are routinely produced by Cs sputter sources operating with a TiH cathode. Recent re-examination of the H_2^- production has lead Golser et al. [1] to attribute this metastability to an extreme centrifugal distortion of the potential energy curves that displaces their equilibrium distances. A model calculation predicts lifetimes up to 0.5 μs for specific rovibrational levels, that would be marginally populated in the tail of the Boltzmann distribution. This explanation was recently challenged [2] by a direct measurement performed in an electrostatic trap, yielding lifetimes for H_2^-, HD^- and D_2^- as long as 8.2 μs, 50.7 μs and 1.89 ms respectively.
As suggested by Aberth et al. [3], a metastable configuration with high spin multiplicity, possibly a $^4\Sigma_g$ state, might be responsible for the ion yield detected in several experiments. Would this state of H_2^- be located right below the metastable state of H_2 and hence have similar energetic properties, a total energy of about 7 eV would be available in the centre-of-mass frame.
In order to clarify the electronic structure of the H_2^- ion, we have set up an experiment to measure the kinetic energy imparted to pairs of H atoms or H and H^- upon spontaneous dissociative detachment and dissociation through the centrifugal barrier, respectively. Experiments conducted with a discharge ion source exclude the electronically excited channel, since no pair of neutrals was observed for the three isotopomers. On the other hand, D_2^- was found to dissociate into D and D^-, with a total kinetic energy release of 22.75 ± 0.12 meV, as measured by time of flight, in good agreement with the value calculated for J=38, i.e. 19 meV [1]. No such dissociation was observed for H_2^- and HD^-.

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Th2-80

LASER SPECTROSCOPY OF SCANDIUM ISOTOPES AND ISOMERS

Yu.P.Gangrsky[1], K.P.Marinova[1], S.G.Zemlyanoi[1], M. Avgoulea[2], J.Billowes[2],
P.Campbell[2], B. Cheal[2], B. Tordoff[2], M. Bissel[3], D.H. Forest[3], M. Gardner[3],
G.Tungate[3], J.Huikari[4], H. Penttilä and J.Äysto[4]

[1]FLNR Joint Institute for Nuclear Research, 141980 Dubna, Moscow Region, Russia
[2]Shuster Building, University of Manchester, Manchester M13 9PL, UK
[3]School of Physics and Astronomy, University of Birmingham, B15 2TT, UK
[4]Accelerator Laboratory, University of Jyväskylä SF-405 51, Finland

Collinear laser spectroscopy experiments on the ScII transition 3d4s $^3D_2 \rightarrow$ 3d4p $^3F_3$ at $\lambda \approx 363.1$ nm were performed on the $^{42\text{-}46}$Sc isotopic chain using an ion guide isotope separator with a cooler-buncher. The hyperfine structures and isotope shifts of five scandium isotopes ($Z = 21$) in the mass region $42 \leq A \leq 46$, with isomeric states in ^{44,45}Sc, have been measured [1,2].

Radioactive isotopes were produced in a fusion ion guide by irradiating a ^{45}Sc target in reactions of the type (d,p), (p,pxn), (p,p′) using 15 MeV deuterons and 25 - 48 MeV protons at 5-10 μA. Laser light was provided by a frequency-doubled Spectra-Physics 380D dye laser locked to a chosen molecular iodine absorption line.

The limits of possible variation of the mean squared charge radii in the scandium isotopic chains were deduced from measured isotope and isomer shifts.

For the studied isotopes of the odd-*Z* element scandium the magnetic dipole and electric quadrupole hyperfine coefficients *A* and *B* of both lower, 3d4s $^3D_2$, and upper, 3d4p $^3F_3$, states are obtained from the hyperfine structures using a χ^2 minimization fitting procedure. The results obtained from these data for the magnetic dipole and electric quadrupole moments of ^{43,44,44m,46}Sc isotopes are in good agreement with those summarised by Stone [3], but has better accuracy. The nuclear moments $\mu(^{45m}\text{Sc})$ and $Q_s(^{45m}\text{Sc})$ are deduced for the first time. The unusually large quadrupole moment of the isomeric state of ^{45}Sc is the most striking feature of the present data.

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Th2-81

VIBRATIONAL RELAXATION OF HIGHLY EXCITED $CO(X^1\Sigma,v)$ MOLECULES ON THE CO_2 IN THE DISCHARGE PLASMA

G.M.Grigorian[1], I.V.Kochetov [2]

[1] *V.A.Fock Research Institute of Physics St.Petersburg University, St.Petersburg, 198504, Russia*
[2] *Troitsk Institute for Innovation and Fusion Research, Troitsk, Moscow Region, 142190, Russia*

The vibrational kinetics of low-temperature plasmas in CO-containing mixtures is attracting attention in modern plasma physics research due to its relevance in different fields, ranging from IR lasers and plasma-based technologies to the study of the processes in planet~~s~~ atmospheres and the interstellar space

The experimental and theoretical investigation described in this paper was undertaken to examine effect of CO_2 on the vibrational relaxation of CO molecules. For the first time, rate constants for vibrational relaxation CO(v>16) on CO_2 molecules have been estimated.

The experimental setup was similar to that described in [1]. The experiments were carried out with a 15-mm diameter discharge tube cooled with running water in conditions typical for a CO-laser performance. He-CO-O_2 and He-CO-Xe mixtures were used. The vibrational distribution of CO molecules in the ground electronic state was determined from the spectra of IR molecular emission at the first and second overtones. For investigation of CO_2 molecules influence on the CO(v) relaxation the different contents of CO_2 gas were added to working gas mixtures. Experimental vibrational distribution functions (VDF) for CO molecules were compared with theoretical ones. The VDF of CO molecules was found by solving the time-independent equations of the vibrational kinetics these molecules together with the Boltzmann equation by the iteration method. More detailed description of theoretical model is present in [1]. On the basis of comparison relaxation rates for high vibrational levels of CO molecules have been estimated.

The investigation of the influence of CO_2 added to He-CO and He-CO-Xe mixtures on the VDF of CO in the discharge plasma has showed that CO_2 molecules may considerably increase the rate of the relaxation of high vibrational levels (v>20) while the lower levels of CO molecule are less sensitive for the presence of CO_2 molecules in the discharge. When the vibration level number is varied from v=17 to v=30 rate constants for vibrational relaxation CO on CO_2 molecules increase more than in order of magnitude. The different channels of the energy transfer between the vibrational levels of the CO and CO_2 molecules have been analyzed.

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Th2-82

FINE-STRUCTURE ENERGY LEVELS AND LIFETIMES IN Co XV

G. P. Gupta[1] and A. Z. Msezane[2]

[1]Department of Physics, S. D. (Postgraduate) College, Muzaffarnagar – 251 001
(Affiliated to Chowdhary Charan Singh University, Meerut - 250 004), INDIA
[2]Department of Physics and Center for Theoretical Studies of Physical Systems
Clark Atlanta University, Atlanta, Georgia 30314, USA
Email: g_p_gupta1@yahoo.co.in

The study of Al-like spectra of ions of the elements of the iron group has received a great deal of attention both experimentally and theoretically. These ions are of particular interest in astrophysics and controlled thermonuclear fusion. Accurate atomic data such as excitation energies, absorption oscillator strengths and radiative decay rates for these cosmically abundant ions are needed to interpret observational data.

We have performed large scale CIV3 calculations of excitation energies from ground states for 98 fine-structure levels as well as of oscillator strengths and radiative decay rates for all electric-dipole-allowed and intercombination transitions among the fine-structure levels of the terms belonging to the $(1s^22s^22p^6)3s^23p$, $3s3p^2$, $3s^23d$, $3p^3$, $3s3p3d$, $3p^23d$, $3s3d^2$, $3s^24s$, $3s^24p$, $3s^24d$, $3s^24f$, and $3s3p4s$ configurations of Co XV, using very extensive configuration-interaction (CI) wave functions [1]. The important relativistic effects in intermediate coupling are incorporated by means of the Breit-Pauli Hamiltonian which consists of the non-relativistic term plus the one-body mass correction, Darwin term, and spin-orbit, spin-other-orbit, and spin-spin operators [2]. The errors, which often occur with sophisticated *ab initio* atomic structure calculations, are reduced to a manageable magnitude by adjusting the diagonal elements of the Hamiltonian matrices. In this calculation we have investigated the effects of electron correlations on our calculated data, particularly on the intercombination transitions, by including orbitals with up to n=5 quantum number. We considered up to three electron excitations from the valence electrons of the basic configurations and included 1164 configurations.

Our adjusted excitation energies, including their ordering, are in excellent agreement with the available experimental results [3] and the recommended data by the National Institute of Standard and Technology (NIST). The mixing among several fine-structure levels is found to be so strong that the correct identification of these levels becomes very difficult. In our CIV3 calculation we identify the levels by their dominant eigenvector [4]. We believe that our very extensive calculations may assist experimentalists in identifying strongly mixed fine-structure levels correctly. From our transition probabilities, we have also calculated radiative lifetimes of the fine-structure levels in Co XV. Our calculated lifetimes for the levels $3s3p^2(^4P)$ are found to be in excellent agreement with the experimental results of Trabert *et al.* [5]. We predict new data for several levels where no other theoretical and/or experimental results are available.

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Th2-83

NUCLEAR ELECTRIC QUADRUPOLE MOMENTS, HFS CONSTANTS FOR HEAVY IONS AND RADIATION TRANSITION PROBABILITIES BETWEEN HFS COMPONENTS FOR IONS OF Fe IN SUPERNOVA

Khetselius O.Yu.

Odessa University, P.O.Box 24a, Odessa-9, 65009, Ukraine

Relativistic calculation of the spectra hyperfine structure parameters for heavy atoms and multicharged ions with account of relativistic, correlation, nuclear, radiative effects is carried out. Calculation scheme is based on gauge-invariant QED perturbation theory with using the optimized one-quasiparticle representation at first in the theory of the hyperfine structure for relativistic atomic systems [1,2]. The correction due to the finite size of a nucleus (the charge distribution in a nucleus is modelled within the Gauss and Fermi models) is accounted for in the zeroth approximation of the perturbation theory in an electric and vacuum-polarization potentials on the non-perturbative basis. Within the new method it is carried out calculating the energies and constants of the hyperfine structure for valent states $6s_{1/2}$, $7s_{1/2}$, $6p_{1/2,3/2}$, $7p_{1/2,3/2}$, $5d_{3/2}$ of cesium^{133}Cs and states $[5p^6]$ $6s_{1/2}, 6p_{1/2}$, $6p_{3/2}$,, $6d_{3/2}$ of *Cs* –like ion of Ba. Nuclear electric quadrupole moments *Q,* the hyperfine structure constants for states of $6s6p\ ^3P_1$ in atom of ^{201}Hg and $7s7p\ ^1P_1, ^3P_1, ^3P_2$ in atom of ^{223}Ra are defined. The key quantitative factor of good agreement between theory and experiment , especially in comparison with alternative theories of the Dirac-Fock type is connected with more correct accounting the inter- electron correlations, nuclear, radiative effects. The contribution due to inter electron correlations to the hyperfine structure constants is about 120-1200 MHz for different states, contribution due to the finite size of a nucleus and radiative contribution is till 2 dozens MHz (for constant *A*). For element ^{201}Hg we have received Q= 380,5 мbarn. It is agreed the best of all with experimental value, received by group Ulm etal (general interval of the experimental values is 300-600 мbarn). For element of ^{223}Ra our value is Q=1,22barn. It is in the limits of last experimental measurements values by Wendt group (ISOLDE Collaboration). The difference between our theory and experiment is connected with non-accounting the nuclear effects contribution (for example, core-polarization ones, which are induced by valent protons of a nucleus), absence of correct data regarding the temporal distribution of magnetization in a nucleus (effect of Bohr-Weisskopf), non-entire accounting for the high order quantum electrodynamics corrections. We present the results of calculating the radiation transition probabilities between hfs components for ions of Fe in Supernova 1987 too [3].

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The line shape of $L_2 - L_2L_3M_{4,5} - M_{4,5}M_{4,5}(M_{4,5})$ satellites in the Auger spectra of solids: an *ab initio* approach.

M. Cini[a], S.Ugenti[a] *,E.Perfetto[b]

[a]*LNF-INFN and Dipartimento di Fisica, Università di Roma Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Rome, Italy.*
[b]*CNISM and Dipartimento di Fisica, Università di Roma Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Rome, Italy.*

Abstract

Several experiments made by Sawatzky et al. in the seventies and by Thurgate et al. in the nineties on the Auger LMM spectra of the transition metals showed structures attributed to $L_2 - L_2L_3M_{4,5} - M_{4,5}M_{4,5}(M_{4,5})$ Coster Kronig satellites. In particular the APECS (Auger PhotoElectron Coincidence Spectroscopy) spectra obtained by Thurgate's group on Ni, Fe, Co and Ga, proved the real existence of these satellites and showed the fact that they may be expected to be atomic-like for high hole-hole coulomb interaction or else when the final state levels are outside the three holes continua, in analogy with the two hole resonances of the Cini-Sawatzky model. With this work we set up an ab initio model aimed for the calculation of such line shapes which is still missing at the state of the art today. To simplify the analysis we started with a closed band situation treated in an Anderson-like model and we used a two-step model to describe the Auger decay. The only other assumption we made consists in taking the one-particle Green's functions appearing in the theory diagonal in the spin and in the magnetic quantum number m_l . We expect that the presence in the spectra of this kind of satellites will be closely related to the break of the independent one-particle picture properly because, to observe the transition we are interested in, we need that the $M_{4,5}$ spectator hole doesn't delocalize before the L_3 decays. For this reason the observation of these three-hole satellites is consistent with an increase in the hole-hole coulomb interaction due to the incomplete screening of the hole created by the initial Coster Kronig event and perhaps the spectator hole must be localized in a two-hole resonance with high probability, which requires strong correlations. With our model we arrive to an exact solution of the problem where the equations are very similar to the ones obtained for the two-hole resonances in the Cini-Sawatzky theory. We present here preliminary results of this model obtained assuming a rectangular band for our test-system.

* *Corresponding author: Tel: +39 06 7259 4868.*
E-mail address: simona.ugenti@roma2.infn.it

Th2-85

INELASTIC PHOTON SCATTERING AS A COMPLEMENTARY DIPOLE (TWO-PHOTON) MECHANISM CONTRIBUTING TO THE ANGULAR DISTRIBUTION OF PHOTOELECTRONS

R.Yu. Kilin, V.A. Kilin, A. Ehresmann[+], K.-H. Schartner[*], H. Schmoranzer[#]

Tomsk Polytechnic University, 634030 Tomsk, Russia
[+] Fachbereich Physik, Universitaet Kassel, D-34132 Kassel, Germany
[*] I.Physikalisches Institut, Justus-Liebig-Universitaet, D-35392 Giessen, Germany
[#] Fachbereich Physik, Technische Universitaet Kaiserslautern, D-67653 Kaiserslautern, Germany

In this work, we point out another electric dipole mechanism of photoionization (PI) or photoexcitation (PE) which has not been accounted for yet, to our knowledge (see, e.g., [1,2] and refs. therein), in theoretical calculations of PI/PE cross sections and photoelectron angular distribution parameters. The mechanism automatically reveals itself in theory through including the additional, here the second, term in the perturbation operator $\hat{H}_{\text{int}}(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N,t) = -\frac{1}{c}\sum_{n=1}^{N}\left(a_{\vec{k}_1,\omega_1} e^{+i(\omega_1 t-\vec{k}_1\vec{r})}(\vec{e}_1\hat{\vec{p}}_n) + a^{*}_{\vec{k}_2,\omega_2} e^{-i(\omega_2 t-\vec{k}_2\vec{r})}(\vec{e}_2\hat{\vec{p}}_n)\right)$. This term is responsible for emitting a secondary photon ω_2 which, if emitted ($\omega_2 \neq 0$), shares the transition energy $E_{tr} = \omega_1 - I$, where ω_1 is the energy of the incident photon and I is the ionization potential, with a photoelectron in an arbitrary proportion. The secondary photon ω_2 can now be considered as a result of inelastic scattering of the initial exciting photon ω_1. It is important to note that the effect of exciting-photon inelastic scattering (EPIS) opens new channels in PI/PE with respect to the single-photon electric dipole PI/PE. Being a two-photon process, EPIS obeys those transition selection rules which are very similar to the ones in quadrupole transitions. As an example, *s*- and *d*- photoelectron partial waves can also be emitted in the n*s*-shell PI due to the EPIS effect, $A(ns^2) + \omega_1 \Rightarrow A^{+}(ns^1) + e_{s,d} + \omega_2$, additionally to the *p*-partial wave in the single-photon dipole PI, $A(ns^2) + \omega_1 \rightarrow A^{+}(ns^1) + e_p$. Since the transition energy can be arbitrarily shared between the photoelectron *e* and the photon ω_2, the contribution of EPIS $\frac{d\sigma_{fq}^{(\vec{e}_1,\vec{e}_2)}(\omega_1)}{d\Omega} = \int_{+0}^{\omega_0} \frac{d\sigma_{fq}^{(\vec{e}_1,\vec{e}_2)}(\omega_1,\omega_2,\varepsilon_q)}{d\omega_2}\,\delta(\omega_1-\omega_2-I_f-\varepsilon_q)\,d\omega_2 d\varepsilon_q$ to the PI cross sections is the integral characteristic, where $\vec{e}$ are the photons polarization and δ represents the energy conservation law. Corresponding corrections should be taken into account in calculations of the photoelectron angular distribution, which is usually described by the well-known formula [3] valid within the two-step model [4]:

$$W(\theta,\varphi) = \frac{W_0}{4\pi}\left(1 + \sum_{k=2,4,\ldots}\alpha_k \sum_{q=-k}^{k} A_{kq}(I)\sqrt{\frac{4\pi}{2k+1}}\,Y_{kq}(\theta,\varphi)\right).$$

The detailed discussion on the topic will be presented at the conference.

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Th2-86

COMPUTATION OF THE MOLECULAR FINE STRUCTURE OF STRONG DIPOLAR MOLECULES

Johannes Deiglmayr[1], Mireille Aymar[2], and Olivier Dulieu[2]

[1] Physikalisches Institut, Albert-Ludwig-Universität Freiburg,
79104 Freiburg im Breisgau

[2] Laboratoire Aimé Cotton, CNRS, bât.505, Campus d'Orsay,
91405 Orsay Cedex, France

Recently the production of ultracold heteronuclear molecules in their electronic ground state either via photoassociation [1] or Feshbach resonances [2] has been achieved. Such heteronuclear molecules, if deeply bound, have a significant permanent electric dipole moment leading to strong, long-range, and alignment dependent intermolecular forces, which offer control by external electromagnetic fields.

We have calculated the *R*-dependent polarizabilities for all heteronuclear dimers in the ground state using a quantum chemistry method based on pseudopotentials for the core representation and effective core polarization potentials, as described in ref. [3].

We also follow a new approach to include spin-orbit coupling in our calculations of molecular potentials: starting from adiabatic potential curves resulting from a full configuration interaction, a diabatization procedure is used to introduce the spin-orbit operator in suitable representation. First results will be shown for Cs_2 and other Cs heteronuclear compounds.

These new insights will be used to find efficient routes to produce and stabilize polar molecules, to model the dynamics of a dipolar gas in an optical dipole trap and to explore external field dependent scattering properties.

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IDENTITY OF MAGNETIC FIELD-INDUCED FRINGE AND TRAJECTORY DISPLACEMENTS, IN ELECTRON INTERFEROMETERS, CHECKED BY PHOTODETACHMENT MICROSCOPY

Christophe Blondel, Walid Chaibi, Christian Delsart and Cyril Drag

*Laboratoire Aimé-Cotton, Centre national de la recherche scientifique, bât. 505,
Univ. Paris-sud, 91405 Orsay cedex, France*

Since the beginning of photodetachment microscopy [1] experiments in 1996, we have made experimental conditions as close as possible to the ideal, pure electric field situation. The Earth magnetic field had been shielded against by a double layer of μ-metal, and the residual magnetic field assumed small enough so as not to perturb the electron interferograms.

The action of a magnetic field $\vec{B}$ in an electron interferometer is actually two-fold. On the one hand, trajectories, hence the envelope of the interference pattern, are displaced by the Lorentz force. On the other hand, an additional phase difference appears, proportional to the magnetic flux enclosed between interfering trajectories, which induces a shift of the fringe pattern. Since the surface enclosed between interfering trajectories varies in a complicated way as a function of the position considered in the ring pattern produced by photodetachment microscopy, the magnetic perturbation of such a pattern could be expected to be a non trivial one, except for the case of parallel electric and magnetic fields, where the first-order magnetic flux is obviously zero. In this situation of parallel fields, the effect of a magnetic field can actually be described completely [2].

To investigate the general case experimentally, we removed a layer of μ-metal, and mounted magnetic coils around the photodetachment microscope to produce magnetic components of the order of a few μT in all directions of space, all over the electron flight region. The striking result of the experiment carried out in these conditions is that trajectories, fringes, hence the whole ring pattern are displaced exactly by the same quantity. Interferograms only undergo a global translation which means that, as far as electron interferometry is concerned, the effect of the magnetic field is zero. A formal demonstration of this property at first order in $\vec{B}$ can be given, which relies only on a far-field approximation and the hypothesis for the field to be uniform.

A practical consequence of this null result is that the robustness of electron affinity measurements carried out by photodetachment microscopy is even better, with respect to stray magnetic fields, than we had initially thought. The most recent data on electron affinity measurements will be recalled at the Conference.

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Th2-88

IS CADMIUM DIMER A TRULY VAN DER WAALS MOLECULE: ROTATIONS AT THE $^{1}0_{u}^{+}(5^{1}P_{1})\leftarrow X^{1}0_{g}^{+}$ AND $^{1}1_{u}(5^{1}P_{1})\leftarrow X^{1}0_{g}^{+}$ TRANSITIONS

M. Strojecki, M. Ruszczak, M. Łukomski and J. Koperski

Smoluchowski Institute of Physics, Jagiellonian University,
ul. Reymonta 4, 30-059 Kraków, Poland

Rotational profiles of the $^{228}Cd_2$ isotopomer recorded in the $(v',v'') = (26,0)$, (27,0), (45,0), (46,0) and (48,0) vibrational bands of the $^{1}0_{u}^{+}(5^{1}P_{1})\leftarrow X^{1}0_{g}^{+}$ transition were investigated (see Fig. 1). As a result, the $B'_{v=26}$=0.0309(5) cm^{-1}, $B'_{v=27}$=0.0308(5) cm^{-1}, $B'_{v=45}$=0.0277(5) cm^{-1}, $B'_{v=46}$=0.0274(5) cm^{-1} and $B'_{v=48}$=0.0271(5) cm^{-1} excited- as well as the $B''_{v=0}$=0.0206(5) cm^{-1} ground-state rotational constants were determined. A multi-band and multi-branch analysis allowed direct determination of absolute values of the R'_e=2.94(3) Å and R''_e=3.77(4) Å excited- and ground-state bond lengths, respectively. Analysis of a rotational profile recorded in the $(v',v'') = (38,0)$ band of the same isotopomer recorded at the $^{1}1_{u}(5^{1}P_{1})\leftarrow X^{1}0_{g}^{+}$ transition allowed estimation the $B'_{v=38}$=0.0317(5) cm^{-1} rotational constant in the $^{1}1_u$ state. The result provides a contribution to the discussion on purity of the ground-state van der Waals bonding and presence of a covalent admixture to the bonding.

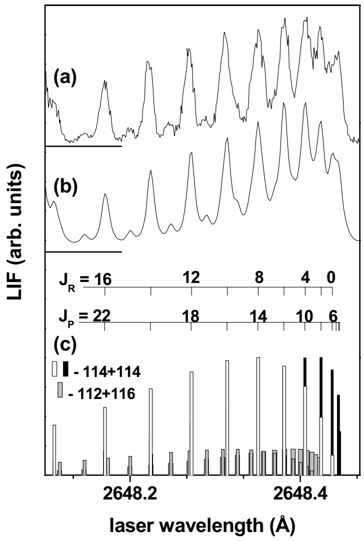


Fig. 1. Rotational profile of the $^{228}Cd_2$ isotopomer recorded in the $(v',v'') = (26,0)$ vibrational band of the $^{1}0_{u}^{+}\leftarrow X^{1}0_{g}^{+}$ transition. (a) Experimental trace, (b) computer simulation obtained as a result of convolution of every rotational transition with a Voigt function corresponding to the 0.08 cm^{-1} bandwidth of the laser beam and 0.12 cm^{-1} Doppler broadening as well as 4 K rotational temperature, (c) *P*-branch (full bars) and *R*-branch (open bars) of the $^{114}Cd^{114}Cd$ isotopomer, *P*- and *R*-branches of the $^{112}Cd^{116}Cd$ isotopomer (grey bars).

Th2-89

DOUBLE AUGER DECAY IN CARBON MONOXIDE AFTER C(1s) EXCITATION OR IONISATION

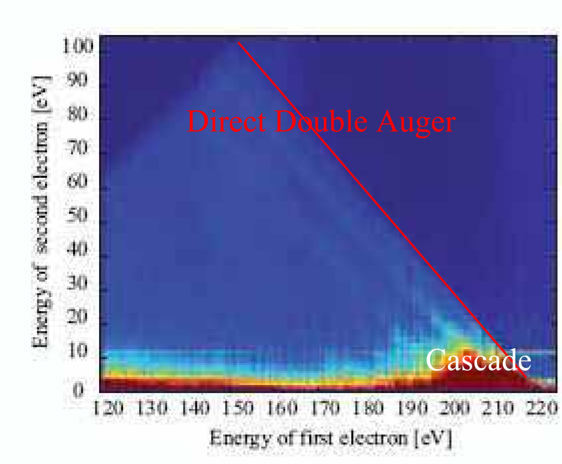
F. Penent[1], P. Lablanquie[1], J. Palaudoux[1], L. Andric[1], M. Braune[2] and J Viefhaus[2]

[1] LCP-MR, CNRS and UPMC, 11 rue Pierre et Marie Curie, 75005 Paris, France
[2] Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

For light atoms or molecules, inner-shell excitation (or ionisation) gives highly excited states of the neutral (or of the ion) that normally decay by emission of one Auger electron. However, two electrons can also be ejected due to direct double Auger decay or cascade processes, when this is energy allowed. We have studied such processes for carbon monoxide molecules by coincidence electron spectroscopy.

Our experiment uses a Magnetic Bottle Time of Flight (MB-TOF) spectrometer which allows the efficient detection in coincidence of all the electrons analysed in energy and is able to characterize double Auger processes [1]. The experiments were performed at BESSY synchrotron (Berlin, Germany) during single bunch operation of the ring (800ns period) that allows TOF measurements.

The figure shows the 2D coincidence spectra between two electrons produced after excitation of the C(1s) electron into the $2\pi^*$ orbital at 287.4 eV photon energy. A continuous line reveals double Auger decay with a random energy sharing between the two electrons. However, the prominent decay process gives an asymmetric energy sharing with fast and slow electrons.



The process releasing the highest energy reveals low energy electrons from autoionising states of oxygen atoms. That allows the identification of the following mechanism:

$$CO + h\nu \rightarrow [C(1s^{-1})O](2\pi^*) \rightarrow CO^{++*} + e^-_{1\ \mathrm{Auger\ fast}} \rightarrow C^+ + O^* \rightarrow O^+ + e^-_{2\ \mathrm{slow}}. (1)$$

Double Auger decay is also observed after carbon K-shell ionisation of CO at 330 eV by detection in coincidence of the photoelectron with two Auger electrons. The direct double Auger decay is observed through continuous energy sharing between the two Auger electrons but, here also, discrete energy lines due to atomic autoionisation are observed at low electron energy. However, contrary to what is observed in (1) on the $2\pi^*$ resonance, the discrete energy spectrum is assigned to C^{+*} autoionising states:

$$CO + h\nu \rightarrow [C(1s^{-1})O]^+ + e^-_{1\ \mathrm{ph}} \rightarrow CO^{++*} + e^-_{2\ \mathrm{Auger\ fast}} \rightarrow C^{+*} + O^+ \rightarrow C^{++} + e^-_{3\ \mathrm{slow}}\ (2)$$

Such high resolution measurements allow a better interpretation of “complete” experiments where ions are detected in coincidence with electrons [2], since such experiments cannot provide both high resolution and efficiency on the coincident electron spectra.

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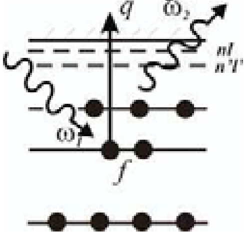
Th2-90

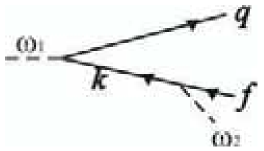
AN APPROACH TO THE DIRECT CALCULATION OF THE ATOMIC FLUORESCENCE SPECTRA INDUCED BY PHOTOEXCITATION

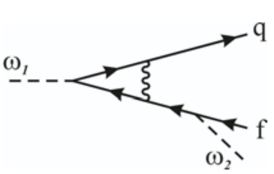
R.Yu. Kilin, V.A. Kilin, A. Ehresmann[+], K.-H. Schartner[*], H. Schmoranzer[#]

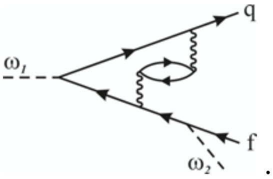
Tomsk Polytechnic University, 634030 Tomsk, Russia
[+] Fachbereich Physik, Universitaet Kassel, D-34132 Kassel, Germany
[*] I.Physikalisches Institut, Justus-Liebig-Universitaet, D-35392 Giessen, Germany
[#] Fachbereich Physik, Technische Universitaet Kaiserslautern, D-67653 Kaiserslautern, Germany

A perturbation theory (PT) approach for calculating the photon-induced fluorescence spectra beyond a two-step approximation is presented. Within the approach, the single-photon excitation of an atom and the subsequent atomic/ionic fluorescing is considered as an indivisible exciting-photon inelastic scattering (EPIS) or Raman scattering process. This is a more general approach than the reasonably valid and commonly used two- (or multi-) step resonance transition model (see, e.g., [1]), since it includes the latter as a particular case. A naive (gedanken) scheme and some lower-order PT diagrams describing the EPIS amplitudes look like:









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As an example, the photoexcitation cross sections (CSs) for a few low-lying *Ne*-states $2s^2 2p^5 np$ [^1S, ^1D], $2s^2 2p^5 nf$ [^1D] and $2s^1 2p^6 ns$ [^1S], $2s^1 2p^6 nd$ [^1D], which may be related to the final states of fluorescence observed in PIFS [1] experiments, and the angular distributions of scattered (secondary) photons have been calculated for different cases of the incident (ω_1<65 eV) and scattered (ω_2) photons' polarization. As it is expected, rich structures of peaks arise in the calculated CSs. Each peak corresponds (within the two-step model) to a transition through a real intermediate state *k*. Since, in the considered transitions, the involved intermediate states are of extremely small natural widths, much less than the energy difference between neighboring peaks, the peaks are found to be high, very narrow and non-overlapping. For intermediate states having widths of approximately the same order of magnitude as the peak spacing, the values of dipole matrix elements entering the EPIS amplitudes and, especially, the ratio ω_2/ω_1, to which the EPIS CS is proportional (in the velocity form), cause small variations of the peak shapes.

The details of the theory and results of the calculations will be presented at the conference.

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Th2-91

FINE-STRUCTURE ENERGY LEVELS, OSCILLATOR STRENGTHS AND LIFETIMES IN Mg-LIKE CHROMIUM

Vikas Tayal and G. P. Gupta

Department of Physics, S. D. (Postgraduate) College, Muzaffarnagar (U.P.)
(Affiliated to Choudhary Charan Singh University), Meerut (U.P), INDIA
Email: g_p_gupta1@yahoo.co.in

Elements in the Mg isoelectronic sequence are astrophysically abundant and accurate atomic data such as energy levels, absorption oscillator strengths and transition probabilities are needed for the interpretation of accurate observational data. These atomic data are also useful for estimating the energy loss through impurity ions in fusion plasmas, and for diagnostic and modeling of the plasmas.

Excitation energies from ground state for 86 fine-structure levels as well as oscillator strengths and radiative decay rates for all electric-dipole-allowed and intercombination transitions among the fine-structure levels of the terms belonging to the $(1s^22s^22p^6)3s^2$, 3s3p, 3s3d, 3s4s, 3s4p, 3s4d, 3s4f, $3p^2$, 3p3d, 3p4s, 3p4p, 3p4d, 3p4f and $3d^2$ configurations of Cr XIII, are calculated using extensive configuration-interaction (CI) wave functions. These wave functions are obtained using the CIV3 computer code of Hibbert [1]. The important relativistic effects are incorporated through Breit-Pauli Hamiltonian [2]. Small adjustments to the diagonal elements of the Hamiltonian matrices have been made. These adjustments improve the accuracy of the mixing coefficients which depends in part on the accuracy of the eigenvalues. This is a justifiable [3] fine-tuning technique and is particularly useful for the calculation of intercombination lines [4]. In this calculation we have investigated the effects of electron correlations on our calculated data, particularly on the intercombination transitions, by including orbitals with up to n=5 quantum number. We considered up to two electron excitations from the valence electrons of the basic configurations and included a large number of configurations to ensure convergence.

Our adjusted excitation energies, including their ordering, are in excellent agreement (better than 0.5%) with the available experimental results [5]. The mixing among several fine-structure levels is found to be very strong. These levels are identified by their dominant eigenvector [6, 7]. From our transition probabilities, we have also calculated radiative lifetimes of some fine-structure levels. Our calculated lifetime for the longer-lived level $3s3p(^3P_1)$ is found to be in excellent agreement with the experimental result of Curtis [8] compared to other calculations.

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Th2-92

SHAPE RESONANCES IN ANION FORMATION IN SF_6 AFTER S 2p SUBSHELL PHOTOIONIZATION

A. A. Pavlychev

Institute of Physics, St. Petersburg State University, St. Petersburg, 198504, Russia

Formation of negative fragments after X-ray excitation of neutral molecular species has received high attention recently (see, e.g. [1-3]). When photon energy approaches to core ionization thresholds the distributions of positively and negatively charged photoions demonstrate complex and different spectral dependences. In the present work relationships between shape resonances and anion yield after inner-shell ionization are examined. The two-step mechanism of anion production is used. In particular, for the shape resonances observed in anion yield [3] above S 2p thresholds in SF_6 one may write
$h\nu + SF_6 \rightarrow SF_6(2p^{-1}) \rightarrow SF_6^{+*} + e^-$
followed by
$SF_6^{+*} \rightarrow SF_5^{2+} + F^-$
Dynamic properties of transient singly ionized and valence excited AB_x^{+*} states play an important role in spectral dependence of anion yield. To describe the T_{2g} and E_g shape resonances in anion yield we take into account coupling of elastic channel with inelastic channels in photoelectron transmission through the molecular region. The elastic channel describes the single-hole ionization and the inelastic channels describe respectively the satellite excitations [4] and the attachment of the photoelectron to the residual cation. Within the optical potential concept (see, e.g. [4]) the cross section Q^- of anion formation is :

$$Q^- = \sigma^+ \alpha\gamma K(1-K)^{-1}.$$

This equation links the cross section Q^- with the cross section σ^+ of single-hole ionization. One may see that Q^- is proportional to σ^+ where α and γ are respectively probabilities of anion formation from the parent SF_6^{+*} state and S 2p-hole Auger decay. The constant K describes coupling of the elastic and inelastic channels. This approach allows us to rationalize both the appearance of the shape resonances in anion yield above S 2p threshold in SF_6 [3] and the suppression of the shape resonance above K thresholds in CO [1]. Important role of molecular vibrations in anion formation in CO_2 is discussed.

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INVESTIGATION OF EXCITATION PROCESSES OF ELECTRONIC STATES OF THE C_2 MOLECULE

G.M.Grigorian

V.A.Fock Research Institute of Physics St.Petersburg University, St.Petersburg, 198504, Russia

One of the features of CO-containing plasmas is high concentrations of C_2 molecules, appeared in the discharge due to plasmachemical reactions. The experimental investigation described in this paper was undertaken to examine excitation channels for electronic states of C_2 molecules. For the first time, correlation between populations of CO vibrational levels and concentration of electronically excited C_2 molecules was detected. Such a correlation may be cased by effective VE-process.
The experimental setup was similar to that described in [1, 2]. The experiments were carried in conditions typical for a gas flow and sealed-off CO-laser performance (in generation as well in amplifier mode). The emission from the positive column of the discharge was recorded with a spectrometer. Concentrations of C_2^* molecules appeared in the discharge plasma were measured in the wide range of experimental conditions. The vibrational distribution of CO molecules in the ground electronic state was determined from the spectra of IR molecular emission at the first and second overtones. Concentration of C_2 molecules in the ground state was measured by the absorption method. Strong correlation has been found in experiments between concentrations of vibrationally excited CO molecules and $d^3\Pi_g$, $e^3\Pi_g$, $C^1\Pi_g$ excited states of C_2 molecule. In particularly, modulation of the intensity of CO lasing oscillation cased marked modulation of the intensity of the emission from these electronically excited states of C_2. The C_2 molecules have several exited electronic states in the vicinity of CO vibrational levels and the correlation observed may be the evidence of the existence of energy transfer VE-process: $CO(v) + C_2 \rightarrow CO(w) + C_2^*$.
The fact that measured in experiments rotational temperatures obtained from analyzing the C_2^* emission have differed from the gas temperature in the plasma is an additional reason for C_2^* excitation channels in addition to an electron impact excitation**.** Estimations for the value of VE-process for $d^3\Pi_g$ state have been made. **R**adial profiles of C_2^* emission and their dependents on the experimental conditions have been analyzed.

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INFLUENCE OF NON-ADIABATIC PERTURBATIONS ON ENERGY, RADIATIVE AND MAGNETIC CHARACTERISTICS OF H_2, HD AND D_2 MOLECULES

S.A. Astashkevich, B.P. Lavrov

Faculty of Physics, St.-Petersburg State University, 198904, Russia.
E-mail: lavrov@pobox.spbu.ru

An influence of non-adiabatic perturbation effects on various observable characteristics of electronic-vibro-rotational (rovibronic) levels of and radiative transitions from the singlet 3d- and the triplet 3s,3d- term complexes of electronic states of hydrogen molecule has been analyzed. In contrast to our previous work [1] we used another quantitative measure of the influence and analyzed the data for all three isotopomers H_2, HD and D_2. As a quantitative measure of the relative perturbation we used the ratio of the difference between perturbed and unperturbed values of certain molecular property under the study to the unperturbed value. As the unperturbed values we have chosen the adiabatic values corresponding to Hund's coupling case *"b"*. As perturbed values of the characteristics we used either directly observed (spectroscopic) data or semi-empirical values obtained from certain primary experimental data in the framework of non-adiabatic model taking into account electronic–rotational and electronic–vibrational interactions. Such primary experimental data were values of the rovibronic terms and the wavenumbers of rovibronic spectral lines [2], the ratios of spontaneous emission transition probabilities for pairs of rovibronic lines having common upper level [3], and the lifetimes of rovibronic levels [4]. The quantitative hierarchy is observed in an influence of non-adiabatic effects on the relative perturbation of various molecular characteristics. In most cases the relative perturbation of transition probabilities and g- factors is 3÷5 orders of magnitude higher (and that of lifetimes are 1÷3 orders higher) than those for rovibronic term values. The rotational quantum number dependences are essentially different for: 1) various characteristics of the same vibronic states; 2) the same characteristics of different electronic states Λ^- and Λ^+). At the same time the perturbations are practically independent from total spin of electrons. Thus, it is shown, that rovibronic transition probabilities and g-factors are more sensitive to the perturbations, and, hence, possess greater information content about intramolecular interactions. Therefore they are more prospective for experimental studies and semi-empirical analysis of non-adiabatic effects.

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Th2-95

ACCURATE CALCULATIONS OF ELECTRONIC PROPERTIES OF ALKALI DIMERS AND ALKALI HYDRIDES

Mireille Aymar and Olivier Dulieu

Laboratoire Aimé Cotton, CNRS, bât.505, Campus d'Orsay,
91405 Orsay Cedex, France

The realization of ultracold samples of dipolar molecules is a current challenge which requires an accurate knowledge of their electronic properties to guide ongoing experiments. Using a standard quantum chemistry approach based on pseudo-potentials for atomic core representation, Gaussian basis sets and effective core polarisation potentials, we have investigated the properties of homonuclear and hetero-nuclear alkali dimers involving all pairs of atoms from Li to Cs, as well as alkali hydrides from LiH to CsH.

In addition to the potential curves for ground and excited states for various symmetries, we have calculated permanent and transition dipole moments as function of the interatomic distance and of the vibrational level. We have also obtained new values of the static polarizabilities for alkali dimers and alkali hydrides. We have extended our studies towards francium diatomic compounds in the perspective of photoassociation of cold francium atoms. .

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Th2-96

A consistent central potential to simulate Methane in scattering calculations

F. Shojaei, M.A. Bolorizadeh*, E. Ghanbari Adivi

Physics Department, Shahid Bahonar University of Kerman, Kerman, Iran, and
Physics Department, Yazd University, Yazd, Iran.

In many interactions involving molecules, the interaction potential is required [1-3] to calculate the physical quantities; e.g. cross sections. A detailed potential for a molecule, neglecting nuclear motions as compared with the electron motion, is:

$$V=\sum_{\substack{i\\ i<j}}\sum_{j}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}-\sum_{\alpha}\sum_{i}\frac{Z_\alpha}{|\mathbf{r}_i-\mathbf{R}_\alpha|}$$

where $\mathbf{r}_i$ and $\mathbf{R}_\alpha$ are the position vector for the i^{th} electron and the α^{th} nucleus of the molecule, respectively. Even for the simplest molecule, H_2^+, this potential is not a simple central one. The calculation of scattering quantities is difficult for a central potential and almost impossible in the case of non-central potentials. Usually the molecules are simplified by a central potential composed of a coulomb interaction and at most another short range potential. This methods, mostly, oversimplifies the interactions. For example, a methane molecule is simplified so that the system is not much different than a carbon atom.

We have substituted the molecular orbital, Φ, into $V=E+\nabla^2\Phi/2\Phi$ to find a central potential to simulate a molecule to be used in scattering calculations. The method is applied to methane (CH_4) where the molecular orbitals $1a_1$, $2a_1$ and $1t_2$ comprising the central carbon orbital and the C-H bands were used [4]. The derived potential observed by an electron of methane is plotted in Figure 1. There is a maximum observed at about 0.6 a.u. showing an attraction from hydrogen atoms of the methane molecule. This maximum is not included in ordinary central potentials used in atomic and/or molecular interactions. The central potential is used to calculate the charge transfer interaction between ion and methane.

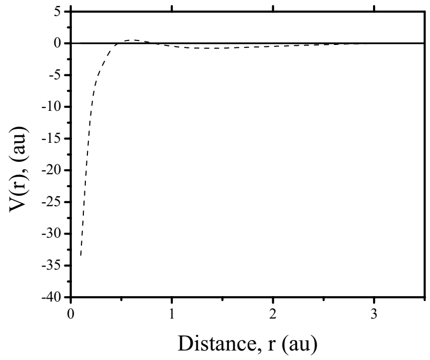

Figure 1. The central potential observed by an electron in a methane molecule.

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* Corresponding Author: mabolori@mail.uk.ac.ir & mabloor04@yahoo.com

Th2-97

THE C1s AND N1s NEXAFS SPECTRA OF FIVE AZA-BENZENES IN THE GAS PHASE

G. Vall-llosera[1], B. Gao[2], H. Ågren[2], E. Rachlew[1], M. de Simone[3], A. Kivimäki[3] and
M. Coreno[4]

[1]Royal Institute of Technology, Department of Physics, AlbaNova University Center,
SE-10691 Stockholm, Sweden.
[2]Theoretical Chemistry, Royal Institute of Technology, AlbaNova University Center,
SE-106 91 Stockholm, Sweden.
[3]Laboratorio Nazionale TASC INFM-CNR, 34012 Trieste, Italy
[4]CNR-IMIP, Montelibretti, 00016 Rome, Italy.

Near edge X-ray absorption fine structure spectroscopy (NEXAFS) has proven to be a sensitive technique for the accurate determination of the electronic structure of matter. The combination of this technique with synchrotron radiation (SR) has the advantage of being site specific due to the possibility of selectively exciting different core levels of different atoms in a molecule. In this work the excitation of C1s and the N1s core levels of five members of the aza-benzenes family by SR have been studied with NEXAFS, and the experimental and theoretical photoabsorption cross-section spectra will be presented. The measurements were conducted on the undulator-based Gas Phase Photoemission beamline at the ELETTRA synchrotron facility, Trieste, Italy. All ions produced along the light path in an inner cell are collected by two equally long electrodes, and the absorption cross section is derived from the data using the Beer-Lambert law.

The aza-benzene family comprises aromatic molecules that are structurally related to benzene wherein one or more CH groups in the six-membered ring is replaced by a nitrogen atom. Our study includes pyridine, which is the simplest derivative with one N substituted, followed by pyridazine, pyrimidine and pyrazine with 2 N substituted in the 1,2-, 1,3- and 1,4- positions and s-triazine which has 3 N substituted in the 1,3,5- positions. Pyrimidine is of particular interest since it provides the basic ring structure for all pyrimidine bases found in DNA or RNA, viz. thymine, cytosine, uracil, as well as radiosensitizing halouracils. Since the electronic structure of these molecules is modified by their different exocyclic functional groups, our study aids to understand the fundamental contribution of the electronic structure of the basic pyrimidine ring to excitations that can lead to degradation and radiation damage of this important class of biomolecules.

Our experimental results show a chemical shift due to the different carbon sites which is also predicted by the theoretical spectra. We give assignments for the different resolved peaks and compare the photoabsorption cross-section of the five different molecules. Fluorescence in the VIS range for these molecules was also collected and will be compared to the photoabsorption spectra.

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Th2-98

THE ATOMIC PARITY VIOLATION EFFECT: CONSISTENT QUANTUM CALCULATION

Khetselius O.Yu.

Odessa University, P.O.Box 24a, Odessa-9, 65009, Ukraine
E-mail: glushkov@paco.net

A consistent QED perturbation theory [1] is adapted to calculation of the atomic parity violation (non-conservation) effect. As method of calculation of the relativistic atomic fields and electron wave functions we have used the relativistic, gauge invariant Dirac-Fock type approach [1]. The potential of Dirac equation includes the the electric and polarization potentials of a nucleus (the Fermi model, the gaussian form of charge distribution in the nucleus and the uniformly charged sphere are considered). There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams (particles screening, particle-hole interaction, mass operator iterations). The magnetic inter-electron interaction is accounted in the lowest (on α constant of hyperfine structure). We present the calculation results for energy levels, hyperfine structure intervals, E1-,M1-transitions amplitudes in heavy atoms of Cs,Sn,Pb. As example let us give here the calculation result for parity non-conserving 6s-7p dipole amplitude in Cs. Our calculation gives value: $D=<6s|Dz|7s>= -0.918\cdot 10^{-11} i|e|a(-Qw/N)$. For comparison let us present other calculation results [2]: $D=-0.91\cdot 10^{-11} i|e|a(-Qw/N)$ by Dzuba etal; .$D=-0.935\cdot 10^{-11} i|e|a(-Qw/N)$ by Bouchiat etal (Paris); $D=-0.935\cdot 10^{-11} i|e|a(-Qw/N)$ by Johnson etal (Indiana). Comparison of calculated D value with measurement of Noeker etal gives the following data of weak nuclear chare in Cs and Wainberg angle: (-Qw/N)=0,918±0,020 (exp.)±0,010 (theor.) and $\sin^2\vartheta_W=0,231\pm0,007$ (exp.)±0,004 (theor.) that is in a good agreement with average world value $\sin^2\vartheta_W=0,230\pm0,005$.

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Th2-99

RADIATIVE LIFETIMES AND TRANSITION PROBABILITIES OF THE NaCs $^1\Pi$ STATES

E.A.Pazyuk[1], A.Zaitsevskii[1], A.V.Stolyarov[1], I. Klincare[2], J. Zaharova[2], M. Tamanis[2], R.Ferber[2]

[1]Department of Chemistry, Moscow State University, Leninskie gory 1/3, 119992, GSP-2, Moscow, Russia
[2]Department of Physics, University of Latvia, Rainis Blvd. 19, Riga LV-1586, Latvia

Radiative lifetimes of excited electronic states and rovibronic transition probabilities of mixed alkali dimers are of important usage since cooling experiments usually include radiative absorption and decay circles. In particular, the low-lying $^1\Pi$ states of NaCs are of interest since photoassociation of the cold colliding atoms via the intermediate spin-orbit coupled $B^1\Pi{\sim}c^3\Sigma^+$ states seems to be preferable [1]. We present here the results of experimental and theoretical investigation of radiative properties of the $(1\text{-}3)^1\Pi$ states of the NaCs molecule.

The radiative lifetimes τ^{rad} for particular rovibronic levels of the $(3)^1\Pi$ and $D(2)^1\Pi$ states of the NaCs molecule have been directly measured in a thermal cell from fluorescence kinetics after modulated laser excitation, see also [2]. The experimental τ^{rad}-values of the $(3)^1\Pi(3 \leq v' \leq 25)$ levels decrease from 29 to 21 ns as the vibrational quantum numbers v' increase. The measured τ^{rad} values for two rotational levels of the $(3)^1\Pi(v'=3)$ state with rotational quantum numbers J'=45 and 106 are 29 ns and 25 ns respectively showing the effect of rotation. The measured τ^{rad}-value of the $D(2)^1\Pi(v'=0; J'=16)$ level is about 37 ns.

The theoretical lifetimes for the lowest $^1\Pi$ states have been evaluated in the framework of a pure "**a**" Hund's coupling case using the approximate sum rule for the vibronic states [3]. The required *ab initio* scalar relativistic (spin-orbit-free) transition dipole moment functions were calculated by many body multipartitioning perturbation theory (MPPT) correlating 18 electrons [4]. The MPPT moments agree very well with their counterparts from 2-electrons core-polarization potential (CPP) calculations [5]. The lifetimes of the $B(1)^1\Pi$ and $(3)^1\Pi$ states are mainly determined by a transition to the ground $X^1\Sigma^+$ state while the additional $D(2)^1\Pi$- $A(2)^1\Sigma^+$ decay channel is important for the $D(2)^1\Pi$ state. All intramolecular perturbations including the pronounced spin-orbit coupling effect were neglected in the present treatment. The theoretical lifetimes coincide with the experimental τ^{rad}-values within 5-10%.

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Th2-100

Transition probabilities for lines originating from 6d and 7s configurations in singly ionized gold

M. Ortiz[a], R. Mayo[a,b], É. Biémont[c,d], P. Quinet[c,d], V. Fivet[d], G. Malcheva [e] and K. Blagoev[e]
[a]Faculty of Physics, Universidad Complutense de Madrid, 28040 Madrid, Spain
[b]CIEMAT, Avda. Complutense 22, 28040 Madrid, Spain
[c]IPNAS (Bât. B15), University of Liège, Sart Tilman, B-4000 Liège, Belgium and
[d]Astrophysics and Spectroscopy, University of Mons-Hainaut,
B-7000 Mons, Belgium
[e] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee, BG- 1784 Sofia, Bulgaria

E-mail: bobcheva@issp.bas.bg

Investigation of stellar abundances of heavy elements (including gold) is important in astrophysics in relation with nucleosynthesis processes. For that purpose, obtaining accurate transition probabilities for singly ionized gold (Au II) lines is timely and justified particularly for the analysis of CP stars spectra.

In the present work, we report on transition probabilities for lines originating from 6d and 7s configurations of Au II.

A Laser Induced Breakdown Spectroscopy (LIBS) method was employed for an experimental determination of transition probabilities. Free gold atoms and ions were produced by laser ablation using a Nd:YAG laser at 10640 Å with 7 ns pulse duration and 160 mJ pulse energy. The spectrum emitted from the laser-produced plasma was registered with a grating monochromator (resolution 0.3 Å). The registration system included also a time-resolved optical multichannel analyzer system (OMA III, EG&G with 1024 channels), which allowed to study the plasma evolution for different delay times after the laser pulse. The experiment was carried out in an argon atmosphere at 8 Torr pressure.

The relative transition probabilities obtained in this way were normalized using the radiative lifetimes of the upper levels calculated in this work.

The theoretical transition probabilities and radiative lifetimes were evaluated with the relativistic Hartree-Fock method as coded by Cowan [1, 2]. This approach takes configuration interaction and core-polarization effects into account.

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Th2-101

THE EFFECTS OF THE PRESENCE OF LOW LYING EXCITED STATES ON 4d PHOTOABSORPTION OF La AND Ce IONS

Nicola Murphy, Lynn Gaynor, Padraig Dunne and Gerry O'Sullivan,

School of Physics, University College Dublin, Belfield, Dublin 4

The photoabsorption spectrum of Xe-like La^{3+} and Ce^{4+} and I-like La^{4+} and Ce^{5+} have been obtained in the extreme ultraviolet (EUV) spectral region with the dual laser plasma (DLP) technique [1]. Photoexcitation from the 4d-subshell is the dominant process in the 80-160 eV energy range. Strong discrete structure, corresponding to 4d np, mf ($n>6$, $m>4$) transitions in La^{3+} appeared at lower laser power densities, but with increasing laser flux the discrete features were suppressed and replaced by broad features in the energy regions of the 4d-5p and 4d-4f transitions. This behaviour can be attributed to the presence of absorption from excited states containing open 5p and 4f subshells in La^{3+} and the onset of similar behaviour in La^{4+}. In Ce, where 4f wavefunction contraction effects are expected to be more significant [2], the effects of excited state absorption are even more pronounced. The transitions responsible were identified with the aid of Hartree-Fock with Configuration Interaction calculations using the Cowan suite of codes [3].

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Th2-102

Theoretical study of E1 spectra of Sn^{+12} to Sn^{+18} ions

Konrad Koc, L. Głowacki and J. Migdałek

Department of Computer Science, Pedagogical University,
ul. Podchorążych 2, 30-084 Kraków, Poland

Transition energies, E1 transition rates and oscillator strength of Sn^{+12} to Sn^{+12} ions have been calculated by using multireference relativistic configuration interaction method based on the no-pair Dirac-Coulomb-Breit Hamiltonian. Analytic basis sets of Gaussian-type functions are employed to expand the upper and lower components of the Dirac four-spinors in the matrix Dirac-Fock self-consistent field and relativistic multireference RCI procedures. Some of the results are compared with values obtained by means of single or multiconfiguration numerical DF SCF calculations.

Th2-103

Electronic transitions in *H*- to *Be* -like ions immersed in electron gas*

Marek Moneta [#]

Uniwersytet Lódzki, Katedra Fizyki Ciała Stałego
Pomorska 149, PL 90-236 Lódż, Poland

Abstract

The electronic characteristics of *H*- to *Be*- like ions immersed in degenerate electron gas were calculated.
The ion was described within the Hartree-Fock-Slater formalism and the medium by the dielectric function.
The ion's electrons repulsion, screening and exchange effects and additionally the self-binding of electron due the polarization of the medium were included in the description.
The results were compared with the reference corresponding characteristics for ions in vacuum.

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[#] marek_moneta@uni.lodz.pl

Th2-104

ON A COMPARISON BETWEEN BREIT-PAULI AND FULLY RELATIVISTIC APPROACHES AT HIGH Z: THE 1s2s2p $^4P^o_{5/2}$ HIGHLY MAGNETIC METASTABLE STATE IN THE Li ISOELECTRONIC SEQUENCE

P. Palmeri[1], P. Quinet[1,2], C. Mendoza[3], M. R. Godefroid[4], P. Indelicato[5]
and N. R. Badnell[6]

[1] Astrophysique et Spectroscopie, Université de Mons-Hainaut, B-7000 Mons, Belgium
[2] IPNAS, Université de Liège, B-4000 Liège, Belgium
[3] Chimie Quantique et Photophysique, Université Libre de Bruxelles, B-1050 Brussels, Belgium
[4] Centro de Física, Instituto Venezolano de Investigaciones Científicas, Caracas 1020A, Venezuela
[5] Laboratoire Kastler Brossel, Ecole Normale Supérieure et Université Pierre et Marie Curie, F-75231 Paris CEDEX 05, France
[6] Department of Physics, University of Strathclyde, G4 0NG Glasgow, UK

The relativistic effects included in the multiconfiguration Breit-Pauli code AUTOSTRUCTURE [1] have been benchmarked with respect to the fully relativistic multiconfiguration Dirac-Fock package MCDFGME [2]. For this, the decay properties of the 1s2s2p $^4P^o_{5/2}$ metastable state have been studied in high-Z ions (up to U^{89+}) along the Li isoelectronic sequence. This state is highly magnetic because it decays through three main magnetic channels: a M1 radiative transition to the $1s^22p$ $^2P^o_{3/2}$ excited state, a M2 radiative transition to the $1s^22s$ $^2S_{1/2}$ ground state and an Auger transition to the ground state of the parent ion, i.e. $1s^2$ $^1S_0$. This latter decay channel is opened thanks to the spin-spin interaction that couples the 1s2s2p $^4P^o_{5/2}$ autoionizing state to the $1s^2\varepsilon f$ $^2F^o_{5/2}$ continuum. The transition energies and the rates of these three channels calculated from both atomic structure codes have been compared along the sequence. The inclusion of kappa-averaged relativistic orbitals [3] in AUTOSTRUCTURE has improved drastically the agreement with MCDFGME at high Z.

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Contact: palmeri@umh.ac.be

Th2-105

RADIATIVE AND AUGER DECAY OF K-VACANCY LEVELS IN THE Ne, Mg, Si, S, Ar AND Ca ISONUCLEAR SEQUENCES

P. Palmeri[1], P. Quinet[1,2], C. Mendoza[3], M.A. Bautista[3], J. García[4] and T.R. Kallman[4]

[1] Astrophysique et Spectroscopie, Université de Mons-Hainaut, B-7000 Mons, Belgium
[2] IPNAS, Université de Liège, B-4000 Liège, Belgium
[3] Centro de Física, Instituto Venezolano de Investigaciones Científicas, Caracas 1020A, Venezuela
[4] Exploration of the Universe Division, NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA

In the X-ray spectra from Chandra and XMM-Newton, K lines and edges from elements such as Ne, Mg, Si, S, Ar, and Ca have been observed where they can become useful items in spectral modelling (see, for instance Ref.[1]). Following our work on the K lines of Fe (see, e.g. Ref.[2]) and on the K-shell photoabsorption of O ions [3], we report new atomic data for K-vacancy levels in the Ne, Mg, Si, S, Ar and Ca isonuclear sequences. Prime objectives are to improve the atomic database of the XSTAR modelling code [4] and to prepare ionic targets for lengthy computations of the photoabsorption cross sections where both radiative and Auger dampings are key effects. In this respect, available atomic structure data sets, namely K-vacancy level energies, A-values and Auger widths, for ions of the first row with electron number $2 \leq N \leq 10$ are far from complete while the second row ($11 \leq N \leq 20$) has hardly been visited. Detailed comparisons with the available experimental and theoretical values will be shown.

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Contact: palmeri@umh.ac.be

Th2-106

Atomic properties of Ca^+, Sr^+, Cd^+, Hg^+, and Ra^+

M.S. Safronova[1], Dansha Jiang[1], and U.I. Safronova[2]

[1]University of Delaware, Newark, Delaware, USA
[2]University of Nevada-Reno, Reno, Nevada, USA

We conducted a systematic study of the atomic properties of Ca^+, Sr^+, Cd^+, Hg^+, and Ra^+ ions using a relativistic all-order method. This method is a linearized coupled-cluster method, where single and double excitations of Dirac-Fock wave functions are included to all orders of perturbation theory. Partial triple excitations are also included in some of the calculations. Reduced electric-dipole matrix elements and transition rates are determined for the ns-$np_{1/2}$, ns-$np_{3/2}$, $np_{1/2}$-n'$d_{3/2}$, $np_{3/2}$-n'$d_{3/2}$, and $np_{3/2}$-n'$d_{5/2}$ transitions, where ns is a ground state. The electric-quadrupole matrix elements are evaluated for the $6d_{3/2}$-7s, $6d_{5/2}$-7s transitions in Ra^+ and $4d_{3/2}$-5s, $4d_{5/2}$-5s transitions in Sr^+. The theoretical lifetimes for the $np_{1/2}$, $np_{3/2}$, $nd_{3/2}$, and $nd_{5/2}$ states are compared with latest available experimental measurements. The energy levels and hyperfine constants are also calculated and compared with experiment. This work provides benchmark values for a large number of yet unmeasured properties.

Contact information: e-mail: msafrono@udel.edu (Marianna Safronova)

Th2-107

OZONE MOLECULE: GLOBAL VARIATIONAL CALCULATION AND ASSIGNMENT OF HIGHLY EXCITED RO-VIBRATIONAL STATES

Vladimir TYUTEREV # , Sergei TASHKUN*, Habib SEGHIR, and Alain BARBE#

#G.S.M.A., UMR CNRS 6089, Université de Reims, BP 1039 - 51687 REIMS Cedex 2, France,
** LTS, Institute of Atmospheric Optics, SB RAS, 634055 TOMSK, Russia*

Accurate ro-vibrational calculations for the ozone molecule in this range represent a "touchstone" for empirical and non-empirical methods [1,2] including those based on high-level *ab initio* electronic structure calculations [3]. A modeling and assignmens of high-resolution ozone spectra near the dissociation limit (6000-8000 cm-1) are known to be extremely challenging due to numerous "exotic" resonances with large ΔV coupling and because of related difficulties in vibrational extrapolations [1]. Recently a breakthrough in very sensitive laser experiments [4,5] on ozone spectra have allowed recording a lot of weak transitions above 6000 cm^{-1}, many of them beeing still non-assigned.

A full comparisons of variational, DVR and Contact Transformation (CT) calculations up to the dissociation limit among these three independent methods and also against recent experimental data for band centers will be presented. In all three cases the same molecular potential function [5] (that provides currently best available agreement with observations) was used, but these methods employ quite different techniques and coordinate systems. The first two methods use numerical integrations in Radau and Jacobi coodinates in a "global" basis, whereas a recent computer assisted CT formulation [6] represents an algebraic perturbational approach extended to multiple and overlappling polyads.

A convergence of this new robust CT algorithm, that allows building non-empirical rovibrational effective Hamiltonians from a molecular potential energy surface to a spectroscopic accuracy are discussed. Examples of calculations for high-order centrifugal distortion and resonance constants and comparison of ro-vibrational calculations up to J=50 vs variational methods and observations are given. In conclusion, this study shows a possibility to achieve an agreement to a spectroscopic accuracy between global DVR-type calculations and non-empirical effective Hamiltonian CT approach that allows a reliable normal mode assignment of highly excited ozone vibrations up to the dissociation limit.

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Th2-108

STORAGE-RING MEASUREMENT OF THE HYPERFINE INDUCED ^{47}Ti^{18+}(2s 2p ^{3}P$_0$ → 2s^2 ^{1}S$_0$) TRANSITION RATE

S. Schippers$^+$, E. W. Schmidt, D. Bernhardt, D. Yu*, A. Müller,
M. Lestinsky†, D. A. Orlov†, M. Grieser†, R. Repnow†, A. Wolf†

Institut für Atom- und Molekülphysik, Justus-Liebig-Universität Giessen, Germany
($^+$) email: Stefan.E.Schippers@iamp.physik.uni-giessen.de
(*) Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, P. R. China
(†) Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Atoms and ions in metastable excited states with very small electromagnetic transition rates are promising systems for realizing ultraprecise atomic clocks, for the diagnostic of astrophysical media regarding the competition of radiative and non-radiative processes, for realizing novel types of cold atomic gases, and for probing fundamental correlation effects in the bound states of few-electron systems. In particular, in alkaline-earth-like and, in general, divalent atoms and ions, having a $(ns)^2\ {}^1S_0$ ground state and a valence shell n, the first excited level above the ground state is the term $ns\,np\ {}^3P_0$. The absence of a total electronic angular momentum J for this level makes its single photon decay to the ground state impossible except for the hyperfine induced decay in the case of a nucleus with a spin $I \neq 0$. For $I \neq 0$ the hyperfine interaction mixes states with different J and the $ns\,np\ {}^3P_0$ term aquires a finite, but long and strongly isotope-dependent radiative lifetime. These hyperfine-dominated decay rates have been treated theoretically for beryllium-, magnesium-, and zinclike ions [1-3] and for divalent heavier atoms [4,5], where the long and isotope-dependent lifetimes are attractive in view of obtaining ultraprecise optical frequency standards and for cold-atom studies.

Hyperfine-induced (HFI) decay rates in divalent $ns\,np\ {}^3P_0$ states were so far determined experimentally only for the atomic-clock transition $5s5p\ {}^3P_0$-$5s^2\ {}^1S_0$ of ^{115}In$^+$ in a radio-frequency ion trap [6], with an $\sim$5% uncertainty, and for the beryllium-like ion N^{3+} [7] using observations from a planetary nebula and yielding an uncertainty of 33%.

Here, a much more accurate measurement of the hyperfine induced $2s\,2p\ {}^3P_0 \rightarrow 2s^2\ {}^1S_0$ transition rate A_{HFI} in berylliumlike ^{47}Ti^{18+} is reported. Resonant electron-ion recombination in a heavy-ion storage ring was employed to monitor the time dependent population of the $^3P_0$ state. The experimental value $A_{\mathrm{HFI}} = 0.56(3)$ s^{-1} [8] is almost 60% larger than theoretically predicted [1].

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POSTERS

Thursday 10/5

3. Few body dynamics

Th3-1

Two-body system at finite temperature

D.U. Matrasulov[1], F.C. Khanna[2,3], Kh.Yu. Rakhimov[1], and Kh.T. Butanov[1]

[1]Heat Physics Department of the Uzbek Academy of Sciences
28 Katartal St., Tashkent 700135, Uzbekistan
[2]Physics Department University of Alberta, Edmonton Alberta, T6G 2J1 Canada
[3]TRIUMF, 4004 Wersbrook Mall, Vancouver, British Columbia, Canada, V6T2A3

Study of the heath-bath effects in the properties of few-particle systems is of importance for many topics of atomic, plasma and particle physics, where quantum properties of a bound system change due to the interaction with environment. Since heath-bath is considered as a system of infinite number of particles, such problems should be solved within the many-body approach.

In this work we solve this problem using a real-time finite-temperature field theory, thermofield dynamics [1,2]. Thermofield dynamics (TFD) is based on two steps:

i) Doubling of the Fock space, which implies switching of the interaction with a heath bath;
ii) Bogolyubov transformations, which makes operators, describing the system properties temperature.

TFD is a powerful tool to explore heath bath effects in the system, whose Hamiltonian can be formally represented in terms of harmonic oscillator annihilation and creation operators.

In our approach we first represent Hamiltonian of the system interacting via Coulomb plus linear potential, in terms of annihilation and creation operators. Then using TFD prescription we calculate numerically temperature-dependent energy spectrum. As follows from the obtained results, the binding energy decreases by increasing of the temperature.

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Th3-2

AB INITIO POTENTIAL SURFACE AND VIBRATIONAL PREDISSOCIATION DYNAMICS OF HeI_2(B) CLUSTER

R. Prosmiti, A. Valdés, P. Villarreal, G. Delgado-Barrio

Instituto de Matemáticas y Física Fundamental, C.S.I.C.,
Serrano 123, 28006 Madrid, Spain

We report here *ab initio* calculations on the $B(^3\Pi)$ excited state of the HeI_2 complex [1]. The lowest triplet $^3A'$ and $^3A''$ states are calculated at the UCCSD(T) level of theory, employing large-core relativistic peudopotentials for the iodine atoms. Spin-orbit coupling effects are not included and the three-dimensional potential energy surface for HeI_2(B) is represented in terms of the average of the $^3A'$ and $^3A''$ adiabats. The UCCSD(T) surface presents a global minimum at the T-shaped configuration, and a secondary one at linear configurations for elongated *r* bond distances.

Spin-free bound state calculations for $J=0$ are carried out for the above surface. The binding energy, and vibrationally averaged structure are determined and compared with the experimental measurements by Levy and coworkers [2], as well as recent experiments by Loomis's group [3].

To our knowledge, this is the first *ab initio* study on the B excited state of HeI_2. For HeI_2(B) complex more experimental data are available from vibrational predissociation dynamics experiments [2,3,4] for low and high υ excitations. Therefore, for a global evaluation of the present *ab initio* PES, further theoretical dynamics simulations are carried out [5]. Spectral blueshifts and vibrational predissociation lifetimes are computed and their comparison with the experimental data is discussed.

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Th3-3

Photoionization microscopy: experiment and simulations.

A. Ollagnier[1], F. Lépine[1], M-A. Lebeault[1], F. Robicheaux[2], M.J.J. Vrakking[3] and C. Bordas[1]

[1] Université Lyon 1 ; CNRS ; LASIM UMR 5579, 43 boulevard du 11 novembre 1918, F-69622 Villeurbanne Cedex, France.
[2] Department of Physics 206 Allison Lab Auburn University, AL 36849-5311
[3]FOM-Institute AMOLF, Kruislaan 407,1098 SJ Amsterdam, The Netherlands

In the 80's Kondratovich, Ostrovsky and Demkov ([1],[2]) proposed an experiment in which the two dimensional flux of electron produced in a photoionization process in the presence of a static electric field is measured with a position sensitive detector placed at a macroscopic distance, perpendicularly to the electric field. They noticed that this electron current is a direct measurement of the square modulus of the transverse component of the electronic wavefunction. This experiment is named "photoionization microscopy" as it provides an image that is a macroscopic projection of the electronic wave function which properties are determined by the short distance motion of the electron around the nucleus.

The first photoionization microscope has been built recently and first experimental results were obtained on Xe atoms ([3],[4]). Ionization with one and two photons was performed and electrons were detected using a state-of-the-art imaging spectrometer. A typical image shows two main structures explained by the topology of electron trajectories. These results have demonstrated that this asymptotic measurement allows one to distinguish between "indirect" electrons scattered by the ionic core and "direct" electrons with trajectories mainly influenced by the electric field. Even more spectacular is the interference pattern observed for both contributions and the smooth evolution of the number of fringes when the ionization wavelength varies. Surprisingly, the structure of the ionization continuum only affects the angular distribution.

These results can be understood intuitively in terms of interferences between several trajectories followed by the electron in order to reach a given position on the detector. A hydrogenic semiclassical model has been able to describe the main features of the experimental results ([5]). However, a complete quantum description of the photoionization microscopy experiment is needed and requires a more refined theoretical description taking into account the effect of the electric field, ionic core, electronic core and ionization process. There, we have recently performed calculations based on wavepacket propagation using a split-operator code. It allows us to study electron dynamics for different atoms and to get a better insight into the relation between interference patterns and electronic motion. In this contribution we will discuss comparisons between experimental results and calculations as well as predictions for photoionization microscopy experiments on hydrogen and non-hygrodenic atoms.

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A classical and quantum mechanical investigation of the role of nondipole effects on the binding of a stripped HD^{2+} molecule

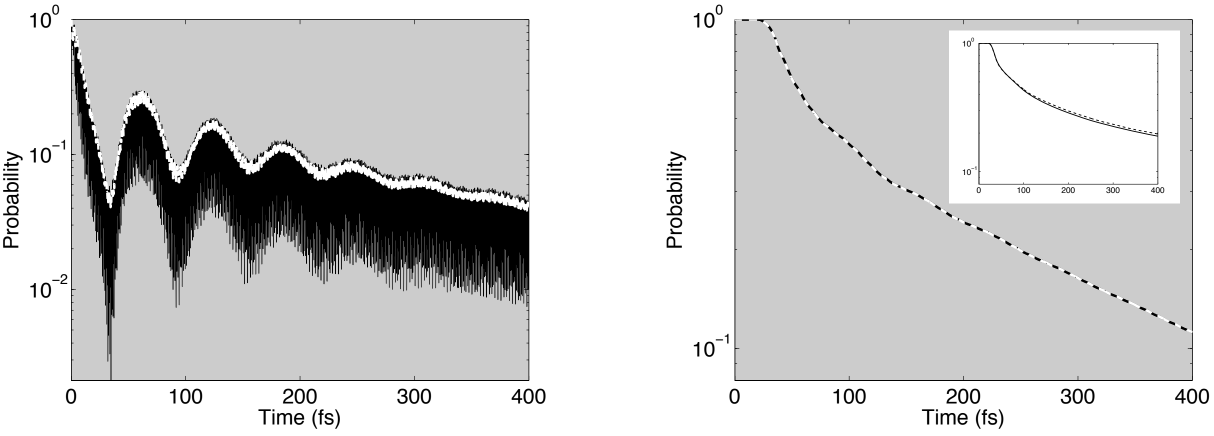
Th3-4

I. Sundvor,[1] L. Sælen,[1] T. Birkeland,[2] S. Selstø,[1] and M. Førre[1]
[1]*Department of Physics and Technology, University of Bergen, N-5007 Bergen, Norway*
[2]*Department of Mathematics, University of Bergen, N-5007 Bergen, Norway*

Quantum control, i.e. the ability to achieve a desired evolution of a quantum system by applying external fields, is a major theme of modern atomic, molecular, and optical sciences.

Recently, it was suggested [1], based on solutions of the time-dependent Schrödinger equation within the dipole approximation, that carefully selected combinations of strong linearly and circularly polarized laser fields could bind two same-sign charges, a proton and a deuteron. The nuclei are bound in the sense that the Coulomb explosion is significantly slowed down when the system is subject to the external fields.

We employ a full quantum mechanical approach to study the binding of two bare nuclei in strong laser fields beyond the dipole approximation. The role of nondipole effects on the binding mechanism is investigated and it is found that in spite of a significant contribution to the dynamics, the nondipole effects do not alter the characteristic lifetime of the system. The results are supported by classical calculations addressing the question of decoupling of the center-of-mass and relative motion.



(a)

(b)

FIG. 1: 1(a) shows the projection of the wave function on the initial wave packet versus time for a case where the nondipole interaction is turned on during 5 fs, and for $\phi_1 = \phi_2 = 0$. The black and white curves show the result of the nondipole and dipole calculations, respectively. 1(b) shows the quantum mechanical probability for the two particles to be less than $10a_0$ apart for the nondipole (dash-dotted line in black) and the dipole calculation (dash-dotted line in white), for the case in 1(a). The inserted figure shows the classical result in the nondipole (solid line) and dipole (dashed line) limit.

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Th3-5

SIGNATURES OF QUANTUM CHAOS IN DOUBLY EXCITED HELIUM

R. Püttner,[1] Y. H. Jiang,[1,#] D. Delande,[2] M. Martins,[1,*] and G. Kaindl[1]

[1]Institut für Experimentalphysik, Freie Universität Berlin, Berlin-Dahlem, Germany
[2]Laboratoire Kastler-Brossel, Université Pierre et Marie, Paris, France
[#]present address: Max-Planck-Institut für Kernphysik, Heidelberg, Germany
[*]present address: Institut für Experimentalphysik, Universität Hamburg, Germany

In the region close to the double-ionization threshold helium approaches the semi-classical limit, i.e. the effective $\hbar$ tends to 0. Since the classical counterpart of the helium atom, the three-body Coulomb system, is non-integrable and exhibits a mixed phase space, quantum chaos is expected in this region of doubly excited resonances. Studies of these resonances below the single ionization threshold (SIT) I_9 of He^+ showed a transition towards quantum chaos by analyzing the distribution of the nearest-neighbor energy spacings (NNS) between the resonances [1].
Now we present the experimental total photoionization cross section up to the SIT I_{15}, together with state-of-the-art complex-rotation calculations revealing an excellent agreement. Based on the calculations the spectral features were assigned using the classification scheme N,K_n, with N (n) being the principal quantum number of the inner (outer) electron and K the angular-correlation quantum number. The quantum number K represents the expectation value for the angle defined by the electrons and the nucleus and can vary from $K=N-1$ to $K=-(N-1)$. The values of K close to the maximal and minimal value can be related to 1-dimensional helium with both electron being on different site (*eZe*-configuration) or on the same site of the nucleus (*Zee*-configuration), respectively.
We studied the validity of the approximate quantum numbers N and K by investigating the statistical properties of the NNS. These studies proved that for the resonances with K close to $N-1$ the quantity $F = N - K$ is a good quantum number. However, a separate consideration of N and K shows a NNS distribution typical for a chaotic system and indicates that the principal (radial) quantum number N already lost its physical meaning below SIT I_{15}. For the resonances with K close to $-(N-1)$ we found that K and N are separately good quantum number. The behavior of the quantum numbers can be understood on the basis of classical 1-dimensional helium since the *Zee*-configuration is known to be stable with respect to perturbations in angular and radial direction, while the *eZe* configuration is only stable with respect to perturbations in angular direction. The existence of good quantum numbers for part of the resonances below SIT I_{14} show that the transition region from integrability to full chaos is much larger than previously assumed. Since F turned out to be a good quantum number for the resonances with K close to $N-1$, the cross section can be described with a small number of only partially overlapping resonances, i.e. we found up to I_{15} no evidence for Ericson fluctuations, which are considered to be an additional signature of quantum chaos.

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Th3-6

INNER-SHELL PHOTODETACHMENT OF NEGATIVE IONS WITH HALF-FILLED NP-SUBSHELL: EFFECT OF STRONG MANY-ELECTRON CORRELATION

G.Yu. Kashenock and V.K. Ivanov

St. Petersburg State Polytechnic University, Russia

The results of theoretical calculations on resonance behavior in inner-shell photodetachment of negative ions with np^3 outer subshell are presented. The main attention is paid to the near-threshold 2s photodetachemnt from Si^-.

Inner-shell photodetachment of negative ions stands out as extremely sensitive probe and theoretical test-bed for important effects of electron-electron interaction because of the weak coupling between photon and target electrons. Many-body effects play a pronounced role here not only between the outer electrons but also between the inner-shell electrons and outgoing electron.

We use the recently developed method (RPAE&DEM) for simultaneous inclusion of the dynamic polarization potential generated in a system "neutral atomic core + electron", dynamic relaxation (screening) and dynamic polarization of a system by external electromagnetic field. The latter is taken into account within the Random Phase Approximation with Exchange (RPAE). The dynamic polarization potential and relaxation are considered within the Dyson equation method. We include the related many-electron corrections step-by-step in order to analyze their particular contributions to calculated observables.

The strong near-threshold resonance in the photodetachment from inner 2s-shell of Si^- is predicted and it is rather similar to the recently investigated resonance in photodetachment from 1s-shell of the carbon negative ion [1]. The complicated nature, as a mixed ("shape- Feshbach") one, of resonance in 1s C^- has been determined. The collective character of the response to the external electromagnetic field in the strongly correlated C^- target is clearly demonstrated, with the dynamical relaxation of the core being the most pronounced of the collective effects. The calculated cross sections are in fair agreement with the recent experimental data [2].

The very new results on inner-shell 2s photodetachment for Si^- negative ion reveal even more complex nature in comparison with 1s C^- since more inner subshells are involved in photodetachment process. Therefore the RPAE correlations become very important together with strong influence of the dynamical relaxation. Because of that the 2s photodetachment cross section reveals the additional peculiarities of the Fano-profile type in the vicinity of 2s threshold.

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DIELECTRONIC RECOMBINATION OF PARTIALLY-FILLED M-SHELL IONS

D. Nikolić,[1] Sh.A. Abdel-Naby,[1] J. Fu,[1] T.W. Gorczyca,[1] N.R. Badnell,[2] and D.W. Savin[3]

[1] Department of Physics, Western Michigan University, Kalamazoo, MI 49008, USA
[2] Department of Physics, The University of Strathclyde, Glasgow, G4 ONG, UK
[3] Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027, USA

Dielectronic recombination (DR) is an important process in modeling the ionization-recombination balance of multiply-charged atomic ions in low-density high-temperature plasmas. For that purpose, we have extended our previous work through L-shell ions to include systematic calculations of the total DR rate coefficients for selected low-charged M-shell ions.

First, we will present results for Al-like S^{3+} using the level resolved distorted-wave atomic structure and collision code AUTOSTRUCTURE. In addition to previous results [1], our present analysis of the total DR rate coefficients is carried out in both the LS and IC-coupling schemes including both $\Delta N = 0$ and $\Delta N > 0$ electron core excitations, and further expanding by including $3s^2n\ell$ and $3s3pn\ell$ (n = 4 and 5) configurations.

Second, we have resolved the long-standing discrepancies between the experimental and theoretical [2-4] DR rate coefficients for Ar-like Sc^{3+} and Ti^{4+} ions: differences in low-lying resonance positions and asymmetry profiles, as well as the overestimation by roughly 60% at the dominant $3p^53d$ ($^1P_1$) Rydberg series limit.

Our new approach enables us to treat accurately DR for open M-shell ions in a computationally feasible manner, and at the same time to achieve good agreement with available storage-ring measurements.

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DIELECTRONIC RESONANCE ENERGIES AND STRENGTHS IN HIGHLY CHARGED IONS TO INVESTIGATE CORRELATED HIGH-FIELD FEW-ELECTRON DYNAMICS AND QED CONTRIBUTIONS

Z. Harman[1], V. Mäckel[1], A.J. González Martínez[1], A.N. Artemyev[1,2],
J.R. Crespo López-Urrutia[1], U.D. Jentschura[1], C.H. Keitel[1], H. Tawara[1],
I.I. Tupitsyn[1,2], J. Ullrich[1]

[1]Max Planck Institute for Nuclear Physics, Saupfercheckweg 1, 69117 Heidelberg, Germany; [2]Department of Physics, St. Petersburg State University, Oulianovskaya 1, Petrodvorets, 198504 St. Petersburg, Russia

The study of dielectronic recombination (DR) with highly charged few-electron ions provides unique possibilities for investigating correlation, quantum electrodynamic (QED) and nuclear effects in many-electron systems as well as for exploring the dynamics of recombination processes. We have calculated resonance energies for KLL recombination channels into highly-charged Fe, Kr, Xe, Ba, W, and Hg ions [1], applying the multiconfiguration Dirac-Fock and the configuration interaction Dirac-Fock-Sturmian methods, and quantum electrodynamic many-body theory with additional screened QED corrections. The theoretical uncertainties of the contributing terms are estimated.

The photorecombination into these highly charged He- to B-like ions has been explored with the Heidelberg electron beam ion trap [2]. The energies of state-selected DR resonances have been determined by monitoring the emitted x-rays and scanning the electron beam energy over the KLL DR region. At the present level of experimental accuracy, it becomes possible to make a detailed comparison to our theoretical approaches. This comparison shows a good overall agreement. However, a few interesting discrepancies are found in specific recombination resonances for initially Li- and Be-like Hg ions, suggesting the need for further theoretical and experimental studies.

Experimental DR strengths have been determined relative to calculated radiative recombination cross sections. DR cross sections have also been calculated in the framework of the multiconfiguration Dirac-Fock (MCDF) method. Such a comparison highlights the significance of relativistic electron-electron correlation and configuration mixing effects in dynamical processes involving heavy ions. Combining the present data of Hg ions with those for other ions available so far, simple scaling formulae for the nuclear charge number dependence of total as well as partial KLL DR strengths for He-like ions have been deduced.

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Th3-9

ON THE DOUBLE EQUIVALENT OF THE C3 DOUBLE CONTINUUM WAVE-FUNCTION

L. U. Ancarani [1] and G. Gasaneo [2]

[1] Laboratoire de Physique Moléculaire et des Collisions,
Université Paul Verlaine - Metz, 57078 Metz, France
[2] Departamento de Fisica, Universidad Nacional del Sur
and Consejo Nacional de Investigaciones Cientificas y Técnicas,
8000 Bahia Blanca, Buenos Aires, Argentina

In this contribution we are interested in the inter-relation between the description of the double continuum final state and of the doubly bound initial state of two-electron atoms. This is particularly important in the theoretical study of the double ionization of helium, whether by electron ((e,3e) experiments) [1] or photon ((γ,2e) experiments) [2] impact. The full three-body Coulomb problem has been extensively studied, but no exact wave-function is known for either the scattering or the bound states. Hence, approximate wave-functions are generally used when calculating double ionization cross sections: a different choice, however, generally leads to different results [1,2]. Moreover, it is well known that having a symmetric description of the initial and final states is desirable since it avoids spurious contributions in the calculated cross sections. In this way, even relatively simple, but correlated, initial and final state wave-functions - as long as the wave-functions include correlation in a "similar" way - can yield calculated cross sections in agreement with experimental data (see, *e.g.*, the recent study of (e,3e) processes [3-6]).

In this report, we investigate the issue of constructing symmetrically double continuum and double bound approximate solutions for two-electron atoms. We have considered the case of the well known and widely used double continuum C3 wave-function [7] (also called 3C or BBK model). The main aim is to find its double bound equivalent (for S-states) in order to have, for the first time, a symmetric description of correlated bound and continuum wave-functions [8]. This, curiously, has not been presented in the literature. The reason is possibly found in the common misbelief that the Pluvinage wave-function [9] is the answer (see, *e.g.*, [3,5,10].

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Th3-10

TWO-CENTER PROBLEM FOR THE DIRAC EQUATION WITH A COULOMB AND SCALAR POTENTIAL

V.V. Bondarchuk, I.M. Shvab

Uzhgorod National University, 54 Voloshin str., Uzhgorod 88000, Ukraine
igor_shvab@yahoo.com

In this work we consider two-center problem for the Dirac equation with Coulomb and Scalar potential:

$$\left(c\vec{\alpha}\vec{p} + \beta(m_0c^2 + \hat{S}) + E - \hat{V}\right)\Psi(\vec{r}) = 0,$$

$$\hat{S} = -\hbar c\left[\frac{\alpha_{S1}}{r_1} + \frac{\alpha_{S2}}{r_2}\right],\ \ \hat{V} = -\hbar c\left[\frac{\alpha_{V1}}{r_1} + \frac{\alpha_{V2}}{r_2}\right].$$

We wish to discuss the dependence of the electron binding energy of the relativistic two-center problem on the value of scalar coupling constants α_S. For solving Dirac equation we use the LCAO-method [1] which was first proposed for Dirac equation to find electron energy [2]. The analytic formula obtained by applying the LCAO method for the relativistic two-center problem enabled us to calculate the energy term over a wide range of the total nuclear charge and a wide range of internuclear distances R.

$$E = E_0 - \frac{4\pi A^2 (R/2)^{2\gamma}\hbar c}{1+S}\left[\left(1-B^2\right)\left\{\alpha_S L - Q_S M\right\} + \left(1+B^2\right)\left\{\alpha_V L - Q_V M\right\}\right].$$

In Figure 1 represent behavior of electron binding energy of Er--Er systems ($\alpha_V = Z\alpha = 68/137$) as function $E_{bin}(R)$ for the three different cases of scalar coupling constant: $\alpha_S < \alpha_V$, $\alpha_S = \alpha_V$ and $\alpha_S > \alpha_V$.

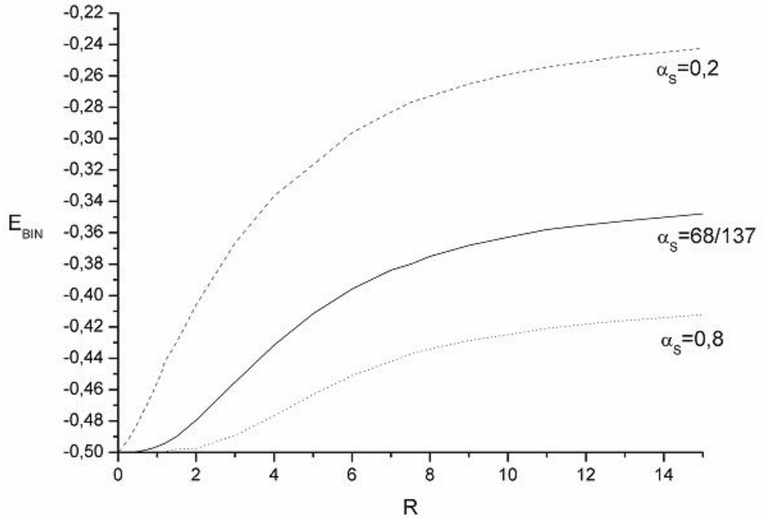

Fig. 1. The binding energy of ground states of the Er-Er system obtained for three different values of α_S ($\hbar = m = c = 1$).

As we see from figure 1 binding energy increases with increasing value α_S.

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Th3-11

Many-Body Dynamics of Repulsively Bound Pairs of Particles in a Periodic Potential

David Petrosyan,[1,2] Bernd Schmidt,[1] James R. Anglin,[1] and Michael Fleischhauer[1]

[1]Fachbereich Physik, Technische Universität Kaiserslautern, D-67663 Kaiserslautern, Germany
[2]Institute of Electronic Structure & Laser, FORTH, 71110 Heraklion, Crete, Greece

Recently, Winkler *et al.* [Nature 441, 853 (2006)] have observed repulsively bound atom pairs in an optical lattice. In a tight-binding periodic potential described by the Bose-Hubbard model, when the on-site repulsion between the particles exceeds their inter-site tunneling rate, such “dimers” are well localized at single sites and are stable over the time scale on which the energy dissipation is negligible. We derive an effective many-body Hamiltonian for a lattice loaded with dimers only, and discuss its implications for dynamics of the system. We show that strong on-site repulsion and nearest-neighbor attraction favor clusters of dimers with minimum surface area and uniform, commensurate filling, representing thus incompressible “droplets” of a lattice liquid.

Th3-12

"A TWO-BODY GREEN FUNCTION TECHNIQUE FOR CALCULTATING TRIPLY DIFFERENTIAL CROSS SECTIONS FOR DOUBLE PHOTOIONIZATIONS OF ATOMS AND MOLECULES"

Authors : Luca Argenti and Renato Colle

Address : Department of Applied Chemistry and Material Science,
University of Bologna
Via Saragozza 8, I-40136 Bologna – Italy
e-mail: colle@sns.it

We present a method, based on the use of two-particle Green functions and projected scattering potentials, for the calculation of triply differential cross sections (TDCS) for double photoionization of atoms and molecules.
The main advantages of the method are the tuneable accuracy of the results and its efficient applicability to molecules.
We apply the method to the calculation of TDCS for double photoionization of helium and other light atoms at energies and geometries covered in recent experiments [1]. We also present preliminary calculations of TDCS for double photoionization of the hydrogen molecule.

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Th3-13

Two-Center Problem for Screened Coulomb and Coulomb plus Confining Potentials

Kh.Yu. Rakhimov and Kh.T. Butanov

Heat Physics Department of the Uzbek Academy of Sciences
28 Katartal St., Tashkent 700135, Uzbekistan

Screened Coulomb potentials play important role in plasma physics to describe electron interaction with atomic nucleus in a plasma environment. Study of interaction of atoms and molecules in plasma environment is an important problem in plasma physics. Binding energy of the electrons in such atoms and molecules is different than that in vacuum because of screening of the Coulomb field of nuclei.

In this work we treat the two center problem with screened Coulomb potential and screened Coulomb plus linear potential. The latter describes the interaction of quarks in hadrons in quark gluon plasma [1]. Using method of linear combination of the atomic orbitals we calculate first the energy term as function of intercenter distance. Inserting the obtained energy term into the Schrödinger equation describing the recoil motion of centers we find binding energy spectrum of this three-particle system via solving numerically this one-center Schrödinger equation. The results show that the binding energy is lower than that in the case of vacuum (nonscreened case).

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Th3-14

INTERFERENCE EFFECTS IN THE PHOTOIONISATION OF H_2

Axel Reinköster [1], Markus Braune [1], Rainer Hentges [1], Sanja Korica [1], Jens Viefhaus [1],
Ralph Püttner [2], Burkhard Langer [3], and Uwe Becker [1]

[1]Fritz-Haber-Institut der MPG, 14185 Berlin
[2]Freie Universität Berlin, Institut für Experimentalphysik, 14195 Berlin
[3]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, 12489 Berlin

Electron-ion-coincidence measurements following H_2 photoionisation by monochromatised synchrotron radiation were performed at BESSY's U125/2-SGM beamline in Berlin. By selecting only the fast H^+ ions in coincidence with hydrogen satellite electrons of continuous energy which match the dissociative final state H^+, the intensity ratio of photoelectrons emitted along the molecular axis and the total ionisation cross section could be determined (Fig. 1). This is the key quantity of the current analysis. The signal shows a variation in the intensity which supports the expected interference patterns due to coherent emission from both H atoms, as also observed in atom-ion collisions [1] and recently for photon impact in N_2 molecules [2]. The resonant feature at ≈20 eV is the so called shape resonance indicating the formation of a standing wave with a wave length of $\lambda=4R$ in agreement with partial cross section measurements [3].

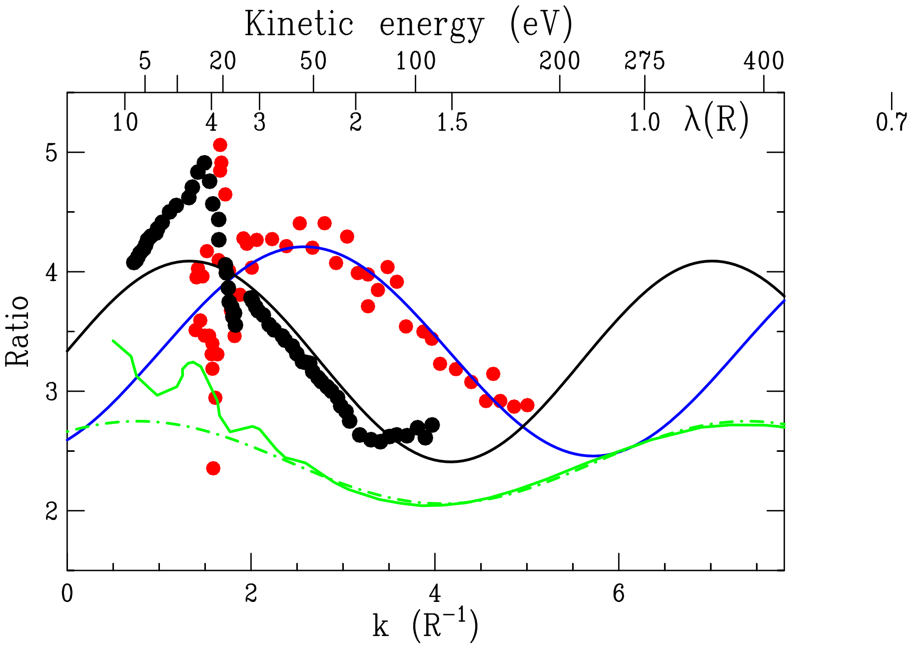

Fig. 1: Intensity variations in the photoionisation of H_2 as a function of the wave vector in units of the inverse bond length. Our data (red circles) are shown together with a fitted Cohen-Fano curve (blue line) and results taken from Chung *et al.* [3] (black circles) and predictions from *ab initio* calculations [4] (green solid line). The black line and the dashed-dotted green line are fitted curves.

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Th3-15

Dissociative double capture in 15N4+ and H2 collisions

Nadine Neumann, Dorota Hant, Lothar Schmidt, Markus Schöffler, Jasmin Titze,
Ottmar Jagutzki and Reinhard Dörner

Institut für Kernphysik, J.W.Goethe Universität, Max von-Laue-Str. 1, 60438
Frankfurt

Because of the high potential energy (up to 30 keV/u) and the low velocity of the ions from the ECR-Source, the main reaction channel in collisions with atoms or molecules is electron capture. The experimental set up will be designed for single capture and double capture with coulomb explosion in molecules, especially fot the following reactions:
$^{15}N^{4+} + H_2 \rightarrow {}^{15}N^{2+} + H^+ + H^+$
The highly charged projectile passes the target molecule in a random distance where Rutheford- and atomic scattering are possible reactions. When the projectile scatters on an electron or the core of the molecule it can be detected out of the center of the beam with a time- and position sensitive MCP-Detector with delay-line anode. The deflection angle of the projectile is a parameter how close the projectile passes the target molecule. The knowledge of this impact parameter is one big advantage of ion-atom and ion-molecule experiment compared to photon-atom or photon-molecule interactions.

Contact:
www.neumann@atom.uni-frankfurt.de

Th3-16

TWO ELECTRON RESONANT EMISSION FROM ATOMS AND CLUSTERS IN THE MULTIPLE SCATTERING APPROACH

F.Da Pieve [a], S.Di Matteo [b], D.Sebilleau [c], R.Gunnella [d], C.R.Natoli [b] and G.Stefani [a]

a) Physics Department, University Roma Tre, via della Vasca Navale 84, 00143 Rome, Italy
b) LNF, National laboratory for nuclear physics, via E.Fermi 40, 00044 Frascati, Rome
c) CNRS, University Rennes, PALMS Laboratory, Campus de Beaulieu 35042 Rennes, France
d) Physics Department, University of Camerino, Italy

The coincidence angular distributions of photoelectrons and Auger electrons can show a high degree of correlations within the electron pair. These correlations depends on the anisotropy induced by photon impact and by detection of the first electron at a specific angle, by the final state quantum numbers like angular momentum and parity, and by energy of the two electrons. Generally, many-body approaches like statistical tensors [1] or graphical technique have been used to describe such correlations, however, such approaches are not suitable for an extension to treat two electrons emission from clusters. We present an alternative approach for the correlation between the two electrons based on the multiple scattering theory in the single particle approach, which allows to consider also the case of emission from a cluster. Multiple scattering theory has been widely used in the past for the interpetation of XAS spectra and photoelectron diffraction patterns. The first tests have been performed on atomic processes: analytical and numerical calculations are presented for the Ar $L_{23}M_{23}M_{23}$ transition and are compared with good agreement with coincidence experimental data [2] collected at ELETTRA synchrotron facility for each of the final angular momentum state ($^1S_0$, ^3P_J, $^1D_2$) of the doubly charged ion. For the solid state we analyzed the coincidence emission from the Ge(100) $L_{23}M_{45}M_{45}$ transition. Numerical results are compared with experimental data collected on the ALOISA beamline at ELETTRA. The coincidence distributions show differences with respect to single electrons diffraction patterns, suggesting both the influence of initial atomic correlation effects [3] (i.e., the rotation due to coincidence emission and detection) and the surface sensitivity of the coincidence technique [4].

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Th3-17

TEMPERATURE EFFECTS ON DISSOCIATIVE ELECTRON ATTACHMENT TO HBr AND DBr

M. Cingel[1], J. Fedor[2], J.D. Skalný[3], J. Horáček[4], A. Stamatovic[1], S. Denifl[1], P. Scheier[1] and T.D. Märk[1]

[1] Institut für Ionenphysik und Angewandte Physik, Leopold Franzens Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria
(michal.cingel@uibk.ac.at)

[2] Present address: Department of Chemistry, University of Fribourg, Chemin de Musee 9, 1700 Fribourg, Switzerland

[3] Department of Experimental Physics, Comenius University, Mlynska dolina, 84245 Bratislava, Slovak Republic

[4] Institute of Theoretical Physics, Charles University, 18000 Prague, Czech Republic

Hydrogen halides constitute an ideal system for testing theoretical models for electron-molecule collisions. Corresponding cross sections (which can be compared to experimental results) include pronounced threshold peaks in the vibrational excitation cross section, step-like features (Wigner cusps) in the dissociative electron attachment (DEA) cross section and distinctly different shapes of the DEA cross section for different vibrational levels of the neutral molecule. The latter feature leads to clearly observable temperature effects [1].

In the present contribution measurements of the Br^- ion yield following dissociative electron attachment to HBr and DBr are summarized. The effusive molecular beam was produced in a temperature controlled capillary heatable up to 650 ºC and perpendicularly crossed with an electron beam. Electrons were formed in a trochoidal electron monochromator with a kinetic energy resolution of about 35 meV. Anions produced were mass analyzed in a quadrupole mass spectrometer and detected in a channeltron.

The ion yield spectra for HBr clearly show the growth of the resonances corresponding to rotationally excited levels of the neutral molecule with increasing temperature. Furthermore, experimental results are in excellent agreement with the non-local resonance model calculations [2].

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Th3-18

coherence and double slit interference in the photo double ionization of H2

Dominique Akoury[1], Katharina Kreidi[1], Thorsten Weber[2], Till Jahnke[1], Rui Alexandre Costa Fraga[1], Nadine Neumann[1], Markus Schoeffler[1], Lothar Schmidt[1], Ottmar Jagutzki[1], Lutz Foucar[1], Tilo Havermeier[1], Horst Schmidt-Boecking[1], Reinhard Doerner[1], Sun Lee[2], Hidehito Adaniya[2], Marcus Hertlein[2], Timur Osipov[2], Mike Prior[2], Ali Belkacem[2], Allen Landers[3], Predrag Ranitovic[4], Lewis Cocke[4]

[1]Institut fuer Kernphysik Frankfurt, Universitaet Frankfurt, Deutschland – [2]LBNL, 1 Cyclotron Road, Berkeley, CA 94720, USA – [3]Department of Physics, Auburn University, Auburn, AL 36849, USA – [4]Department of Physics, Kansas State University, Manhattan, KS 66506, USA

The emission of photoelectrons from a diatomic homonuclear molecule generates a system, which is reminiscent to the classical double slit. From a sequence of H2 double slit experiments, interference structures in the angular distribution of the electrons with respect to the molecular axis have been observed. In this experiment the COLTRIMS technique has been used, and the momenta of the electrons and the recoils have been measured in coincidence for four different photon energies. For lower photon energies above threshold the double ionization is caused mostly by electron scattering, whereas for higher photon energies above threshold the shake off process gets important. Depending on whether the double ionization was initialized by electron scattering or shake off the energy sharing of the electrons is quite equal or very unequal. In case there is a fast and a slow electron the interference structure has been observed in the fast electron. In case both electrons have similar energies the interference structure has been found in the dielectron.

Th3-19

THE 2D TWO-COULOMB-CENTRE PROBLEM IN THE DIRAC EQUATION FRAMEWORK

V.V. Bondarchuk, I.M. Shvab

Uzhgorod National University, 54 Voloshin str., Uzhgorod 88000, Ukraine
igor_shvab@yahoo.com

In this work we have calculated by means of perturbation theory the asymptotic expansions of the eigenvalues (potential curves) $E(R)$ of the two-dimensional two-Coulomb-centre problem Z_1eZ_2 in the limits of united ($R \to 0$) and separated ($R \to \infty$) atoms with the precision $O(R^3)$ and $O(R^{-3})$, respectively.

To illustrate applications of the obtained asymptotic formulas we use them to calculate electron states of the simplest two-center systems. To estimate the contribution of the dimensionality factor in potential curves in the united atom limit, we consider the relation $Q1(Z,R) = E_{3D}^{bin} / E_{2D}^{bin}$ between three-dimensional and two-dimensional expression for the binding energy when $Z_1 = Z_2$. Figure presents a relative contribution of the dimensionality factor of the ground state energy values for the three-dimensional $3D$ and two-dimensional $2D$ molecule ion calculated by the asymptotic formula (2.15) [2] for the three-dimensional case and our formula. As is seen from Figure 1, the term relation $Q1(Z,R)$ increases as Z increases and R is rather small.

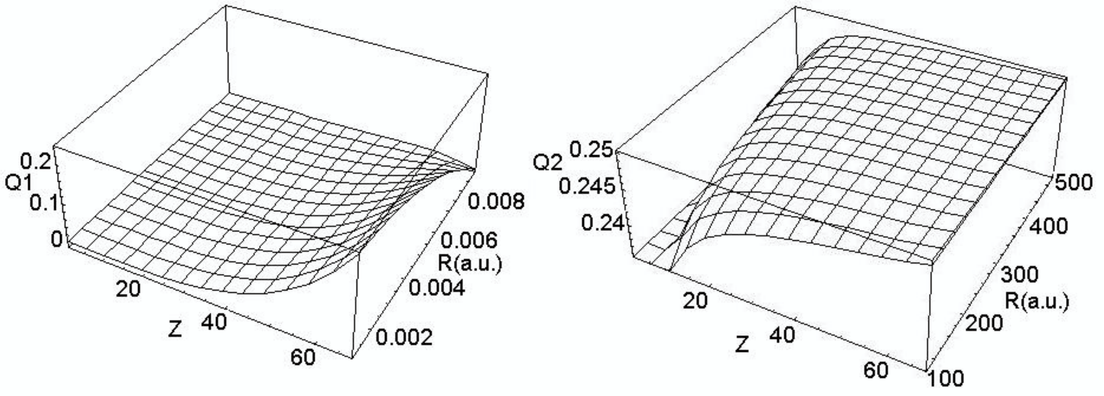

Figure1. The relative contribution $Q1(Z,R)$ and $Q2(Z_1,R)$ of the ground state energy values for the $3D$ and $2D$ molecule ion in the united- and separated atom limit accordingly.

Figure 1 presents an analogous relative contribution $Q2(Z_1,R) = E_{3D}^{bin} / E_{2D}^{bin}$ of the dimensionality factor of the ground state energy values for the $3D$ and $2D$ molecule ion in the separating atom limit, calculated by the asymptotic formula (2.26) [2] for the three-dimensional case and our formula. The data in this figure show that, as the Z and R increase, the term relation $Q2(Z_1,R)$ increases and asymptotically tend to value 0.25.

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Th3-20

METHYL-SUBSTITUTED PYRIDINE-WATER COMPLEXES REVISITED

C. G. Floare

[1] *National Institute for R & D of Isotopic and Molecular Technologies, 71 - 103 Donath Str., 400293, Cluj-Napoca, Romania.*

We have recently reported a reversible liquid-solid transition upon heating of a simple solution composed of a-cyclodextrin (a-CD), water and 4-methylpyridine [1-3]. This phenomenon is due to an extraordinarily strong negative temperature coefficient of the solubility of a-CD in the mixture of 4MP and a small quantity of water.

In this contribution we present a part of our work to study this system where we investigated the hydrogen bonding in pyridine and a set of methyl substituted pyridine-water complexes. We used density functional theory (DFT) and second-order Møller-Plesset perturbation theory (MP2).

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Th3-21

A TRUE NATURE OF HELIUM DOUBLE PHOTOIONIZATION AMPLITUDES

S Cvejanović*&, M Wiedenhoeft#, J. Viefhaus*, and U. Becker*

*Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany
&Department of Physics, Medical Faculty, Brace Branchetta 20, 51000 Rijeka, Croatia
#Department of Physics, Western Michigan University, Kalamazoo, USA

As the most fundamental 3-body Coulomb system, double photoionization of He serves as a testing ground for investigating electron correlation dynamics[1]. In the triple differential cross section for a (γ,2e) interaction the dynamical information is generally inseparable from the effects of the quantum symmetry, preventing easy comparison between experiments employing different detection geometry and/or photon polarisation. That inspired attempts to extract dynamic information from the measured or calculated cross sections using the general cross section parametrisation of Huetz [2], which introduces two symmetrized dynamic amplitudes, each a function of E_1, E_2 and θ_{12}. To enforce uniqueness of the fit a relatively simple amplitude model had to be chosen, either by fixing the functional form of its θ_{12} dependency[3], or by limiting the number of terms in the expansion over the standard angular functions[4]. The parametrisation model[3] postulates a Gaussian dependency over θ_{12} for both amplitudes at small energies, but at higher energies allows for an additional uncorrelated contribution when the energy asymmetry increases, in agreement with the physical insight about the angular correlations within different ionisation mechanisms (Wannier - knockout - shake-off). In fitting our extensive sets of TDCS measured over a wide range of excess energies E (20 - 160eV) but for not too-extreme energy asymmetry ($E/E_i \leq 10$), we found the parametrisation model[3] very satisfactory and the dynamical evolution of derived parameters in good overall agreement with those calculated[5]. But what about the amplitude phase variation with θ_{12}, which was not allowed for in the parametrisation? Are the rather irregularly appearing structures in the wings of the calculated[5] amplitudes artefacts due to exclusion of higher angular momenta? Only by simultaneously fitting the three separate TDCS obtained under widely different kinematical conditions (for the circular polarisation and for the alternative choices of electron energies under linear polarisation) but identical dynamics (E_1 = 4 eV, E_2 = 76 eV) we reached a required sensitivity of the fit to the small effects of the phase variation in the amplitude wings. Our results fully confirmed the calculations[5], showing for the first time a minor deficiency of the amplitude parametrisation model[3].

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POSTERS

Thursday 10/5

4. General Physics

Th4-1

DECOMPOSITION OF THE BOSE DISTRIBUTION OF BLACK-BODY RADIATION IN TERMS OF FERMION BINARY PHOTONS

Sándor Varró

Research Institute for Solid State Physics and Optics
H-1525 Budapest, PO Box 49, Hungary
E-mail: varro@sunsev.kfki.hu

It is shown that the energy of a mode of a chaotic thermal radiation field, following the continuous exponential distribution as a classical random variable, can be decomposed into a sum of its fractional part and of its integer part. The integer part is a discrete random variable, we call it Planck variable, whose distribution is just the Bose distribution. The fractional part is the "dark part" represented by the "dark variable" with a continuous distribution of finite support. Interestingly, the average energy of the dark part approaches from below the zero-point energy for large temperatures. It is proved that the Bose distribution is infinitely divisible, and the irreducible decomposition of it is given. This means that the Planck variable can be decomposed into an infinite sum of independent binary random variables representing the "binary photons" of energies 1-, 2-, 4-, 8-, etc. times the original photon energy. The average energies of these binary photons are given by Fermi distributions with zero chemical potential. According to our analysis, the black-body radiation can be viewed as a mixture of statistically and thermodynamically independent fermion gases consisting of binary photons [1], [2]. The binary photons have wave-particle fluctuations of fermions, and these combine to give the wave-particle fluctuation of the original bosonic photons, expressed by Einstein's fluctuation formula.

Acknowledgement

This work has been supported by the Hungarian National Scientific Research Foundation, OTKA, Grant No. T048324.

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Th4-2

MONTE CARLO SIMULATIONS OF NON-MARKOVIAN OPEN SYSTEMS

J. Piilo, S. Maniscalco, and K.-A. Suominen

Department of Physics, University of Turku, FI-20014 Turku, Finland

We discuss various types of Monte Carlo simulation methods which are commonly applied to solve the dynamics of Markovian [1] and non-Markovian open quantum systems [2]. A long standing issue in the simulations of non-Markovian systems has been the development of Monte Carlo wave-function method working in the Hilbert space of the reduced system only and without auxiliary states. We demonstrate the existence of Monte Carlo wave-function method for a certain class of simple non-Markovian and non-Lindblad-type systems and discuss the ongoing research for generalizing the method.

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Th4-3

MEASUREMENT INDUCED MANIPULATION OF THE QUANTUM-CLASSICAL BORDER

Sabrina Maniscalco, Jyrki Piilo, and Kalle-Antti Suominen

Department of Physics, University of Turku, 20014 Turku, Finland

During the last three decades a huge number of experiments have confirmed the predictions of quantum theory. At the same time many technological applications based on its most peculiar features, such as entanglement, have been discovered. Nevertheless, various aspects concerning the foundations of quantum mechanics still remain to be clarified. Among them, the transition from a microscopic probabilistic world into a macroscopic deterministic one, also known with the pictorial name of quantum-classical border. The consensus today is that classical behaviour is an emergent property of quantum systems induced by their interaction with the environment.

In this paper we focus on a paradigmatic open quantum system, namely the quantum Brownian motion model in a harmonic potential. Such a system, namely a damped harmonic oscillator, possesses a classical limit and it is therefore possible to monitor the transition from quantum to classical dynamics caused by decoherence induced by the environment.We demonstrate how appropriate sequences of nonselective measurements of the energy of such system give rise to quantum Zeno or anti-Zeno effects, allowing to manipulate the quantum-classical border by prolonging or shortening, respectively, the persistence of quantum features in the initial state [1].

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Th4-4

PHASE SPACE SUB-PLANCK STRUCTURES: EXPERIMENTAL REALIZATION IN TIME-FREQUENCY DOMAIN

Ludmiła Praxmeyer (1), Piotr Wasylczyk (2), Czesław Radzewicz (2),
Krzysztof Wódkiewicz (3,4)

(1) Theoretical Physics Division, Sofia University, James Bourchier 5 blvd,
1164 Sofia, Bulgaria (e-mail: lpraxm@gmail.com)
(2) Institute of Experimental Physics, Warsaw University, ul. Hoża 69,
00-681 Warsaw, Poland
(3) Institute of Theoretical Physics, Warsaw University, ul. Hoża 69,
00-681 Warsaw, Poland
(4) Department of Physics and Astronomy, University of New Mexico,
Albuquerque NM 87131, USA

It was shown by Zurek [1] that sub-Planck structures in phase space - an unexpected sign of quantum interference - play a surprisingly important role in the distinguishability of quantum states. A sub-Planck phase space shift applied to a superposition of coherent states is sufficient to produce a state which is orthogonal to the unshifted one. This seems counter-intuitive because such superpositions of coherent states overlap significantly. Nevertheless, a very small shift causes that the original and shifted superpositions are orthogonal to each other, which makes them - at least in principle - distinguishable. The effect was originally studied for a superposition of four coherent states [1] and then in [2,3] it was shown that superpositions of just two coherent states lead to a similar result.

Both in classical optics and quantum mechanics the linear superposition principle is the basis of all interference phenomena. Thus, it should not surprise one that if quantum wave packets are replaced by light pulses, the effects similar to sub-Planck structures, i.e. sub-Fourier structures, should be observed. We present experimental data of the frequency resolved optical gating (FROG) measurements of light pulses revealing interference features which correspond to sub-Planck structures in phase space [4]. For superpositions of pulses a small, sub-Fourier shift in the carrier frequency leads to a state orthogonal to the initial one, although in the representation of standard time-frequency distributions these states seem to have a non-vanishing overlap.

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Th4-5

THE UNIVERSAL VIEW OF THE HAMILTONIAN OF THE EXCANGE INTERACTION FOR THE SYSTEM OF PARTICLES WITH ARBITRARY SPINS.

E.Orlenko

St.Petersburg State Polytechnic University. Polytechnicheskaya St.29, St.petersburg
195251.Russia.

On the base of the arrangement symmetry for the system of identical particles the universal type Hamiltonian of the exchange interaction in the spin representation is developed. For the case of spin ½ the developed Hamiltonian comes to the Heisenberg form.

The magnetic phenomena, connected with the spin ordering in the system of spins, different from ½, are very actual in the low temperature physics at last time. The magnetic properties of the degenerated atomic gases have been studying very intensive. The atoms of Rb87 have spin j=2, atoms of Na23 have spin j=1, K40 has j=9/2, all these systems show us the macroscopic quantum magnetic properties. For the description and explanation of these spin-ordering phenomena there is necessary to develop and to use the spin Hamiltonian, which is different from the Heisenberg Hamiltonian, because of its connection with symmetry properties of spin ½ particles.

In the simplest case of many-particles system with only two-particle interaction the Hamiltonian taking into account pair interactions and acting on spin functions could be presented as

$$\hat{H} = N(N-1)K + \underset{k<l}{\quad} A_{kl}\hat{P}_{j_k,j_l}\cdot, \quad (1)$$

where the projection operator in a polynomial presentation:

$$\hat{P}_{j,j} = c_1\left(\hat{\vec{j}}_1\cdot\hat{\vec{j}}_2\right)^{2j} + c_2\left(\hat{\vec{j}}_1\cdot\hat{\vec{j}}_2\right)^{2j-1} + \ldots c_{2j}\left(\hat{\vec{j}}_1\cdot\hat{\vec{j}}_2\right) + c_{2j+1} \quad . \; (2)$$

For the two-particle system, which spins are $j_1 = j_2 = j$, the total spin J may have eigenvalues: $(2j),(2j-1),\ldots 0$ - in summary $2j+1$ - eigenvalues. For obtaining the operator we are requesting:

$$\boxed{\hat{P}_{jj}\left|J,J_z\right\rangle = \pm 1\left|J,J_z\right\rangle} \; (3)$$

We have a system of $(2j+1)$ linear equations from (3) for determination of free coefficients:

$$(2j+1)\left\{\begin{array}{l} c_1\overline{\left(\hat{\vec{j}}_1\cdot\hat{\vec{j}}_2\right)}^{2j} + c_2\overline{\left(\hat{\vec{j}}_1\cdot\hat{\vec{j}}_2\right)}^{2j-1} + \ldots c_{2j}\overline{\left(\hat{\vec{j}}_1\cdot\hat{\vec{j}}_2\right)} + c_{2j+1} \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \end{array}\right|_J = \pm 1 \qquad (4)$$

This system has only one, unique solution with determinate coefficients:

$$c_1 = \frac{\Delta_1}{\Delta},\ldots$$

$$c_{2j+1} = \frac{\Delta_{2j+1}}{\Delta}$$

where $\Delta = \begin{vmatrix} \left(j^2\right)^{2j}, & \left(j^2\right)^{2j-1}, \ldots\ldots\ldots\ldots 1 \\ \left(j(j-2)\right)^{2j}, & \left(j(j-2)\right)^{2j-1}, \ldots\ldots 1 \\ \ldots\ldots\ldots\ldots\ldots\ldots & \ldots\ldots\ldots\ldots\ldots\ldots 1 \\ \left(-j(j+1)\right)^{2j}, & \left(-j(j+1)\right)^{2j} \ldots 1 \end{vmatrix}$, and determinants Δ_k could be obtained by changing the *k*-column in general determinant Δ by the column of free radicals from the right part .

For example, we can represent the Hamiltonians of exchange interaction for the systems of particles with spins $j=1$, $j=3/2$, $j=2$.

For particles with spin $j=1$ the operator $\hat{P}_{11}$ has a view:

$$\hat{P}_{11} = \hat{\vec{j}}_1 \cdot \hat{\vec{j}}_2 + (\hat{\vec{j}}_1 \cdot \hat{\vec{j}}_2)^2 - 1 \quad , \tag{5}$$

and Hamiltonian of a system N pair interacting bosonic particles with spins j=1 has a view [6]

$$\hat{H}_{int} = (K-A)\frac{N(N-1)}{2} + A \underset{k<l}{} \left[(\hat{\vec{j}}_k \cdot \hat{\vec{j}}_l)^2 + (\hat{\vec{j}}_k \cdot \hat{\vec{j}}_l) \right] \tag{6}$$

For particles system with spins j=3/2 an operator $\hat{P}_{3/2,3/2}$:

$$\hat{P}_{3/2,3/2} = -\frac{2}{9}(\hat{\vec{j}}_1 \cdot \hat{\vec{j}}_2)^3 - \frac{11}{18}(\hat{\vec{j}}_1 \cdot \hat{\vec{j}}_2)^2 + \frac{9}{8}(\hat{\vec{j}}_1 \cdot \hat{\vec{j}}_2) + \frac{67}{32}. \tag{7}$$

Then Hamiltonian of a system of N particles in interacting:

$$\hat{H}_{\text{int}} = \frac{N(N-1)}{2}K - A \underset{k<l}{} \{\frac{2}{9}(\hat{\vec{j}}_k \cdot \hat{\vec{j}}_l)^3 + \frac{11}{18}(\hat{\vec{j}}_k \cdot \hat{\vec{j}}_l)^2 - \frac{9}{8}(\hat{\vec{j}}_k \cdot \hat{\vec{j}}_l) - \frac{67}{32}\}. \tag{8}$$

Transposition operator $\hat{P}_{2,2}$ for particles with spins j=2 will be represented in the form:

$$\hat{P}_{22} = \frac{1}{36}(\hat{\vec{j}}_1 \cdot \hat{\vec{j}}_2)^4 + \frac{1}{6}(\hat{\vec{j}}_1 \cdot \hat{\vec{j}}_2)^3 - \frac{13}{36}(\hat{\vec{j}}_1 \cdot \hat{\vec{j}}_2)^2 - \frac{5}{2}(\hat{\vec{j}}_1 \cdot \hat{\vec{j}}_2) - 1 \quad , \tag{9}$$

then Hamiltonian for the bosonic system of N particles with spins j=2:

$$\hat{H}_{int} = (K-A)\frac{N(N-1)}{2} +$$

$$+\frac{A}{6} \underset{k<l}{} \left\{ \frac{1}{6}(\hat{\vec{j}}_k \cdot \hat{\vec{j}}_l)^4 + (\hat{\vec{j}}_k \cdot \hat{\vec{j}}_l)^3 - \frac{13}{6}(\hat{\vec{j}}_k \cdot \hat{\vec{j}}_l)^2 - 15(\hat{\vec{j}}_k \cdot \hat{\vec{j}}_l) - 6 \right\}.$$

It is easy to see, that all Hamiltonians, described many-particles system with spins of particles different from ½ contain non-linear inputs of scalar product operators. These inputs are the reason of nonlinear magnetic phenomena which take place in spin bosonic systems [4].

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Th4-6

EINSTEIN COEFFICIENTS FOR ACTIVATION BARRIER

Anatoly V. Stepanov

National Ozone Monitoring Research and Educational Centre, Byelorussian State University, Minsk 220064, Belarus

Analytical calculation of Einstein coefficients is made for activation barrier of the Boltzmann–Arrhenius model and an activation process model. For the activation process model an activation barrier is shown to have discrete energy structure due to its thermodynamic equilibrium with thermal radiation. This structure is determined by interaction of conformation substates of a molecule with thermal radiation. The Boltzmann–Arrhenius model represents an activation process as a result of the work of high-energy spectral components of thermal equilibrium radiation. The process is realized by overcoming a potential barrier with continuous energy structure. However, it is shown, that such process is essentially non-equilibrium and hard to achieve at thermal equilibrium radiation [1].

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Th4-7

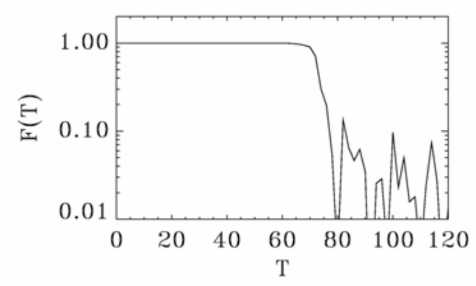
Loschmidt echo in a system of interacting electrons

G. Manfredi and P.-A. Hervieux

Institut de Physique et Chimie des Matériaux de Strasbourg,
GONLO, 23 rue du Loess, 67034 Strasbourg, France

In a famous controversy with Ludwig Boltzmann at the dawn of modern statistical mechanics, Joseph Loschmidt pointed out that, if one reverses the velocities of all particles in a physical system, the latter would evolve back to its initial state, thus violating the second law of thermodynamics. The main objection to this line of reasoning is that velocity reversal is an extremely unstable operation and that tiny errors would quickly restore "normal" entropy increase. Nevertheless, time reversal is indeed possible, as was shown in spin echo experiments performed since the 1950s.

Loschmidt's idea has recently experienced a resurgence of interest in the context of quantum information theory. Indeed, any attempt at coding information using quantum bits is prone to failure if a small coupling to the environment destroys the unitary evolution of the wave function (decoherence). In order to estimate the robustness of a physical system, the following procedure has been suggested: a single quantum particle evolves under the action of a chaotic Hamiltonian H_0 until a time T; then, it is evolved backwards in time until $2T$ with the original Hamiltonian plus a small perturbation (the "environment"). The square of the scalar product of the initial and final states defines the *Loschmidt echo* or *fidelity* of the system. Theoretical and numerical studies showed that the Loschmidt echo decays exponentially with the time delay T.



What happens when one deals, not with a single particle, but with a large system of interacting particles, such as the electrons in a metallic or semiconductor nanostructure? In order to answer this question, we devised a quantum hydrodynamic model that includes electron-electron interactions via the self-consistent Coulomb field. The results of our numerical experiments were intriguing: the fidelity does not decay exponentially, but rather stays close to unity until a critical time, after which it drops abruptly (see figure). This unusual behaviour is related to the fact that the unperturbed Hamiltonian H_0 depends on the electron density n_e. When the perturbation induces a small change in n_e, H_0 is itself modified, which in turns affects n_e, and so on. Thanks to this "snowball effect", the perturbed and unperturbed solutions can diverge very fast. This effect could be a generic feature of interacting many-particle systems. If so, it would have an impact on the decoherence properties of solid-state quantum computation devices, which may then behave differently in the single-electron and many-electron regimes.

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G. Manfredi, P.-A. Hervieux, Phys. Rev. Lett., 97, 190404 (2006)

POST-DEADLINE ABSTRACTS[*]

FORMATION AND TIME-RESOLVED FLUORESCENCE OF $Cs^{*}He_n$ EXCIPLEXES IN SOLID ^{4}He
A. Hofer, P. Moroshkin, A. Weis Mo 7/5, (Clusters and Nanoparticles)

SELF-SUSTAINED OSCILLATING MODE OF OPERATION OF A HOLLOW CATHODE DISCHARGE AT POSITIVE DYNAMIC RESISTANCE
V. Steflekova, E. Dimova and D. Zhechev Mo 7/5, (Plasma)

ONE- AND TWO-PHOTON COHERENT CONTROL OF ATOMIC IONIZATION YIELDS IN THE PRESENCE OF A DC FIELD
A. Bolovinos, S. Cohen Mo 7/5, (Coherent Control)

EXACT SOLUTION OF THE THREE-BODY SCHRÖDINGER EQUATION FOR COULOMB PROBLEMS
S. Paul Thu 10/5, (Few body dynamics)

TWO-COLOR PUMP-PROBE STUDIES COMBINING EUV FREE ELECTRON AND IR/VISIBLE LASER RADIATION
P. Radcliffe, S. Düsterer, H. Redlin, A. Azima, W. Li, J. Feldhaus, J. Dardis, K. Kavanagh, H. Luna, J. Pedregosa Gutierrez, P. Yeates, E.T. Kennedy, J.T. Costello, A. Delserieys, C.L.S. Lewis, R. Taïeb, A. Maquet, A.N. Grum-Grzhimailo, E.V. Gryzlova, S.I. Strakhova, D. Cubaynes, D. Glijer, and M. Meyer
Mo 7/5, (Coherent Control)

AB INITIO STUDY OF THE PHOTODISSOCIATION OF METHANE
Rob van Harrevelt Mo 7/5, (Molecular dynamics)

TWO-PHOTON IONIZATION OF He USING EXTERIOR COMPLEX SCALING
F. Morales, F. Martín, C.W. McCurdy, Dan Horner Thu 10/5, (Few body dynamics)

OZONE MOLECULE: GLOBAL VARIATIONAL CALCULATION AND ASSIGNMENT OF HIGHLY EXCITED RO-VIBRATIONAL STATES
Vladimir Tyuterev, Sergei Tashkun, Habib Seghir, and Alain Barbe
Thu 10/5, (Atomic and Molecular Spectroscopy)

PHOTODISSOCIATION OF ALKALI DIMER MOLECULES AND DIATOMIC BUBBLES IN SOLID ^{4}HE
P. Moroshkin, A. Hofer, and A. Weis Mo 7/5, (Clusters and Nanoparticles)

ATOM-DIMER RESONANCE IN AN ULTRACOLD GAS
F. Ferlaino, M. Mark, M. Berninger, J. G. Danzl, S. Knoop, T. Kraemer, H. Schöbel, H. C. Nägerl, and R. Grimm We 9/5, (Cold atoms and molecules)

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[*] Last update: 30/04/2007

STRUCTURAL PATTERNS IN FULLERENES: C_{20} TO C_{102}

Yang Wang, Goar Sánchez, Sergio Díaz-Tendero, Fernando Martín and Manuel Alcamí Mo 7/5, (Clusters and Nanoparticles)

STATE SELECTIVE DIFFERENTIAL CROSS SECTIONS FOR SINGLE ELECTRON CAPTURE IN H^+-, He^+- and He^{2+} -COLLISIONS WITH He

M.S. Schöffler, J. Titze, L.Ph.H. Schmidt, O. Jagutzki, T. Jahnke, R. Dörner, H. Schmidt-Böcking and I. Mancev Thu 10/5, (Few body dynamics)

MESOSCOPIC COHERENT QUANTUM DYNAMICS IN THE STRONG BLOCKADE REGIME

Tilman Pfau

PAULI'S APPROACH OF HYDROGEN ATOM IN NONCOMMUTATIVE QUANTUM MECHANICS

Y. Grandati, A. Bérard, H. Mohrbach, H. Boumrar and F. Menas

We 9/5, (Precision Measurements)

FORMATION AND TIME-RESOLVED FLUORESCENCE OF Cs*He$_n$ EXCIPLEXES IN SOLID ^{4}He

A. Hofer, P. Moroshkin, A. Weis

Physics Department, University of Fribourg, Switzerland

Solid He is an environment that is very well suited to study weakly bound complexes. Recently we have shown that the formation of exciplexes (excited state complexes) in solid ^{4}He [1] is different from exciplex formation in cold He gas or on He nanodroplets. Laser excited Cs atoms in solid He can bind 7 He atoms, whereas in less dense environments only the Cs*He$_2$ exciplex is observed. Cs atoms in solid ^{4}He excited to the 6P$_{1/2}$ or 6P$_{3/2}$ state decay via three different channels: i) atomic D$_1$ (6P$_{1/2}$ - 6S$_{1/2}$) fluorescence at 880 nm, ii) formation and fluorescence (at 950 nm) of Cs*He$_2$ and iii) formation and fluorescence (at 1400 nm) of Cs*He$_7$. The D$_2$ (6P$_{3/2}$ - 6S$_{1/2}$) emission is completely quenched due to the exciplex formation.

More recently we carried out time-resolved fluorescence studies of all three possible decay channels of excited Cs in solid He. The Cs atoms were excited by 10 ns laser pulses. We recorded pulse shapes of the different fluorescence channels. Figure 1 shows a measurement of the time-resolved fluorescence from the small Cs*He$_2$ and from the terminal Cs*He$_7$ exciplex and also for the atomic D$_1$ emission. The thin line shows the recorded laser pulse.

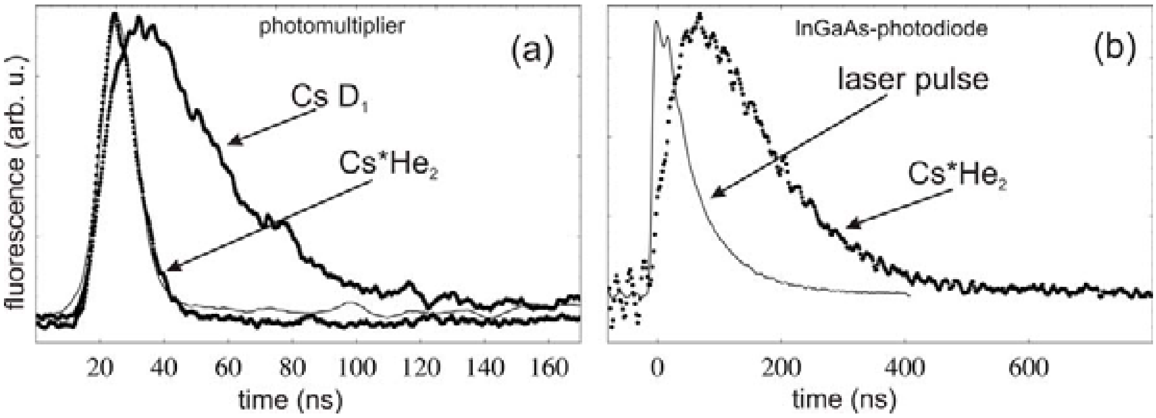

Fig.1 (a) Pulse shape of the atomic D$_1$ fluorescence and the Cs*He$_2$ exciplex (bold dotted line) compared to the laser pulse (thin line) (b) same for the Cs*He$_7$ exciplex. Note the slower time response of the InGaAs detector.

The lifetime of the Cs*He$_2$ exciplex is shorter than the atomic lifetime but it can not be resolved with the present system. We can conclude that this complex is only a transient product in the formation of the Cs*He$_7$ exciplex which has a lifetime of 95 ns. The Cs*He$_7$ exciplex emission is shifted to the red by 500 nm with respect to the D$_1$ emission, but the (trivial) ω^3 scaling only partly explains the measured lifetime. We will present formation and decay paths of the different complexes.

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SELF-SUSTAINED OSCILLATING MODE OF OPERATION OF A HOLLOW CATHODE DISCHARGE AT POSITIVE DYNAMIC RESISTANCE

V. Steflekova, E. Dimova and D. Zhechev

Institute of Solid State Physics, BAS, 72 Tzarigradsko Chaussee,
1784 Sofia, Bulgaria
spectron@issp.bas.bg

Earlier a light-induced oscillating mode of operation of a Hollow Cathode Discharge (HCD) was observed under i-V region of negative dynamic resistance $r_{din}=\partial U/\partial I<0$ [1].In some cases self-sustained oscillations arise under region of $r_{din} >0$, where the electric circuit transforms the energy of the feed continuous discharge current into oscillating one. This transformation may be analyzed qualitatively within the frames of the glow discharge equivalent electrical scheme (RCL)[2], i.e. whether a small deviation η from the selected working point $\{i_{0,} V_0\}$ can rise in amplitude.

Generally, the discharge current i related to the voltage V may be expressed as $i = g_a V + C\frac{dV}{dt} + V\frac{dC}{dt}$, where g_a is the plasma active conductivity. Since $i = i_0 + \eta$ the voltage across the discharge $V = V_0 + \frac{dV}{di}\eta = V_0 + r_{dyn}\eta$.

Having taken in mind also the relations $L\frac{di}{dt} + Ri + V = U$ and $L\frac{d\eta}{dt} + R\eta + r_{dyn}\eta = 0$ a standard equation of the type

$$a\,(\partial\eta/\partial t)^2 + b(\partial\eta/\partial t) + d = 0$$

may be worked out. The positive solution of interest $\partial\eta/\partial t >0$ takes place at $d < 0$, where the coefficients a, b and d represent functions of some coefficients and gas discharge medium parameters. The inequality d < 0 is found to require reasonable date values. Thus, our analysis represents an adequate approach in the comprehension of the spontaneous self-sustained oscillations in a HCD.

The National Fund of Scientific Research (Contract F 1210/02) supported this investigation.

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ONE- AND TWO-PHOTON COHERENT CONTROL OF ATOMIC IONIZATION YIELDS IN THE PRESENCE OF A DC FIELD

A. Bolovinos, S. Cohen

Atomic & Molecular Physics Laboratory, Physics Department, University of
Ioannina, GR–45110 Ioannina, Greece

Phase control refers to the interference between alternative transition amplitudes generated by two mutually coherent laser fields and manipulated through the external adjustment of their relative phase [1]. Total ionization yields of dipole allowed transitions of isolated atomic systems may be controlled by involving only odd or only even number of photons for each excitation pathway. However, photoelectron angular distributions may be modified by the coherent control scheme involving one and two photon transitions (with frequencies 2ω and ω, respectively). Nevertheless, for extending the application of this simplest scheme to the manipulation of total ionization yields, some theoretical investigations have explored the implication of external static electric fields which mix states of opposite parity [2]. A relevant experimental study appeared very recently [3] where this scheme was employed using the low excited 8s state of Cs and electric field strengths ~4kV/cm.

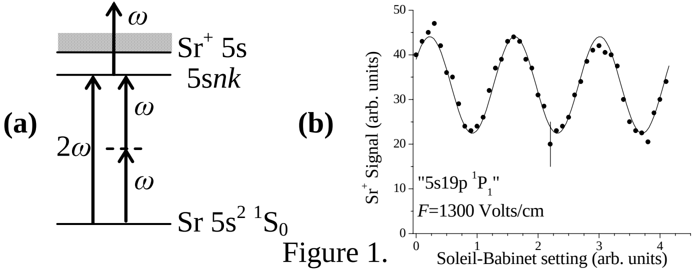

Figure 1.

In the present work we experimentally demonstrate one- and two-photon phase sensitive coherent control of total ionization rates in the presence of a DC electric field via bound Rydberg states of the strontium atom (Figure 1(a)). A pulsed Nd:YAG pumped dye laser (~5 ns duration λ~440 nm), is frequency doubled in a BBO crystal. The visible and UV beams propagate collinearly and pass through a Soleil-Babinet compensator for manipulating their relative phase. Subsequently they are focused by an f=25 cm concave mirror into a Sr atomic beam in a typical time-of-flight set-up. The laser-atom interaction takes place in the presence of an F=50-2000 Volts/cm field which both breaks the parity selection rule and accelerates the produced photoions to the detector. Several zero-field 5s*nl* ($n\approx$17-20, l=s,p,d,…) Rydberg states may be either one- or two-photon excited. Note that the UV beam alone cannot photoionize them. In the presence of the static field, the total ion signal is controlled by the field strength F (determining the relative character composition of the final 5s*nk* Stark states) and the intensities and relative phase of the two laser beams. As shown in Figure 1(b), the contrast is 50% or better, which is very encouraging, considering the fact that the visible beam linear polarization is perpendicular to F and may induce final state background excitations.

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Exact Solution of the three-body Schrődinger Equation for Coulomb Problems

S . Paul
Quantum Optics and Quantum Information Division, Physical Research Laboratory
India

ABSTRACT

The study of the dynamics of three charged particles moving in the three-body continuum is one of the fundamental problems in atomic physics. In the present work, based on hyperspherical partial wave approach [1], an analytical wave function is constructed which represents an exact solution of three-body Schrődinger equation.

The exact final state unsymmetrized wave function is given by

$$\Psi_f^{(-)}(r_1,r_2,\hat{r}_1,\hat{r}_2)=\sum_{l_2,l_2,n} A_{l_1,l_2}^{n}\, f_{l_1,l_2}^{n}(r_1,r_2)Y_{l_1,l_2}^{LM}(r_1,r_2,\hat{r}_1,\hat{r}_2),$$

where the radial wave function for two charged particles is

$$f_{l_1,l_2}^{n}(r_1,r_2)=\frac{1}{(P\sqrt{r_1^2+r_2^2})^{3/2}}\, j_\mu(P\sqrt{r_1^2+r_2^2})P_{l_2,l_2}^{n}(\tan^{-1}(r_2/r_1)),$$

$$\mu=2n+l_1+l_2 \text{ and } P=\sqrt{p_1^2+p_2^2}\,.$$

The coefficients A_{l_1,l_2}^{n} involved in final state wave function can be easily calculated from a set of homogeneous linear equations

$$\sum_{\lambda'}\alpha_{\lambda\lambda'}C_{k\lambda'}A_{\lambda'}=0, \text{ where } \lambda=(l_1,l_2,n).$$

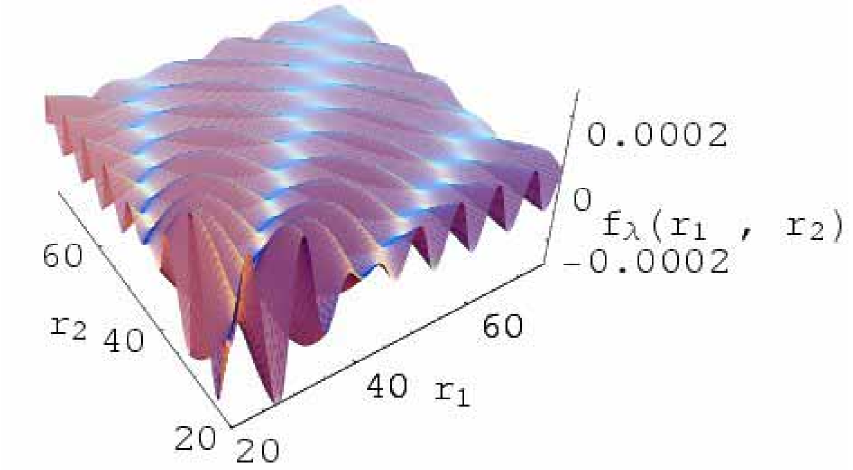

Figure 1: Radial part $f_\lambda(r_1,r_2)$ of the unsymmetrized final state wave function for $l_1=1, l_2=1, n=3$ and $P=1$

In the above equation, the symmetric charge matrix $[\alpha_{\lambda\lambda'}]$ depends on the parameters (L,S,M,l_1,l_2,n) and the matrix $[C_{k\lambda'}]$ is obtained from the inner product of two spherical Bessel functions. For a particular process as electron-hydrogen-ionization merely a few sets of values of the coefficients are necessary to calculate all the differential cross-sections for various energies. The process can also be prolonged for application to the problems more than three bodies.

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Two-color pump-probe studies combining EUV Free Electron and IR/visible Laser radiation

P. Radcliffe[1], S. Düsterer[1], H. Redlin[1], A. Azima[1], W. Li[1], J. Feldhaus[1], J. Dardis[2], K. Kavanagh[2], H. Luna[2], J. Pedregosa Gutierrez[2], P. Yeates[2], E.T. Kennedy[2], J.T. Costello[2], A. Delserieys[3], C.L.S. Lewis[3], R. Taïeb[4], A. Maquet[4], A.N. Grum-Grzhimailo[5], E.V. Gryzlova[5], S.I. Strakhova[5], D. Cubaynes[6], D. Glijer[6], and M. Meyer[6]

[1] *HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany*
[2] *NCPST and School of Physics, Dublin City University, Glasnevin 6, Dublin, Ireland*
[3] IRCEP, Queen's University Belfast, BT71NN, United Kingdom
[4] *LCP-MR, Université Pierre et Marie Curie, F-75006 Paris, France*
[5] *Institute of Nuclear Physics, Moscow State University, Moscow 119992, Russia*
[6] *LIXAM, Centre Universitiare Paris-Sud, Bât. 350, F-91405 Orsay, France*

The Free Electron Laser in Hamburg (FLASH) was used in combination with the synchronized femtosecond optical laser to investigate the photoionization of rare gases in an optical dressing field, so-called Above Threshold Ionization (ATI), and the photoinduced fragmentation of H_2 molecules. The experiments were carried out using a magnetic bottle electron spectrometer enabling us to record electron spectra for each individual FLASH pulses. FLASH provided short light pulses (about 20 fs) at 25.5 and 13.8 nm respectively, which were combined with 120 fs pulses from the optical laser (800nm).

The measurements of the ATI signal, i.e. of sidebands in the photoelectron spectrum, were used to optimize the spatial and the temporal overlap between the pulses. The sidebands, which arise from the interaction of the electron with both the FLASH and the optical laser photons, are extremely sensitive to the overlap of the pulses and to the stability of the set-up. We have undertaken first time-resolved measurements of the photoinduced fragmentation of molecular hydrogen. The dissociation of the molecules was induced by the FLASH pulses and the formation of excited atomic fragments, i.e. hydrogen atoms with the electron in the Rydberg states (n=3,4,...), was probed through photoionization by the optical laser. In the region of temporal overlap between the two pulses, a very fast increase of the signal was observed indicating a fast dissociation process (less than 100fs). For longer time delays the signal is determined by the lifetime of the excited hydrogen atoms.

In an application, we investigated the dependence of the sideband intensity from the relative orientation of the linear polarization vectors of both radiation fields. The amplitude of these variations is mainly determined by the ratio of the emission of 'p' and 'f' ('s' and 'd') electrons in the 5p (1s) ionization of Xe (He). The results provide therefore insights into the electronic interactions during ionization.

Ab initio study of the photodissociation of methane.

Rob van Harrevelt

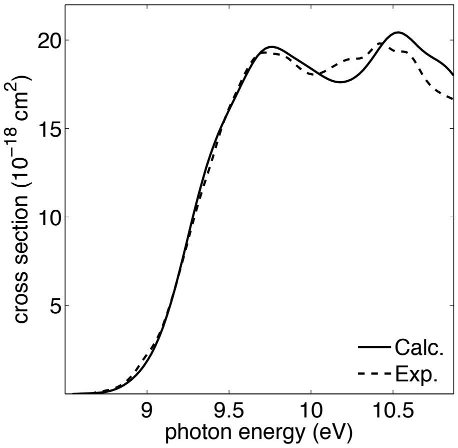
Institute of Theoretical Chemistry, Radboud University Nijmegen, the Netherlands.

r.vanharrevelt@science.ru.nl

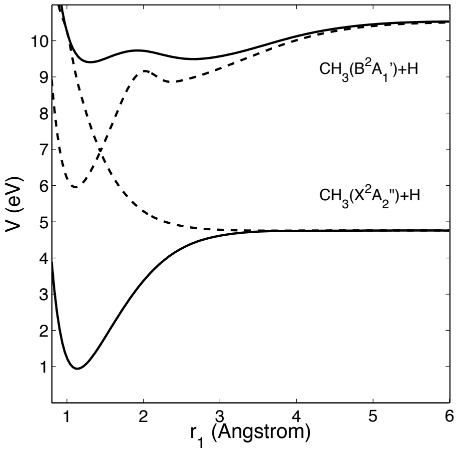
The ultraviolet absorption band in the 8.8-11.4 eV photon energy range has been assigned to a $1t_2 \rightarrow 3s$ Rydberg transition [1]. The absorption spectrum is composed to two diffuse broad bands, centered at 9.7 and 10.4 eV. Vibrations of e and t_2 lift the degeneracy of the 1^1T_2 state. Of the resulting adiabatic potential energy surfaces, V_1, V_2 and V_3, only the V_1 surface is dissociative. Possible products on the V_1 surface are $CH_3(\tilde{B}^2A_1')$+H and $CH_2(\tilde{a}^1A_1)$+H_2 [2]. However, experiments [3] suggest that most products are formed on the ground state (V_0) potential energy surface. The aim of this poster is to explain these experimental findings.

To study the absorption spectrum, a three-valued potential energy surface is constructed based on an expansion in powers of the nuclear displacements [4]. The parameters are fitted to results of multi-reference configuration interaction (MRSD-CI) calculations. The cross section is calculated using the multiconfiguration time-dependent Hartree approach. The result is in good agreement with experiment [1]. The calculations suggest that the two broad bands correspond to the different Jahn-Teller components.

The poster also discusses the importance of conical intersections between the V_0 and V_1 surfaces at planar geometries [5] for the photofragmentation process. Cuts through the potential energy energy surface have been calculated using the MRSD-CI approach.



Calculated and experimental [1] photodissociation cross sections.



Energies V_0 and V_1 along the $CH_4 \rightarrow CH_3$+H path. r_1 is the C-H1 bond length. Solid lines: C_{3v} pathway. Dashed lines: planar pathway.

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TWO-PHOTON IONIZATION OF He USING EXTERIOR COMPLEX SCALING

[1]*F. Morales,* [1]*F. Martín,* [2,3] *C.W. McCurdy,* [2] *Dan Horner*

[1]*Departamento de Química, Universidad Autónoma de Madrid, 28049, Madrid, Spain*
[2] *Lawrence Berkeley National Laboratory, Computing Sciences, Berkeley, CA 94720, USA*
[3] *Department of Applied Science, University of California, Davis, Livermore, CA 95616, USA*

Having successfully studied the problem of one-photon double ionization of He and H_2 by using the exterior complex scaling (ECS) method in combination with B-spline basis functions (see Refs. 1,2,3 and references therein), a subject of intense study over the last decade, our group now tries to study single and double ionization by the simultaneous absorption of two photons using an extension of this method. This offers a new challenge, as complexity increases, and current publications (see Ref. 4 and references therein) on He do not even agree on the magnitude of the total cross sections.

A particular aspect of double ionization in He is that the total number of photons absorbed (two in this case) is larger than the number of photons required (one) to ionize the system by emission of a single electron. This process is called above threshold ionization (ATI) and is known to be difficult to describe because it implies continuum-continuum transitions. The evaluation of the fully differential cross sections will allow us to understand if the emission of the two electrons is sequential or not a question that has been the subject of intense debate in the last two years. It will be also interesting to compare the calculated cross sections with those of the one photon case. At the conference, we will present the details of our method to treat ionization by absorption of two photons and will present results for total ionization cross sections for He.

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OZONE MOLECULE:
GLOBAL VARIATIONAL CALCULATION AND ASSIGNMENT OF HIGHLY EXCITED RO-VIBRATIONAL STATES

Vladimir TYUTEREV #, Sergei TASHKUN *, Habib SEGHIR, and Alain BARBE#

#G.S.M.A., UMR CNRS 6089, Université de Reims, BP 1039 - 51687 REIMS Cedex 2, France,
* LTS, Institute of Atmospheric Optics, SB RAS, 634055 TOMSK, Russia

Accurate ro-vibrational calculations for the ozone molecule in this range represent a "touchstone" for empirical and non-empirical methods [1,2] including those based on high-level ab initio electronic structure calculations [3]. A modeling and assignmens of high-resolution ozone spectra near the dissociation limit (6000-8000 cm-1) are known to be extremely challenging due to numerous "exotic" resonances with large ΔV coupling and because of related difficulties in vibrational extrapolations [1]. Recently a breakthrough in very sensitive laser experiments [4,5] on ozone spectra have allowed recording a lot of weak transitions above 6000 cm^{-1}, many of them beeing still non-assigned.

A full comparisons of variational, DVR and Contact Transformation (CT) calculations up to the dissociation limit among these three independent methods and also against recent experimental data for band centers will be presented. In all three cases the same molecular potential function [5] (that provides currently best available agreement with observations) was used, but these methods employ quite different techniques and coordinate systems. The first two methods use numerical integrations in Radau and Jacobi coodinates in a "global" basis, whereas a recent computer assisted CT formulation [6] represents an algebraic perturbational approach extended to multiple and overlappling polyads.

A convergence of this new robust CT algorithm, that allows building non-empirical rovibrational effective Hamiltonians from a molecular potential energy surface to a spectroscopic accuracy are discussed. Examples of calculations for high-order centrifugal distortion and resonance constants and comparison of ro-vibrational calculations up to $J=50$ vs variational methods and observations are given. In conclusion, this study shows a possibility to achieve an agreement to a spectroscopic accuracy between global DVR-type calculations and non-empirical effective Hamiltonian CT approach that allows a reliable normal mode assignment of highly excited ozone vibrations up to the dissociation limit.

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PHOTODISSOCIATION OF ALKALI DIMER MOLECULES AND DIATOMIC BUBBLES IN SOLID ^{4}HE

P. Moroshkin, A. Hofer, and A. Weis
Physics Department, University of Fribourg, Switzerland

We present experimental and theoretical studies of laser photodissociation of cesium dimers isolated in a solid ^{4}He matrix. The dissociation products (excited Cs atoms and Cs^*He_N exciplexes) are detected via their spectrally and time-resolved fluorescence. We have found several new features of this emission as compared to that of laser-excited Cs atoms in solid He under the same conditions [1]: (i) a reduced spectral shift of the $6P_{1/2}$ – $6S_{1/2}$ (D_1) fluorescence, (ii) the appearance of $6P_{3/2}$ – $6S_{1/2}$ (D_2) fluorescence which is otherwise completely quenched, (iii) a shortening of the lifetime of the excited $6P_{1/2}$ state (partial quenching).

It is well known that alkali atoms in condensed helium reside in small cavities called atomic bubbles [1]. We attribute the new features to a different trapping site structure: a diatomic bubble that contains one excited and one ground-state Cs atom or one Cs_2 molecule with a large internuclear separation. The excess kinetic energy of the dissociation products is transferred to surrounding He atoms and dissipated in the crystal.

Our analysis of Cs-Cs and Cs-He interactions shows that the observed effect is not due to a C_6/R^6 van der Waals interaction between two Cs atoms, residing each in its own bubble, but that it can be explained if the two atoms represent a molecule bound by a long-range C_3/R^3 dispersion interaction [2]. In the latter case each of the two Cs atoms is in a 50:50 coherent superposition of the $6P$ and $6S$ states. Any bubble deformation that is not symmetric with respect to a reflection in a plane separating the Cs atoms, should result in a collapse of the diatomic wavefunction into one $6P$ and one $6S$ atom. From the measured decay times of the D_1 and D_2 fluorescence we conclude that this happens on a time scale of several nanoseconds and that the bubble distortion responsible for this quenching is in fact the formation of a Cs^*He_N exciplex.

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Atom-dimer resonance in an ultracold gas

F. Ferlaino[1], M. Mark[1], M. Berninger[1], J. G. Danzl[1], S. Knoop[1], T. Kraemer[1], H. Schöbel[1], H. C. Nägerl[1], and R. Grimm[1,3]
[1]*Institut für Experimentalphysik, Innsbruck, Austria*
[3]*Institut für Quantenoptik und Quanteninformation,Innsbruck, Austria*

Abstract

The unique scattering properties of an ultracold Cesium gas give rise to an extremely rich molecular energy structure which can be experimentally accessed via magnetically tunable Feshbach resonances [1]. We present our studies on the collisional dynamics between ultracold Feshbach Cs_2 molecules and in an atom-dimer mixture.

Starting with a Cs gas at 250 K in a crossed dipole trap we create Cs_2 molecules using low-field d- and g-wave Feshbach resonances. By a fine tuning of the magnetic field, we have the complete control about the molecular quantum states accessed and we can populate all dimer states up to binding energies of 10 MHz and magnetic fields up to 55 G [2]. We show that molecular states with high relative angular momentum $\ell = 8$ can be populated for which direct Feshbach association of these states is not feasible, due to negligible coupling with the s-wave threshold.

Among the different molecular states, a shallow triplet-dominated s-wave state is found to be of particular interest in connection with the physics of universal halo states. We first investigate the collision properties between these molecules finding a non-intuitive dependence of the two-body loss rate on the magnetic field. We then study the atom-dimer collisions by combining the s-wave molecules with atomic ensemble of Cs atoms in their hyperfine ground state. We observe a resonant enhancement in the inelastic atom-dimer collision rate at a scattering length of 400 Bohr radii which indicate a crossing with a trimer state. The existence of such a trimer state is particularly relevant in connection with the Efimov physics. The evidence for a tri-atomic Efimov quantum states has already been experimentally observed in an ultracold Cs gas for $a < 0$ [3]. The observation of an atom-dimer resonance opens the question of wether this might represent an Efimov trimer in the molecular side ($a > 0$) of the Efimov scenario.

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STRUCTURAL PATTERNS IN FULLERENES: C_{20} TO C_{102}

Yang Wang, Goar Sánchez, Sergio Díaz-Tendero, Fernando Martín and Manuel Alcamí

Departamento de Química, C-9, Universidad Autónoma de Madrid, Cantoblanco,
28049 Madrid, Spain

The structures of different fullerene isomers, C_n, with sizes between n = 20 and n = 102 have been obtained by fully optimizing their geometries at the B3LYP/6-31G* level of theory [1,2]. For the most stable classical isomers, we have studied the evolution of different parameters, as bond distances, sphericity, HOMO-LUMO gap or the formation enthalpy with the size of the system.

A classification of the bonds in the fullerenes in 9 different motifs permits to gain insight in the factors determining the fullerene stability. A simplified model that assumes a fixed energy per bond is able to reproduce the calculated formation enthalpies. This model also permits to conclude that fullerenes presenting spherical aromaticity [3] have an enhanced stability between 25 and 40 kcal/mol.

The role of different motifs, as the presence of pentagon-pentagon bonds, in the case of C_n fullerenes with n < 70 or the presence of pyrene substructures in the case of the larger fullerenes, has important consequence for their stability and reactivity.

An analysis of the structure and stability of different isomers has also been performed. In some cases as C_{50} [4] or C_{52}^{2+} [5] the most stable isomer does not follow the pentagon adjacency penalty rule. We have explained these exceptions by introducing a "sphericity rule" in the case of fullerenes with $2(N+1)^2$ π electrons.

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State selective differential cross sections for single electron capture in H^+-, He^+- and He^{2+}-collisions with He

M. S. Schöffler[1*], J. Titze[1], L. Ph. H. Schmidt[1], O. Jagutzki[1], T. Jahnke[1], R. Dörner[1],
H. Schmidt-Böcking[1] and I. Mancev[2]

[1] Institut für Kernphysik, Universität Frankfurt, 60486 Frankfurt, Germany
[2] Department of Physics, University Nis, 18000 Nis, Serbia

Using the COLTRIMS technique (COLd Target Recoil Ion Momentum Spectroscopy), the differential cross sections for single electron capture in collisions of H^+, He^+ and He^{2+} projectiles with helium have been measured over a wide range of energies (40 – 1000 keV/u). At highest projectile energies there are evidences for the electron-nuclear-Thomas-process. The experimental data are in good agreement with new theoretical results from a four-body one-channel distorted wave models (CDW-BFS, CDW-BIS and BDW) [1].

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* electronic address: schoeffler@atom.uni-frankfurt.de

Mesoscopic coherent quantum dynamics in the strong blockade regime

Tilman Pfau
5. Physikalisches Institut, Univesität Stuttgart, Germany

Blockade effects on the single quantum level are at the heart of quantum devices like single-electron transistors. The blockade mechanisms are based on strong interactions like the Coulomb interaction in case of single electrons. Neutral atoms excited into a Rydberg state experience abnormally strong interactions that lead to the corresponding blockade effect for single Rydberg atoms. In this poster we report on measurements of a strong van der Waals blockade, showing that only one out of several thousand atoms within a blockade volume can be excited. In addition, our experimental results clearly demonstrate the coherent nature of the excitation of magnetically trapped ultra cold atoms into a Rydberg state, confirming for the first time the predicted dependence of the collective Rabi frequency on the square root of the mesoscopic system size. This collective coherent behaviour is generic for all mesoscopic systems which are able to carry only one single excitation quantum.

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Pauli's approach of hydrogen atom in Noncommutative Quantum Mechanics

Y. Grandati[a], A. Bérard[a], H. Mohrbach[a], H. Boumrar[b] and F. Menas[b].

[a] LPMC-ICPMB, IF CNRS N° 2843
Université Paul Verlaine-Metz
1 Bd Arago, 57078 Metz Cedex 3, France

[b] LPCQ – Université Mouloud Mammeri de Tizi Ouzou, Algérie.

We explore the possible extension of the Pauli's calculation for the energy spectrum of a non commutative hydrogene atom. Our approach, based on the use of the Runge-Lenz vector, can be seen as a perturbative correction of the standard calculation.

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List of Participants[*]

1.	Janne	Ahokas	Department of Physics, University of Turku 20014 Turku Finland jmiaho@utu.fi
2.	John	Alexander	School of Maths and Physics, Queen's University Belfast Belfast, UK jalexander08@qub.ac.uk
3.	Michael	Allan	Department of Chemistry, University of Fribourg Fribourg, Switzerland michael.allan@unifr.ch
4.	S.Y. Yousif	Al-Mulla	University of Borås, College of Engineering, Physics and Mathematics Group, 50190 Borås Sweden samir.al-mulla@hb.se
5.	Janis	Alnis	Max-Planck-Institute of Quantum Optics Hans-Kopfermann-Str. 1 85748 Garching Germany janis.alnis@mpg.mpg.de
6.	Aurelia	Alonso Medina	Dpto. Física Aplicada, EUIT. Industrial Universidad Politιcnica de Madrid (UPM) Madrid, Spain aurelia.alonso@upm.es
7.	Stuart C.	Althorpe	Department of Chemistry, University of Cambridge Lensfield Road, Cambridge, CB2 1EW UK. sca10@cam.ac.uk
8.	M. Ya.	Amusia	Racah Institute of Physics, the Hebrew University, Jerusalem 91904, Israel and Ioffe Physical-Technical Institute St.-Petersburg 194021, Russia amusia@012.net.il
9.	Lorenzo	Ancarani	Laboratoire de Physique Moléculaire et des Collisions Université Paul Verlaine – Metz 57078 Metz, France ancarani@univ-metz.fr
10.	Lars H	Andersen	Department of Physics & Astronomy, University of Aarhus DK-8000 Aarhus C Denmark LHA@phys.au.dk
11.	Jens Ulrik	Andersen	University of Aarhus DK-8000 Aarhus C Denmark jua@phys.au.dk
12.	Pontus	Andersson	Department of Physics, Gothenburg University SE-412 96 Gothenburg Sweden pontus.andersson@physics.gu.se

---

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13.	Philippe	Antoine	Laboratoire de Physique Atomique Moléculaire et Optique Universite Catholique de Louvain, UCL chemin du cyclotron, 2 B-1348 Louvain-la-Neuve Belgium antoine@pamo.ucl.ac.be
14.	Cenap	Ates	Max Planck Institute for the Physics of Complex Systems Nöthnitzer Str. 38, 01187 Dresden Germany cenap@pks.mpg.de
15.	Damir	Aumiler	Institute of Physics, Bijenička 46, 10 000 Zagreb Croatia aumiler@ifs.hr
16.	Lorenzo	Avaldi	CNR-IMIP Area della Ricerca di Roma 1 CP10, 00016 Monterotondo Scalo Italy lorenzo.avaldi@imip.cnr.it
17.	Hamlet	Avetissian	Department of Quantum Electronics, Yerevan State University, 1 A. Manukian, 375025 Yerevan Armenia avetissian@ysu.am
18.	Mireille	Aymar	Laboratoire Aimé Cotton, CNRS, Universite Paris-Sud 11 Bât.505, Campus d'Orsay, 91405 Orsay Cedex France mireille.aymar@lac.u-psud.fr
19.	Vladimir	Azriel	Institute of Energy Problems of Chemical Physics RAS Leninski prospect 38, Bldg.2 Moscow 119334 Russia Azriel_Vladimir@mail.ru
20.	Xavier	Baillard	LNE-SYRTE, Observatoire de Paris 61 Avenue de l'Observatoire, 75014 Paris France xavier.baillard@obspm.fr
21.	Richard	Balog	Department of Physics & Astronomy, University of Aarhus Ny Munkegade, Aarhus, 8000 C Denmark balog@phys.au.dk
22.	Caroline	Banahan	National Centre for Plasma Science and Technology (NCPST) & School of Physical Sciences, Dublin City University Glasnevin, D9 Ireland caroline.banahan@gmail.com
23.	Paolo	Barletta	Department of Physics and Astronomy, University College London, Gower St., London WC1E 6BT U.K. paolo@theory.phys.ucl.ac.uk
24.	Mark	Bason	Department of Physics, Durham University Rochester Building, Science Laboratories South Road, Durham DH1 3LE, U.K. m.g.bason@durham.ac.uk
25.	Marion	Batz	Johannes Gutenberg-Universität, Institut für Physik Mainz, Germany batz@uni-mainz.de
26.	Dominik	Bauer	Max-Planck-Institut für Quantenoptik Hans-Kopfermann-Straße1 , D-85748Garching Germany dominik.bauer@mpg.mpg.de
27.	Uwe	Becker	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin Germany becker@fhi-berlin.mpg.de

28.	Fabian	Beil	Fachbereich Physik, University of Kaiserslautern Germany beil@physik.uni-kl.de
29.	Ali	Belkacem	Chemical Sciences Division Lawrence Berkeley National Laboratory Berkeley, CA 94720, USA abelkacem@lbl.gov
30.	Simon	Bell	sbell@physics.unimelb.edu.au
31.	Attila	Bende	National Institute for R&D of Isotopic and Molecular Technologies, I.N.C.D.T.I.M Cluj-Napoca Molecular and Biomolecular Physics Department Donath Street, No 71-103, Ro-400293, Cluj-Napoca Romania bende@s3.itim-cj.ro
32.	Manolis	Benis	IESL-FORTH P.O. Box 1385 711 10 Heraklion, Crete Greece benis@iesl.forth.gr
33.	Chloe	Berenguer	Lab. de Physique des Gaz et des Plasmas, UMR 8578 Université Paris-sud 91405 Orsay France sophie.granon@pgp.u-psud.fr
34.	Silvia	Bergamini	The Open University England s.bergamini@open.ac.uk
35.	Nikolay	Bezuglov	V. A. Fock Institute of Physics Saint-Petersburg State University 198904 St. Petersburg Russia bezuglov@pobox.spbu.ru
36.	Emile	Biémont	Institut de Physique Nucléaire, Atomique et de Spectroscopie (IPNAS), Université de Liège Sart Tilman, Bât. B15 , B-4000 Liège Belgium and Service d'Astrophysique et de Spectroscopie Université de Mons-Hainaut 20 Place du Parc B-7000 Mons Belgium E.Biemont@ulg.ac.be
37.	Douglas	Blackie	Imperial College London UK Douglas.Blackie01@ic.ac.uk
38.	Rainer	Blatt	Institut für Experimentalphysik, Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria, and Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften, Otto-Hittmair-Platz 1, A-6020 Innsbruck, Austria Rainer.Blatt@uibk.ac.at
39.	Klaus	Blaum	Physics Department Johannes Gutenberg-University Mainz 55099 Mainz Germany blaumk@uni-mainz.de
40.	Christophe	Blondel	Laboratoire Aimé-Cotton, Centre national de la recherche scientifique, bât. 505, Univ. Paris-sud 91405 Orsay cedex France christophe.blondel@lac.u-psud.fr

41.	Kaspars	Blushs	Institute of Atomic Physics and Spectroscopy University of Latvia Riga, Latvia kblush@latnet.lv
42.	Sergey	Bobashev	Ioffe Physico-Technical Institute Polytekhnicheskaya 26 194021 St. Petersburg Russia s.bobashev@mail.ioffe.ru
43.	Madalina	Boca	Department of Physics, University of Bucharest MG11, Bucharest, Magurele 077125 Romania boca@barutu.fizica.unibuc.ro
44.	Paola	Bolognesi	CNR-IMIP Area della Ricerca di Roma1 00016 Monterotondo Scalo Italy paola.bolognesi@imip.cnr.it
45.	Christian	Bordas	Université Lyon 1, CNRS ; LASIM UMR 5579 43 boulevard du 11 novembre 1918 F-69622 Villeurbanne Cedex, France bordas@lasim.univ-lyon1.fr
46.	Adam	Börzsönyi	Department of Optics University of Szeged P.O.Box 406, Szeged 6701 Hungary badam@titan.physx.u-szeged.hu
47.	William	Bryan	Department of Physics and Astronomy University College London London, U.K. w.bryan@ucl.ac.uk
48.	Adam	Buczek	Poznan University of Technology ul. Nieszawska 13B, 60-965 Poznan, Poland adam.buczek@put.poznan.pl
49.	Chris	Calvert	School of Mathematics and Physics Queen's University Belfast Belfast, U.K. c.calvert@qub.ac.uk
50.	Thomas	Carette	Chimie quantique et Photophysique Université Libre de Bruxelles B 1050 Brussels, Belgium tcarette@ulb.ac.be
51.	Dimitris	Charalambidis	IESL-FORTH and Phys. Dept., Univ. of Crete 711 10 Heraklion, Crete, Greece chara@iesl.forth.gr
52.	Viacheslav	Chernuchkin	Voronezh State University Russia albert@phys.vsu.ru
53.	Mihaela	Ćirišan	Faculty of Sciences, Department of Physics Trg Dositeja Obradovica 4 21000 Novi Sad Serbia djurovic@uns.ns.ac.yu ; mihaela@uns.ns.ac.yu
54.	Robert	Clark	Nuclear Data Section International Atomic Energy Agency IAEA Vienna, Austria r.e.h.clark@iaea.org
55.	Emanuele	Coccia	Dept. of Chemistry and CNISM, CASPUR, University "La Sapienza", Rome 00185 Rome, Italy coccia@caspur.it

56.	Gam	Coenegracht	-
57.	Samuel	Cohen	Atomic & Molecular Physics Laboratory Physics Department, University of Ioannina GR–45110 Ioannina Greece scohen@uoi.gr
58.	Cristobal	Colón	Dpto. Física Aplicada, EUIT.Industrial Universidad Politécnica de Madrid (UPM), Madrid Spain cristobal.colon@upm.es
59.	Anne	Crubellier	Laboratoire Aimé Cotton, CNRS Universite Paris-Sud 11 bât.505, Campus d'Orsay 91405 Orsay Cedex France anne.crubellier@lac.u-psud.fr
60.	Roman	Čurík	J.Heyrovský Institute of Physical Chemistry Dolejškova 3, Prague 8 Czech Republic roman.curik@jh-inst.cas.cz
61.	Jean	Dalibard	Laboratoire Kastler Brossel Ecole Normale Supérieure, 24 rue Lhomond, 75005 Paris France jean.dalibard@lkb.ens.fr
62.	John	Dardis	National Centre for Plasma Science and Technology (NCPST) and School of Physical Sciences Dublin City University Dublin 9, Ireland john.dardis@gmail.com
63.	Rebeca	de Nalda	CSIC Instituto de Quimica-Fisica "Rocasolano" Serrano 119, 28006 Madrid Spain r.nalda@iqfr.csic.es
64.	Kieran	Deasy	Dept. of Applied Physics and Instrumentation Cork Institute of Technology Cork, Ireland kieran.deasy@cit.ie
65.	Piero	Decleva	Dipartimento di Chimica, Università di Trieste Trieste, Italy decleva@univ.trieste.it
66.	Pierre	Defrance	Department de Physique Université Catholique de Louvain Chemin du Cyclotron 2 B-1348 Louvain-la-Neuve Belgium defrance@pamo.ucl.ac.be
67.	Benjamin	Deguilhem	Laboratoire de Chimie et Physique quantique, I.R.S.AM.C. Université Paul Sabatier 118 Route de Narbonne F-31062 Toulouse Cedex France deguilhem@irsamc.ups-tlse.fr
68.	Maarton	DeKieviet	Physics Department, Heidelberg University Heidelberg Germany maarten@physi.uni-heidelberg.de
69.	Natalia	Del Fatti	LASIM, Université Lyon 1 – CNRS Universite Claude Bernard Lyon 1 43 Bd. du 11 Novembre 1918 6922 Villeurbanne France delfatti@lasim.univ-lyon1.fr

70.	Christian	Delsart	Laboratoire Aimé-Cotton Centre national de la recherche scientifique, bât. 505 Univ. Paris-sud 91405 Orsay cedex France christian.delsart@lac.u-psud.fr
71.	Jerzy	Dembczyńskí	Faculty of Technical Physics Poznan University of Technology Nieszawska 13B 60-965 Poznan Poland jerzy.Dembczynski@put.poznan.pl
72.	Stephan	Denifl	Institut für Ionenphysik und Angewandte Physik Leopold Franzens Universität Innsbruck Technikerstr. 25 A-6020 Innsbruck Austria stephan.denifl@uibk.ac.at
73.	Moncef	Derouich	Institut d'Astrophysique Spatiale, Universite Paris-Sud 11 Batiment 121, F-91405 Orsay France moncef.derouich@ias.u-psud.fr
74.	Michele	Desouter-Lecomte	Laboratoire de Chimie Physique Unité Mixte de Recherche 8000 CNRS et Université Paris-Sud-11 91405 Orsay Cedex France mdesoute@lcp.u-psud.fr
75.	Alan	Dickinson	School of Natural Sciences (Physics) Newcastle University Newcastle upon Tyne NE1 7RU U.K. A.S.Dickinson@ncl.ac.uk
76.	Emilia	Dimova	Institute of Solid State Physics, BAS, 72 Tzarigradsko Chaussee, 1784 Sofia, Bulgaria edimova@issp.bas.bg
77.	Adi	Diner	Weizmann Institute of Science Rehovot, 76100 Israel adi.diner@weizmann.ac.il
78.	Slobodan	Djeric	Stahl Electronics Kellerweg 23 67582 Mettenheim Germany s.djeric@stahl-electronics.com
79.	Stevica	Djurović	Faculty of Sciences, Department of Physics University of Novi Sad Trg Dositeja Obradovica 4 21000 Novi Sad Serbia djurovic@uns.ns.ac.yu
80.	Wolfgang	Domcke	Department of Chemistry Technical University of Munich Germany wolfgang.domcke@ch.tum.de
81.	Peter	Domokos	Research Institute of Solid State Physics and Optics Hungarian Academy of Sciences H-1525 Budapest, P.O.Box49 Hungary domokos@szfki.hu
82.	Michael	Drewsen	Department of Physics and Astronomy University of Aarhus Denmark drewsen@phys.au.dk

83.	Padraig	Dunne	School of Physics, University College Dublin Belfield, Dublin 4 Ireland padraig.dunne@ucd.ie
84.	Kevin	Dunseath	Equipe SIMPA, Laboratoire PALMS, UMR 6627 CNRS , Université de Rennes 1 Campus de Beaulieu F-35042 Rennes Cedex France kevin.dunseath@univ-rennes1.fr
85.	Dassia	Egorova	Department of Chemistry Technical University of Munich Lichtenbergstr, 4 D-85747 Garching Germany egorova@web.de
86.	Arno	Ehresmann	Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology University of Kassel D-34109 Kassel Germany ehresmann@physik.uni-kassel.de
87.	Aigars	Ekers	Institute of Atomic Physics and Spectroscopy University of Latvia Zellu Str. 8 LV-1002 Riga Latvia aigars.ekers@lu.lv
88.	Mikhail	Emelin	Institute of Applied Physics, RAS 46 Ulyanov Street 603950, Nizhny Novgorod Russia emelin@ufp.appl.sci-nnov.ru
89.	Agapi	Emmanouilidou	ITS, University of Oregon, Eugene, Oregon 97403-5203 USA agapi@uoregon.edu
90.	Alev	Er	Istanbul University Faculty of Science Physics Department, 34118 Vezneciler, Istanbul Turkey alever82@gmail.com
91.	Wolfgang E.	Ernst	Institute of Experimental Physics Graz University of Technology Petersgasse 16 A-8010 Graz Austria wolfgang.ernst@tugraz.at
92.	Stavros	Farantos	IESL-FORTH P.O. Box 1385 71110 Heraklion, Crete Greece farantos@iesl.forth.gr
93.	Olivier	Faucher	Institut Carnot de Bourgogne UMR 5209 CNRS- Université de Bourgogne BP 47870, 21078 Dijon Cedex France olivier.faucher@u-bourgogne.fr
94.	Francesca	Ferlaino	Leopold Franzens Universität Innsbruck Technikerstraße 25 A-6020 Innsbruck Austria francesca.ferlaino@uibk.ac.at

95.	Vanessa	Fivet	Service d'Astrophysique et de Spectroscopie Université de Mons-Hainaut 20 Place du Parc B-7000 Mons Belgium vanessa.fivet@umh.ac.be
96.	Raymond	Flannery	Georgia Institute of Technology Atlanta USA r.flannery@physics.gatech.edu
97.	Calin Gabriel	Floare	National Institute for R & D of Isotopic and Molecular Technologies, I.N.C.D.T.I.M Cluj-Napoca 71 - 103 Donath Str. 400293, Cluj-Napoca Romania cfloare@gmail.com
98.	Viorica	Florescu	Department of Physics University of Bucharest MG11, Bucharest Magurele 077125 Romania flor@barutu.fizica.unibuc.ro
99.	Lutz	Foucar	Institut für Kernphysik, University Frankfurt Max von Laue Strasse 1 D-60438 Frankfurt Germany foucar@atom.uni-frankfurt.de
100.	Emmanuel	Foumouo	Laboratoire de Physique Atomique Moléculaire et Optique (unité PAMO) Université Catholique de Louvain 2, chemin du Cyclotron B-1348 Louvain-la-Neuve Belgium foumouo@pamo.ucl.ac.be
101.	Mikhail V.	Frolov	Department of Physics Voronezh State University Voronezh 394006 Russia frolov@phys.vsu.ru
102.	Boguslaw	Furmann	Chair of Quantum Engineering and Metrology Faculty of Technical Physics Poznań University of Technology Poland boguslaw.furmann@put.poznan.pl
103.	Werner	Fuβ	Max-Planck-Institut für Quantenoptik D-85741 Garching Germany w.fuss@mpg.mpg.de
104.	Naceur	Gaaloul	Laboratoire de Photophysique Moléculaire du CNRS Bâtiment 210, Université Paris-Sud 91405 Orsay cedex France naceur.gaaloul@ppm.u-psud.fr
105.	Gustavo	García	Departamento de Física Atómica Molecular y Agregados Instituto de Matemáticas y Física Fundamental CSIC Serrano 113-b, 28006 Madrid Spain g.garcia@imaff.cfmac.csic.es
106.	Alberto	García-Vela	Instituto de Matemáticas y Física Fundamental-IMAFF, C.S.I.C Serrano 123, 28006 Madrid, Spain garciavela@imaff.cfmac.csic.es

107.	Henri-Pierre	Garnir	IPNAS, Université de Liège Sart Tilman B15 B-4000 Liège Belgium hpgarnir@ulg.ac.be
108.	Alexandre	Gauguet	SYRTE, CNRS UMR 3630, L'Observatoire de Paris 61 avenue de l'Observatoire de Paris 75014 Paris France alexandre.gauguet@obspm.fr
109.	Michael	Geissler	Department of Physics and Astronomy Queen´s University Belfast BT7 1NN UK m.geissler@qub.ac.uk and Max Planck Institute of Quantum Optics Garching, Germany michael.geissler@mpg.mpg.de
110.	Savas	Georgiou	IESL-FORTH P.O. Box 1385 71110 Heraklion, Crete Greece pkontol@iesl.forth.gr
111.	Gustav	Gerber	Experimentelle Physik I Physikalisches Institut Universitaet Wuerzburg Am Hubland D-97074 Wuerzburg Germany gerber@physik.uni-wuerzburg.de
112.	Trant T.	Gien	Department of Physics and Physical Oceanography Memorial University of Newfoundland St John's, NL A1B 3X7 Canada ttg@warp.nfld.net
113.	Bertrand	Girard	Université Paul Sabatier - Toulouse 3 Laboratoire de Collisions - Agrégats - Réactivité (UMR 5589 CNRS - UPS) IRSAMC (FR 2568 CNRS -UPS) 118 Route de Narbonne Bat. 3R1 b4 31062 Toulouse cedex 9, France bertrand.girard@irsamc.ups-tlse.fr
114.	Nicolas	Gisin	Group of Applied Physics University of Geneva 20, rue de l'Ecole de Medecine CH-1211 Geneva 4 Switzerland Nicolas.Gisin@physics.unige.ch
115.	Michel	Godefroid	Chimie quantique et Photophysique, Université Libre de Bruxelles, B 1050 Brussels, Belgium mrgodef@ulb.ac.be
116.	Leticia	González	Institut für Chemie und Biochemie Freie Universität Berlin Takustrasse 3 D-14195 Berlin Germany leti@chemie.fu-berlin.de
117.	John	Goold	Physics Department University College Cork Cork, Ireland jgoold@phys.ucc.ie

118.	Yves	Grandiani	Université Paul Verlaine-Metz LPMC ICPMB (FR 2843) Institut de Physique 1 rue Arago, 57078 Metz Cedex France grandati@univ-metz.fr
119.	Tasko	Grozdanov	Institute of Physics P.O. Box 57 11001 Belgrade Serbia tasko@phy.bg.ac.yu
120.	Stephane	Guérin	Institut Carnot de Bourgogne UMR Universite de Bourgogne 5209 CNRS BP47870, 21078 Dijon cedex France sguerin@u-bourgogne.fr
121.	Romain	Guérout	Laboratoire Aimé Cotton du CNRS Bâtiment 505 Université de Paris-Sud F-91405 Orsay France romain.guerout@lac.u-psud.fr
122.	Jonas	Gurell	Department of Physics Stockholm University Albanova, SE-10691 Stockholm Sweden jonas.gurell@physto.se
123.	John L.	Hall	JILA, University of Colorado and NIST Boulder CO 80309-0440 USA jan@HallStableLasers.com or jhall@jila.colorado.edu
124.	Jan Petter	Hansen	Department of Physics and Technology University of Bergen Allégaten 55, 5007 Bergen Norway janpetter.hansen@ift.uib.no
125.	Klavs	Hansen	Dept. of Physics Göteborg University SE-41296 Göteborg Sweden klavs@physics.gu.se
126.	Zoltan	Harman	Max-Planck-Institut für Kernphysik Heidelberg Germany zoltan.harman@mpi-hd.mpg.de
127.	James	Harries	JASRI / SPring-8 Kouto 1-1-1 Sayou, Hyogo 679-5198 Japan
128.	Alex	Harvey	Department of Physics and Astronomy University College London Gower Street London, WC1E 6BT UK alexh@theory.phys.ucl.ac.uk
129.	Oded	Heber	Weizmann Institute of Science PO Box 26 Rehovot 76100 Israel oded.heber@weizmann.ac.il
130.	Elke	Heinecke	Institute of Optics and Atomic Physics Technical University of Berlin D-10623 Berlin Germany elke@kalium.physik.tu-berlin.de

131.	Edouard	Hertz	Institut Carnot de Bourgogne UMR 5209 CNRS-Université de Bourgogne BP 47870, 21078 Dijon Cedex France edouard.hertz@u-bourgogne.fr
132.	Paul-Antoine	Hervieux	Institut de Physique et Chimie des Matıriaux de Strasbourg, Universite Louis Pasteur GONLO, 23 rue du Loess 67034 Strasbourg France paul-antoine.hervieux@ipcms.u-strasbg.fr
133.	Atsunari	Hiraya	Department of Physical Science Graduate School of Science Hiroshima University 1-3-1 Kagamiyama Higashi-hiroshima, 739-8526 Japan hiraya@sci.hiroshima-u.ac.jp
134.	Tim H.	Hoffmann	Fachbereich Physik Techn. Universität Kaiserslautern 67653 Kaiserslautern Germany thoffman@rhrk.uni-kl.de
135.	Stephen	Hogan	Laboratorium für Physikalische Chemie, Swiss Federal Institute of Technology Zurich (ETH Zurich), HCI E213 Wolfgang-Pauli-Strasse, 10 CH-8093 Zurich Switzerland seho@xuv.phys.chem.ethz.ch
136.	Klaus	Højbjerre	Department of Physics and Astronomy University of Aarhus Denmark klaush@phys.au.dk
137.	Anne	Holm	Department of Physics and Astronomy University of Aarhus Denmark aish@phys.au.dk
138.	Jiri	Horáček	Institute of Theoretical Physics, Charles University 18000 Prague Czech Republic jiho@matfyz.cz
139.	Rainer	Hörlein	Max-Planck-Institut für Quantenoptik D-85748 Garching Germany rainer.hoerlein@mpq.mpg.de
140.	Zoltan	Horváth	Department of Optics and Quantum Electronics University of Szeged H-6720 Dóm tér 9, Szeged Hungary z.horvath@physx.u-szeged.hu
141.	Hartmut	Hotop	Fachbereich Physik Techn. Universität Kaiserslautern 67653 Kaiserslautern Germany hotop@physik.uni-kl.de
142.	Chantal	Houée-Levin	LCP, UMR 8000 F-91405 Orsay France Chantal.houee-levin@lcp.u-psud.fr
143.	Karel	Houfek	Institute of Theoretical Physics Faculty of Mathematics and Physics Charles University in Prague Prague Czech Republic houfek@mbox.troja.mff.cuni.cz

144.	Padraig	Hough	National Centre for Plasma Science and Technology and School of Physical Sciences, Dublin City University Glasnevin, Dublin 9 Ireland padraighough@gmail.com
145.	Jony J.	Hudson	Centre for Cold Matter The Blackett Laboratory Imperial College London London SW7 2BW U.K. jony.hudson@imperial.ac.uk
146.	Michael	Huels	Ion Reaction Laboratory Dept. of Nuclear Medicine and Radiobiology Faculty of Medicine and Health Sciences University of Sherbrooke Sherbrooke, Quebec Canada michael.huels@usherbrooke.ca
147.	Bogdan Catalin	Ibanescu	Department of Chemistry University of Fribourg Switzerland bogdancatalin.ibanescu@unifr.ch
148.	Stefan	Jaksch	Institut für Ionenphysik und Angewandte Physik Leopold-Franzens-Universität Innsbruck Technikerstrasse 25 A-6020 Innsbruck Austria stefan.jaksch@uibk.ac.at
149.	Andrey	Jarmola	Department of Physics and Institute of Atomic Physics and Spectroscopy University of Latvia Rainis Blvd. 19 Riga LV-1586 Latvia jarmola@latnet.lv
150.	Brana	Jelenkovic	Institute of Physics University of Belgrade 11080, Belgrade Serbia branaj@phy.bg.ac.yu
151.	Bogumił	Jeziorski	Faculty of Chemistry University of Warsaw Pasteura 1 02-093 Warsaw Poland jeziorsk@chem.uw.edu.pl
152.	Christine	Joblin	CESR, CNRS – Université Toulouse III Observatoire Midi-Pyrénées 9 Av. du Colonel Roche 31028 Toulouse cedex 04 France christine.joblin@cesr.fr
153.	Per	Johnsson	FOM-Institute AMOLF Kruislaan 407 1098 SJ Amsterdam The Netherlands p.johnsson@amolf.nl
154.	Gerald	Jordan	Photonics Institute Vienna Univ. of Technology Gusshausstrasse 27/387 1040 Vienna Austria gerald.jordan@tuwien.ac.at

155.	Brandon	Jordon-Thaden	Max-Planck-Institut für Kernphysik D-69117 Heidelberg Germany brandon.jordon-thaden@mpi-hd.mpg.de
156.	Christian	Jungen	Laboratoire Aimé Cotton du CNRS Bâtiment 505 Universit´e de Paris-Sud F-91405 Orsay France christian.jungen@lac.u-psud.fr
157.	Nikolay	Kabachnik	Institute of Nuclear Physics Moscow State University Moscow 119992 Russia and Fakultät für Physik Universität Bielefeld Universitätsstrasse 25 D-33615 Bielefeld Germany nkabach@mail.ru
158.	Costas	Kalpouzos	IESL-FORTH P.O. Box 1385, 711 10 Heraklion, Crete Greece kalpouzo@iesl.forth.gr
159.	Manfred	Kappes	Institut für Nanotechnologie, Forschungszentrum Karlsruhe 76021 Karlsruhe, Germany; Institut für Physikalische Chemie, Universität Karlsruhe 76128 Karlsruhe, Germany manfred.kappes@chemie.uni-karlsruhe.de
160.	Victor	Kartoshkin	A.F.Ioffe Psysico-Technical Institute Russian Academy of Sciences Polytechnical str.26 194021 St.-Petersburg Russia victor.kart@mail.ioffe.ru
161.	Konstantinos	Katsonis	Lab. de Physique des Gaz et des Plasmas UMR 8578, Université Paris-sud 91405 Orsay France konstantinos.katsonis@u-psud.fr
162.	Spyros	Kaziannis	Department of Physics University of Ioannina 45110 Ioannina Greece skaziannis@in.gr
163.	Mark	Keil	Department of Physics Ben-Gurion University of the Negev Be'er Sheva Israel mkeil@netvision.net.il ; keil@bgu.ac.il
164.	Ryszard	Kepa	Atomic and Molecular Physics Laboratory Institute of Physics University of Rzeszów 35-959 Rzeszów Poland rkepa@univ.rzeszow.pl
165.	Anatoli	Kheifets	Research School of Physical Sciences The Australian National University Canberra ACT 0200 Australia a.kheifets@anu.edu.au
166.	Victor	Kilin	Tomsk Polytechnic University 634030 Tomsk Russia vak@tpu.ru ; vak.49@mail.ru

167.	Teodora	Kirova	Institute of Atomic Physics and Spectroscopy University of Latvia Riga, Latvia teo@lu.lv
168.	Theofanis	Kitsopoulos	IESL-FORTH and University of Crete P.O. Box 1385, 711 10 Heraklion, Crete Greece theo@iesl.forth.gr
169.	Mikael	Kjellberg	Dept. of Physics, Göteborg University SE-41296 Göteborg Sweden mikael.kjellberg@physics.gu.se
170.	Jens	Klein	Department of Physics, University of Kaiserslautern 67653 Kaiserslautern Germany jeklein@physik.uni-kl.de
171.	Łukasz	Kłosowski	Nicolaus Copernicus University Institute of Physics, Grudziądzka 5/7, 87-100 Toru Poland iklos@fizyka.umk.pl
172.	Horst	Knöckel	Inst.f. Quantenoptik, Leibniz University of Hannover Welfengarten 1 30167 Hannover Germany knoeckel@iqo.uni-hannover.de
173.	Konrad	Koc	Department of Computer Science Pedagogical University Academic Computer Centre CyfroNet ul. Podchorążych 2 30-084 Kraków Poland sfkoc@cyf-kr.edu.pl
174.	Wojciech	Koczorowski	Poznan University of Technology ul. Nieszawska 13B 60-965 Poznan Poland wojciech.koczorowski@put.poznan.pl wojtekk@phys.put.poznan.pl
175.	Thorsten	Köhler	Department of Physics University of Oxford Clarendon Laboratory, Parks Road Oxford, OX1 3PU U.K. t.koehler1@physics.ox.ac.uk
176.	Servaas	Kokkelmans	Department of Physics Eindhoven University of Technology P.O. Box 513 5600 MB Eindhoven The Netherlands s.kokkelmans@tue.nl
177.	Nikolai	Kolatchevsky	P.N. Lebedev Physics Institute Leninsky prosp. 53 Moscow, 119991 Russia kolik@lebedev.ru Max-Planck-Institute of Quantum Optics Hans-Kopfermann-Str. 1, 85748 Garching, Germany
178.	Iannis	Kominis	IESL-FORTH and Phys. Dept., Univ. of Crete 711 10 Heraklion, Crete Greece ikominis@iesl.forth.gr

179.	Konstantin	Korovin	Ioffe Physico-Technical Institute Russian Academy of Sciences 19402, 1 Saint-Petersburg Russia
180.	Jouko	Korppi-Tommola	Department of Chemistry University of Jyvaskyla P.O. Box 35 FIN-40014 Finland ktommola@jyu.fi
181.	Kirill	Koshelev	Hamburger Sternwarte University of Hamburg Hamburg, Germany ; Petersburg Nuclear Physics Institute Gatchina, Russia stgb335@hs.uni-hamburg.de
182.	Galya	Koshenock	Department of Experimental Physics, St.Petersburg Polyechnical University Polytekhnicheskaya 29 195251 St.Petersburg, Russia galya.abroad@mail.ru
183.	Kyriaki	Kosma	Max-Planck-Institut für Quantenoptik D-85741 Garching Germany kok@mpq.mpg.de
184.	Igor	Kostyukov	Institute of Applied Physics RAS Uljanova 46 603950 Nizhny Novgorod Russia
185.	Svetlana	Kotochigova	Department of Physics Temple University Philadelphia, PA 19122 ; National Institute of Standards and Technology 100 Bureau Drive stop 8423, Gaithersburg Maryland 20899 USA skotoch@temple.edu
186.	Attila	Kovács	Department of Optics and Quantum Electronics University of Szeged H-6720 Dóm tér 9, Szeged Hungary a.pkovacs@physx.u-szeged.hu
187.	Krzysztof	Kowalski	Institute of Physics Polish Academy of Sciences Al. Lotnikσw 32/46 02-668 Warsaw Poland krkowal@ifpan.edu.pl
188.	Ference	Krausz	Max-Planck-Institut für Quantenoptik Hans-Kopfermann-Strasse 1 D-85748 Garching Germany ferenc.krausz@mpq.mpg.de
189.	Vladyslav	Kravchenko	Department of Physics Taras Shevchenko National University of Kiev, Kiev Ukraine krav@univ.kiev.ua
190.	Aleksandar J.	Krmpot	Institute of Physics University of Belgrade Pregrevica 118, 1080 Belgrade- Zemun, Serbia krmpot@phy.bg.ac.yu

191.	Axel	Kuhn	University of Oxford Clarendon Laboratory U.K. a.kuhn1@physics.ox.ac.uk
192.	Anne	Lafosse	Laboratoire des Collisions Atomiques et Moléculaires, CNRS Université Paris-Sud (UMR 8625, FR LUMAT), Bât. 351 F-91405 Orsay Cedex France lafosse@lcam.u-psud.fr anne.lafosse@u-psud.fr
193.	Peter	Lambropoulos	IESL-FORTH and Phys. Dep. Univ. of Crete 711 10 Heraklion, Crete Greece labro@iesl.forth.gr
194.	Lutz	Lammich	Department of Physics and Astronomy, University of Aarhus Denmark lutz@phys.au.dk
195.	Guillaume	Laurent	Departamento de Química C-9, Universidad Autónoma de Madrid 28049 Madrid Spain guillaume.laurent@uam.es
196.	Sydney	Leach	LERMA, Observatoire de Paris-Meudon L92195 Meudon France sydney.leach@obspm.fr
197.	Pierre	Lemonde	LNE-SYRTE, Observatoire de Paris 61 Avenue de l'Observatoire, 75014 Paris, France Pierre.Lemonde@obspm.fr
198.	Franck	Lépine	Université Lyon 1 CNRS ; LASIM UMR 5579 43 boulevard du 11 novembre 1918 F-69622 Villeurbanne Cedex France lepine@lasim.univ-lyon1.fr
199.	Anton	Lindahl	Department of Physics Gothenburg University SE-412 96 Gothenburg Sweden anton.lindahl@physics.gu.se
200.	Eva	Lindroth	Atomic Physics, Fysikum, Stockholm University S-106 91 Stockholm Sweden lindroth@physto.se
201.	Mihaela Laura	Lipciuc	Laser Centre and Department of Chemistry Vrije Universiteit de Boelelaan 1083 1081HV Amsterdam The Netherlands lipciuc@few.vu.nl
202.	Martin	Lisowski	FEMTOLASERS Produktions GmbH Fernkorngasse 10, A-1100 Vienna Austria info@femtolasers.com
203.	Igor	Litvinyuk	J.R. Macdonald Laboratory, Physics Department Kansas State University Manhattan, Kansas 66506 USA ivl@phys.ksu.edu

204.	Kopin	Liu	Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica P. O. Box 23-166 Taipei 10617 Taiwan kpliu@gate.sinica.edu.tw
205.	Sergio	López-López	Instituto de Matematicas y Fisica Fundamental-IMAFF, C.S.I.C Serrano 123, 28006 Madrid, Spain slopez@imaff.cfmac.csic.es
206.	Pablo	López-Tarifa	Departamento de Química, C-9, Universidad Autónoma de Madrid Cantoblanco, 28049 Madrid Spain pablo.lopez@uam.es
207.	Jerome	Loreau	Service de Chimie Quantique Universite Libre de Bruxelles Brussels Belgium jloreau@ulb.ac.be
208.	Erik	Lötstedt	Max-Planck-Institut für Kernphysik Saupfercheckweg 1 D-69117 Heidelberg Germany erik.loetstedt@mpi-hd.mpg.de
209.	Peter	Lundin	Department of Physics Stockholm University Albanova, SE-10691 Stockholm Sweden peppe@physto.se
210.	Zaal	Machavariani	Department of Exact and Natural Sciences, Physics Division Tbilisi State University Chavchavadze Av. 3 Tbilisi 0128 Georgia zaalmachavariani@hotmail.com
211.	Javier	Madroñero	Physik Department Technische Universität München 85747 Garching Germany jmadrone@ph.tum.de
212.	Harri	Mäkelä	Department of Physics, University of Turku FI-20014 Turun yliopisto Finland harmak@utu.fi
213.	Galina	Malcheva	Institute of Solid State Physics Bulgarian Academy of Sciences 72 Tzarigradsko Chaussee, BG- 1784 Sofia Bulgaria bobcheva@issp.bas.bg
214.	Laurence	Malegat	LIXAM (Laboratoire d'Interaction du rayonnement X Avec la Matière) UMR8624 du CNRS, Université Paris-Sud, Bat. 350, 91405 ORSAY cedex France laurence.malegat@lixam.u-psud.fr
215.	Alice	Malhador	Institute of Physics UK kate.hooper@iop.org
216.	Sabrina	Maniscalco	Department of Physics University of Turku 20014 Turku Finland sabrina.maniscalco@utu.fi

217.	Sven	Mannervik	Department of Physics, Stockholm University Albanova, SE-10691 Stockholm Sweden mannervik@physto.se
218.	Fabio	Marinetti	Department of Chemistry and CNISM University “La Sapienza”, Rome CASPUR Rome Italy marinett@caspur.it
219.	Bratislav	Marinković	Institute of Physics Pregrevica 118 11080 Belgrade Serbia marinkov@phy.bg.ac.yu
220.	Emilio	Mariotti	Università di Siena, Dipartimento di Fisica via Roma 56 Siena, I-53100 Italy mariotti@unisi.it
221.	Fernando	Martín	Dep. de Química, C-9 Universidad Autónoma de Madrid 28049-Madrid Spain fernando.martin@uam.es
222.	Michal	Matuszewski	Department of Physics, Warsaw University Hoza 69, PL-00-681 Warsaw Poland mmatu@fuw.edu.pl and Laser Physics Centre Research School of Physical Sciences and Engineering Australian National University Canberra ACT 0200 Australia
223.	Ronald	McCarroll	Laboratoire de Chimie Physique - Matière et Rayonnement (UMR 7614 du CNRS) Université Pierre et Marie Curie 75231-Paris Cedex 05, France mccarrol@ccr.jussieu.fr
224.	W. Leo	Meerts	Molecular- and Biophysics Group Institute for Molecules and Materials, Radboud University Nijmegen P.O. Box 9010 6500 GL Nijmegen The Netherlands leo.meerts@science.ru.nl
225.	Christoph	Meier	Laboratoire Collisions, Agrégats et Réactivité, IRSAMC Université Paul Sabatier Toulouse France chris@irsamc.ups-tlse.fr
226.	Frans	Meijer	University College Dublin Ireland frans.meijer@ucd.ie
227.	Gerard	Meijer	Fritz-Haber-Institut Faradayweg 4-6 Berlin Germany meijer@fhi-berlin.mpg.de
228.	Frederic	Merkt	Laboratorium für Physikalische Chemie Swiss Federal Institute of Technology Zurich (ETH Zurich) Switzerland merkt@xuv.phys.chem.ethz.ch
229.	Tony	Merrigan	Centre for Plasma Physics Queen’s University Belfast U.K. tmerrigan01@qub.ac.uk

230.	Kaspars	Miculis	Dept. of Physics, University of Latvia LV-1586 Riga Latvia michulis@latnet.lv
231.	Katsumi	Midorikawa	Laser Technology Laboratory, RIKEN 2-1 Hirosawa, Wako Saitama 351-0198 Japan kmidori@riken.jp
232.	Jacek	Migdalek	Pedagogical University of Cracow Academic Computer Centre CyfroNet 30-084, Krakow Poland sfmigdal@cyf-kr.edu.pl
233.	Florina	Mihailescu	National Institute for Laser, Plasma and Radiation Physics Laser Dept. P.O.Box MG-36, Bucharest, 077125 Romania andreea.mihailescu@inflpr.ro
234.	Andrej	MIhelič	Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia andrej.mihelic@ijs.si
235.	Marina	Mijailović	Institute of Physics, University of Belgrade 11080, Belgrade Serbia lekic@phy.bg.ac.yu
236.	Aleksandar	Milosavljević	Institute of Physics Pregrevica 118 11080 Belgrade Serbia
237.	Otilia	Mó	Departamento de Química, C-9 Universidad Autónoma de Madrid Cantoblanco, 28049-Madrid Spain otilia.mo@uam.es
238.	Albert	Mollema	KVI Atomic Physics, University of Groningen Zernikelaan 25 9747 AA Groningen the Netherlands mollema@kvi.nl
239.	Klaus	Mølmer	Lundbeck Foundation Theoretical Center for Quantu System Research Department of Physics and Astronomy University of Aarhus DK 8000 Aarhus C.m Denmark moelmer@phys.au.dk
240.	Marcin	Molski	Adam Mickiewicz University of Pozna PL 60-780 Pozna ul. Grunwaldzka 6 Poland marcin@rovib.amu.edu.pl
241.	Michel	Mons	Laboratoire Francis Perrin URA CEA-CNRS 2453 Service des Photons, Atomes et Molécules, CEA Saclay, Bât 522 Gif-sur-Yvette Cedex France mmons@cea.fr
242.	Peter	Moroshkin	University of Fribourg, Department of Physics, Chemin du Musee 3, CH 1700, Fribourg, Switzerland peter.moroshkin@unifr.ch

243.	Robert	Moshammer	Max-Planck-Institut für Kernphysik Saupfercheckweg 1 69117 Heidelberg Germany r.moshammer@mpi-hd.mpg.de robert.moshammer@mpi-h.mpg.de
244.	Albert	Moto	obengeb@yahoo.com
245.	Tetsuya	Mukai	NTT Basic Research Laboratories 3-1, Morinosato-Wakamiya Atsugi, Kanagawa 243-0198 Japan ; tetsuya@will.brl.ntt.co.jp CREST, Japan Science & Technology Agency 4-1-8 Honcho, Kawaguchi Saitama 332-0012, Japan
246.	Jordi	Mur Petit	Laboratoire Aimé Cotton, CNRS - Univ.Paris-Sud 91405 Orsay France jordi.mur@lac.u-psud.fr
247.	Domhnall	Murphy	Centre for Theoretical Atomic Molecular and Optical Physics Queens University Belfast Belfast BT71NN Northern Ireland domhnall.murphy@qub.ac.uk
248.	Hanns-Christoph	Nägerl	Institut für Experimentalphysik und Forschungszentrum Quantenphysik, Universität, Innsbruck, Technikerstrasse 25, 6020 Innsbruck, Austria. Christoph.Naegerl@ultracold.at
249.	David	Nagy	Research Institute of Solid State Physics and Optics Hungarian Academy of Sciences, H-1525 Budapest P.O. Box 49, Hungary nagyd@optics.szfki.kfki.hu or nagyd@szfki.hu
250.	Adi	Natan	Department of Physics of Complex Systems Weizmann Institute of Science, Rehovot, 76100 Israel
251.	Andre	Nauts	Unité de Physique Atomique, Moléculaire et Optique (PAMO) Département de Physique. UCL Faculté des Sciences 2, Chemin du Cyclotron 1348 Louvain-la-Neuve Belgium nauts@pamo.ucl.ac.be
252.	Roy	Newell	Department of Physics and Astronomy, University College London, London, UK w.r.newell@ucl.ac.uk
253.	Olga	Nikolayeva	Institute of Atomic Physics and Spectroscopy and Department of Physics, University of Latvia, 19Rainis blvd., LV-1586, Riga, Latvia onikolay@latnet.lv
254.	Georgios M.	Nikolopoulos	IESL-FORTH P.O. Box 1385 71110 Heraklion, Crete Greece nikolg@iesl.forth.gr
255.	Steffen	Novotny	Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany steffen.novotny@mpi-hd.mpg.de
256.	Oldrich	Novotny	Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany oldrich.novotny@mpi-hd.mpg.de

257.	Robert	Nyman	Institut d'Optique, Campus Polytechnique RD 128, 91127 Palaiseau France robert.nyman@institutoptique.fr
258.	Martin	Oberst	Department of Physics, University of Kaiserslautern, 67653 Kaiserslautern Germany oberst@physik.uni-kl.de
259.	Oleg	Obolensky	A.F. Ioffe Physical Technical Institute, 194021 St. Petersburg Russia oleg@mail.ioffe.ru or Oleg@rpro.ioffe.rssi.ru
260.	Jenny	Öjekull	Department of Chemistry, Atmospheric Science, Göteborg University Sweden ojekull@chem.gu.se
261.	Thomas	Oksenhendler	FASTLITE, Bat 403, Ecole Polytechnique, 91128 Palaiseau France thoksen@fastlite.com
262.	Karoly	Osvay	Department of Optics, University of Szeged, P.O.Box 406, Szeged 6701, Hungary osvay@physx.u-szeged.hu and Max Born Institute, Max-Born-Str. 2A, D-12489 Berlin, Germany osvay@mbi-berlin.de
263.	Ipek K.	Öztürk	Istanbul University Faculty of Science Physics Department, 34118 Vezneciler, Istanbul Turkey ikanat@istanbul.edu.tr
264.	Krzysztof	Pachucki	Institute of Theoretical Physics, Warsaw University Hoża 69, 00-681 Warsaw, Poland krp@fuw.edu.pl
265.	Adriana	Pálffy	Max-Planck-Institut f¨ur Kernphysik, Heidelberg, Germany palffy@mpi-hd.mpg.de
266.	Alexander	Patzer	Institute of Optics and Atomic Physics Technical University of Berlin D-10623 Berlin Germany alexp@kalium.physik.tu-berlin.de
267.	Gillian	Peach	Department of Physics and Astronomy University College London Gower Street, London WC1E 6BT, U.K. g.peach@ucl.ac.uk
268.	Henrik	Pedersen	Max-Planck-Institut für Kernphysik 69117 Heidelberg Germany henrik.pedersen@mpi-hd.mpg.de
269.	Francis	Penent	LCP-MR, Univ. Pierre et Marie Curie 6 CNRS (UMR 7614), 11 rue Pierre et Marie Curie 75231 Paris Cedex 05 France penent@ccr.jussieu.fr
270.	Annemieke	Petrignani	Max-Planck-Institut für Kernphysik 69117 Heidelberg Germany a.petrignani@mpi-hd.mpg.de

271.	David	Petrosyan	IESL-FORTH P.O. Box 1385 71110 Heraklion, Crete Greece dap@iesl.forth.gr
272.	Victor	Petrunin	Physics and Chemistry Department, University of Southern Denmark, 5230 Odense M Denmark vvp@fysik.sdu.dk
273.	Tilman	Pfau	University of Stuttgart, 5. Physikalisches Institut Pfaffenwaldring 57 room 4.162 D-70550 Stuttgart, Germany t.pfau@physik.uni-stuttgart.de
274.	Jyrki	Piilo	Department of Physics, University of Turku FI-20014 Turku Finland jyrki.piilo@utu.fi
275.	Pierre	Pillet	Laboratoire Aimé Cotton, CNRS Bât. 505, Univ Paris-Sud 91405 Orsay cedex France Pierre.Pillet@lac.u-psud.fr
276.	Pepijn	Pinkse	Max-Planck-Institut-für Quantenoptik, Hans-Kopfermannstr. 1 D-85748 München Germany pepijn.pinkse@mpg.mpg.de
277.	Michal	Piotrowicz	The Open University Physics and Astronomy Department Walton Hall, Milton Keynes, MK7 6AA UK m.piotrowicz@open.ac.uk
278.	Bernard	Piraux	Laboratoire de Physique Atomique, Moléculaire et Optique (unité PAMO), Université Catholique de Louvain, 2, chemin du Cyclotron, B-1348 Louvain-la-Neuve Belgium piraux@pamo.ucl.ac.be
279.	Misra	Prabhakar	Department of Physics & Astronomy, Howard University Washington D.C. 20059 U.S.A. pmisra@howard.edu
280.	Dave	Pritchard	Department of Physics, 4-304 Massachusetts Institute of Technology 77 Massachusetts Avenue Cambridge, MA 02139 USA dpritch@MIT.edu
281.	Rita	Prosmiti	Instituto de Matemáticas y Física Fundamental, C.S.I.C., Serrano 123, 28006 Madrid Spain rita@imaff.cfmac.csic.es
282.	Laurence	Pruvost	Laboratoire Aimé Cotton, CNRS II, bat 505, campus d'Orsay 91405 Orsay, France laurence.pruvost@lac.u-psud.fr
283.	Pascal	Quinet	Astrophysique et Spectroscopie Université de Mons-Hainaut B-7000 Monsm Belgium and IPNAS, Université de Liège Sart Tilman (Bât. B15), B-4000 Liège Belgium pascal.quinet@umh.ac.be quinet@umh.ac.be

284.	Ismanuel	Rabadán	Depatamento de Química, Universidad Autónoma de Madrid, 28049 Madrid, Spain ismanuel.rabadan@uam.es
285.	Andrzej	Raczyński	Instytut Fizyki, Uniwersytet Mikołaja Kopernika, Toruń, Poland raczyn@fizyka.umk.pl
286.	Paul	Radcliffe	Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, 22607 Hamburg, Germany paul.radcliffe@desy.de
287.	T. Peter	Rakitzis	Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas 71110 Heraklion-Crete, Greece and Department of Physics, University of Crete P.O. 2208, 71003 Voutes-Heraklion, Greece ptr@iesl.forth.gr
288.	Merijn	Reijnders	Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven The Netherlands M.P.Reijnders@tue.nl
289.	Gerhard	Rempe	Max-Planck Institute for Quantum Optics Hans-Kopfermann-Str. 1, D-85748 Garching Germany gerhard.rempe@mpq.mpg.de
290.	Yong-joo	Rhee	Laboratory for Quantum Optics, Korea Atomic Energy Research Institute P.O. BOX 105 Yuseong, Daejeon 305-600 Korea yjrhee@kaeri.re.kr
291.	Thomas	Rizzo	Laboratoire de chimie physique moléculaire, Ecole Polytechique Fédérale de Lausanne Station 6, CH-1015 Lausanne Switzerland thomas.rizzo@epfl.ch
292.	Octavio	Roncero	Inst. de Matemáticas y Física Fundamental, C.S.I.C. Unidad Asociada UAM-CSIC Serrano 123, 28006 Madrid, Spain oroncero@imaff.cfmac.csic.es
293.	Jan Michael	Rost	Max Planck Institute for the Physics of Complex Systems Nöthnitzer Str. 38, 01187 Dresden Germany makolies@pks.mpg.de
294.	Arnaud	Rouzee	Institut Carnot de Bourgogne UMR 5209 CNRS-Université de Bourgogne BP 47870, 21078 Dijon Cedex France Arnaud.Rouzee@u-bourgogne.fr
295.	Martin-W.	Ruf	Fachbereich Physik, Technische Universität Kaiserslautern, 67653 Kaiserslautern Germany ruf@physik.uni-kl.de
296.	Igor	Ryabtsev	Institute of Semiconductor Physics, SB RAS 630090, Novosibirsk Russia ryabtsev@isp.nsc.ru
297.	Sergey	Rykovanov	Max-Planck Institute for Quantum Optics Hans-Kopfermannstr. 1, D-85748 Garching Germany sergey.rykovanov@mpq.mpg.de
298.	Lene	Sælen	Department of Physics and Technology, University of Bergen, N-5007 Bergen, Norway lene@ift.uib.no

299.	Marianna	Safronova	Department of Physics and Astronomy, 223 Sharp Lab, University of Delaware, Newark, Delaware 19716 USA msafrono@udel.edu
300.	Giuseppe	Sansone	National Laboratory for Ultrafast and Ultraintense Optical Science CNR-INFM, Department of Physics, Politecnico, Piazza L. daVinci 32, 20133 Milano Italy giuseppe.sansone@polimi.it
301.	Oliver	Scharf	Chimie quantique et Photophysique, Université Libre de Bruxelles, B 1050 Brussels Belgium oscharf@ulb.ac.be
302.	Stefan	Schippers	Institut für Atom- und Molekülphysik, Justus-Liebig-Universität Giessen, Germany Stefan.E.Schippers@iamp.physik.uni-giessen.de or stefan.schippers@uni-giessen.de
303.	Thomas	Schlathölter	University of Groningen, KVI, Zernikelaan 25, NL-9747AA Groningen, The Netherlands tschlat@kvi.nl
304.	Peter	Schmelcher	Physikalisches Institut, Universität Heidelberg, Philosophenweg 12, 69120 Heidelberg, Germany and Theoretische Chemie, Institut für Physikalische Chemie, Universität Heidelberg, INF 229, 69120 Heidelberg, Germany peter.schmelcher@pci.uni-heidelberg.de
305.	Bernd	Schmidt	Fachbereich Physik, Technische Universität Kaiserslautern, D-67663 Kaiserslautern, Germany bschmidt@physik.uni-kl.de
306.	Horst	Schmidt-Böcking	Institut für Kernphysik, Universität Frankfurt, 60486 Frankfurt, Germany schmidtb@hsb.uni-frankfurt.de
307.	Wieland	Schöllkopf	Fritz-Haber-Institut, Faradayweg 4-6, Berlin, Germany wschoell@fhi-berlin.mpg.de
308.	Reinhold	Schuch	Stockholm University, Atomic Physics, AlbaNova, 10691 Stockholm, Sweden schuch@physto.se
309.	Anna M.	Schulenburg	Laboratorium für Physikalische Chemie, ETH Hönggerberg, CH-8093 Zürich, Switzerland schulenburg@xuv.phys.chem.ethz.ch
310.	Martin	Schultze	Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany. martin.schultze@mpq.mpg.de
311.	Emanuele	Scifoni	Laboratoire d'Astrophysique de Grenoble, University Joseph Fourier, Grenoble, France emanuele.scifoni@obs.ujf-grenoble.fr
312.	Matti	Selg	Institute of Physics of the University of Tartu, Riia 142, 51014 Tartu, Estonia
313.	Vladimir	Shabaev	Department of Physics, St.Petersburg State University, Oulianovskaya 1, Petrodvorets, 198504 St.Petersburg, Russia shabaev@pcqnt1.phys.spbu.ru

314.	Jacob-Friis	Sherson	QUANTUM, Johannes Gutenberg University, Mainz, Germany sherson@uni-mainz.de
315.	Fujio	Shimizu	Institute for Laser Science, University of Electro-Communications, 1-5-1 Chofugaoka, Chofu, Tokyo 113-8585, Japan fshimizu@ils.uec.ac.jp
316.	Farideh	Shojaei	Physics Department, Shahid Bahonar University of Kerman, Kerman, Iran fshojaei@mail.uk.ac.ir
317.	Borja	Sierra	Facultad de Ciencia y Tecnologva Departamento de Química Física, Universidad del País Vasco Apdo. 644. 48080 Bilbao Spain borja@iesl.forth.gr
318.	Bruno	Silva	Department of Physics and Astronomy, University College London, Gower St., London WC1E 6BT, UK b.silva@ucl.ac.uk
319.	Roger	Silverans	Catholic University of Leuven Belgium roger.silverans@fys.kuleuven.be
320.	John	Simons	Chemistry Department, Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, UK john.simons@chem.ox.ac.uk
321.	Manolis	Skatzakis	IESL-FORTH P.O. Box 1527 GR711 10 Heraklion, Crete Greece; Dept., Univ. of Crete PO Box 2208, GR71003 Heraklion, Crete, Greece
322.	Przemek	Sobocinski	KVI, Rijksuniversiteit Zernikelaan 25, 9747AA Groningen The Netherlands sobocinski@kvi.nl
323.	Przemek	Sobocinski	University of Groningen, KVI, Rijksuniversiteit, Zernikelaan 25, 9747AA Groningen, The Netherlands sobocinski@kvi.nl
324.	Dimitris	Sofikitis	I.E.S.L.-FO.R.T.H. PO Box 1385, 711 10 Heraklion (Crete), Greece; Department of Physics, Univ. of Crete, PO Box 2208, GR71003 Heraklion (Crete), Greece sofdim@iesl.forth.gr
325.	Andrey	Solov'yov	Frankfurt Institute for Advanced Studies, Johann Wolfgang Göthe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany solovyov@fias.uni-frankfurt.de
326.	Ilia A.	Solov'yov	Frankfurt Institute for Advanced Studies Johann Wolfgang Göthe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main Germany ilia@fias.uni-frankfurt.de
327.	Frederik	Spiegelhalder	Institut für Quantenoptik und Quanteninformation Österreichische Akademie der Wissenschaften Innsbruck, Austria frederik.spiegelhalder@ultracold.at
328.	Rajesh	Srivastava	Department of Physics, Indian Institute of Technology, Roorkee, 247667, India rajsrfph@iitr.ernet.in
329.	Ewa	Stachowska	Poznan University of Technology, Chair of Quantum Engineering and Metrology ul. Nieszawska 13B, 60-965 Poznan, Poland ewa.stachowska@put.poznan.pl

330.	Viorica	Stancalie	National Institute for Laser, Plasma and Radiation Physics, Laser Dept., P.O.Box MG-36, Bucharest, 077125 ROMANIA viorica.stancalie@inflpr.ro
331.	Henrik	Stapelfeldt	Department of Chemistry, University of Aarhus, Denmark henriks@chem.au.dk
332.	Calvin	Stubbins	Department of Physics, Franklin & Marshall College, Lancaster, Pennsylvania, USA calvin.stubbins@email.fandm.edu
333.	Juergen	Stuhler	TOPTICA PHOTONICS AG Lochhamer Schlag 19, D-82166 Graefelfing/Munich Germany juergen.stuhler@toptica.com
334.	Dominique	Sugny	Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne BP 47870, 21078 Dijon, France dominique.sugny@u-bourgogne.fr
335.	Ihor	Sydoryk	Institute of Atomic Physics and Spectroscopy, University of Latvia, LV-1586 Riga, LATVIA ihor@lanet.lv
336.	Gustaw	Szawioła	Poznan University of Technology, Quantum Engineering and Metrology ul. Nieszawska 13B, 60-965 Poznań, Poland gustaw.szawiola@put.poznan.pl
337.	Gabriel	Taban	Department of Applied Physics, Eindhoven University of Technology, PO Box 513, 5600 MB Eindhoven, The Netherlands g.taban@tue.nl
338.	Marion	Tacconi	University of Rome La Sapienza, Department of Chemistry, Piazzale A Moro 5, 00185 Rome Italy tacconi@caspur.it
339.	Junko	Takahashi	Meiji Gakuin University, 1518 Kamikurata, Totsuka, Yokohama 244-8539 Japan juntaka@law.meijigakuin.ac.jp
340.	Maris	Tamanis	Department of Physics and Institute of Atomic Physics and Spectroscopy, University of Latvia, Rainis Boulevard 19, LV-1586 Riga, Latvia tamanis@latnet.lv
341.	Michael	Tarbutt	Centre for Cold Matter, The Blackett Laboratory, Imperial College London, London SW7 2BW, U.K. m.tarbutt@imperial.ac.uk
342.	Genevieve	Tastevin	Laboratoire Kastler Brossel, Ecole Normale Supérieure, Paris, France tastevin@lkb.ens.fr
343.	Swaraj	Tayal	Department of Physics, Clark Atlanta University, Atlanta, USA stayal@cau.edu
344.	Kenneth	Taylor	Queen's University Belfast Belfast BT7 1NN, UK k.taylor@qub.ac.uk
345.	Ioannis	Thanopulos	Department of Chemistry 6174 University Blvd. University of British Columbia Vancouver, B.C. V6T 1Z3, Canada ioannis@chem.ubc.ca

346.	Petko	Todorov	Institute of Electronics, BAS, boul. Tzarigradsko Shosse 72, 1784 Sofia, Bulgaria petkoatodorov@yahoo.com
347.	Yoni	Toker	Department of Particle Physics, Weizmann Institute of Science PO Box 26, Rehovot 76100, Israel ytoker@weizmann.ac.il
348.	Sean	Tokunaga	Centre for Cold Matter, Blackett Laboratory, Imperial College London, SW7 2BW, UK sean.tokunaga@imperial.ac.uk
349.	Luca	Tomassetti	Università di Ferrara, Dip. di Fisica, via del Paradiso 12 Ferrara, I-44100, Italy tomassetti@fe.infn.it
350.	Boyan	Torosov	Department of Physics, Sofia University, James Bourchier 5 blvd., 1164 Sofia, Bulgaria torosov@gmail.com
351.	Elmar	Träbert	Ruhr University Bochum Germany traebert@ep3.rub.de
352.	Friederike	Trimborn	Technische Universität Kaiserslautern D-67663 Kaiserslautern, Germany witthaut@physik.uni-kl.de
353.	George	Tsakiris	Max-Planck-Institut für Quantenoptik, Hans-Kopfermannstr. 1, D-85748 Garching, Germany george.tsakiris@mpq.mpg.de
354.	Vladimir	Tyuterev	Université de Reims, G.S.M.A., UMR CNRS 6089, BP 1039 - 51687 REIMS Cedex 2, France vladimir.tyuterev@univ-reims.fr
355.	Paris	Tzallas	I.E.S.L.-FO.R.T.H. PO Box 1385, GR711 10 Heraklion (Crete), Greece ptzallas@iesl.forth.gr
356.	Wim	Ubachs	Laser Centre Vrije Universiteit Amsterdam The Netherlands wimu@few.vu.nl
357.	Thomas	Udem	Max-Planck-Institut für Quantenoptik Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany thu@mpq.mpg.de
358.	Stefan	Ulmer	Physics Department, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany ulmers@uni-mainz.de
359.	Edvards	Valbahs	University of Latvia Rainis Blvd. 19 Riga LV-1586 Latvia edvards@lu.lv
360.	Gemma	Vall-Llosera	Royal Institute of Technology Department of Physics AlbaNova University Center SE-10691 Stockholm Sweden solrosfroet@gmail.com
361.	Sebastiaan	van de Meerakker	Fritz-Haber-Institut der Max-Planck-Gesellschaft Faradayweg 4-6 14195 Berlin Germany basvdm@fhi-berlin.mpg.de

362.	Hugo	van der Hart	Queen's University Belfast Belfast U.K. h.vdhart@qub.ac.uk
363.	Rob	Van Harrevelt	Radboud University Nijmegen P.O. Box 9010 6500 GL Nijmegen The Netherlands r.vanharrevelt@science.ru.nl
364.	Yulian	Vanne	AG Moderne Optik Institut für Physik Humboldt-Universität zu Berlin Hausvogteiplatz 5-7 D 10117 Berlin Germany yulian.vanne@physik.hu-berlin.de
365.	Sándor	Varró	Research Institute for Solid State Physics and Optics Hungarian Academy of Sciences PO Box 49 H-1525 Budapest Hungary varro@sunserv.kfki.hu
366.	Genko	Vasilev	Department of Physics Sofia University James Bourchier 5 Boulevard 1164 Sofia Bulgari gvasilev@phys.uni-sofia.bg
367.	Sergey	Vasiliev	Department of Physics, University of Turku 20014 Turku Finland servas@utu.fi
368.	Wim	Vassen	Laser Centre Vrije Universiteit Amsterdam The Netherlands w.vassen@few.vu.nl
369.	Fernande	Vedel	PIIM UMR6663 Université de Provence-CNRS Centre de Saint Jérome Case C21, 13 397 Marseille Cedex 20 France fern@up.univ-mrs.fr ; fernande.vedel@up.univ-mrs.fr
370.	Michalis	Velegrakis	I.E.S.L.-FO.R.T.H. PO Box 1385, GR711 10 Heraklion (Crete) Greece vele@iesl.forth.gr
371.	Simone	Veronesi	Università di Siena Dip. di Fisica Institute of Inorganic Methodologies and Plasmas via Roma 56 Siena, I-53100 Italy simone.veronesi@imip.cnr.it
372.	Leif	Veseth	Department of Physics University of Oslo Norway leif.veseth@fys.uio.no
373.	Jacques	Vigué	Laboratoire Collisions, Agrégats Réactivité, IRSAMC UMR 5589 CNRS – Université Paul Sabatier Toulouse 3 118 Route de Narbonne 31062 Toulouse cedex France jacques.vigue@irsamc.ups-tlse.fr

374.	Pablo	Villarreal	Instituto de Matemáticas y Física Fundamental (CSIC) Serrano 123 E-28006-Madrid Spain p.villarreal@imaff.cfmac.csic.es
375.	Nikolay	Vitanov	Department of Physics Sofia University James Bourchier 5 Boulevard 1164 Sofia Bulgaria vitanov@phys.uni-sofia.bg
376.	Edward	Vliegen	Laboratorium für Physikalische Chemie, Swiss Federal Institute of Technology Zurich (ETH Zurich) Switzerland vliegen@xuv.phys.chem.ethz.ch
377.	Wolfgang	Von Klitzing	I.E.S.L.-FO.R.T.H. PO Box 1385, GR711 10 Heraklion (Crete), Greece wvk@iesl.forth.gr
378.	Marc	Vrakking	FOM-Institute AMOLF Kruislaan 40 1098 SJ Amsterdam The Netherlands vrakking@amolf.nl
379.	Edgar JD	Vredenbregt	Department of Applied Physics Eindhoven University of Technology PO Box 513 5600 MB Eindhoven The Netherlands e.j.d.vredenbregt@tue.nl
380.	Wolfgang	Wagner	Forschungszentrum Dresden-Rossendorf Institute of Radiation Physics Germany w.wagner@fzd.de
381.	Fengyan	Wang	IESL – FORTH P.O. Box 1385 711 10 Heraklion, Crete Greece fywang@iesl.forth.gr
382.	Yang	Wang	Departamento de Química, C-9, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid Spain yang.wang@uam.es
383.	Matthias	Weidemüller	Physics Institute Albert-Ludwig University Freiburg 79104 Freiburg Germany m.weidemueller@physik.uni-freiburg.de
384.	Antoine	Weis	Physics Department University of Fribourg Switzerland antoine.weis@unifr.ch
385.	Michael	Wernli	Dipartimento di Chimica and CNISM Università ”la Sapienza”, Rome P.le Aldo Moro 5 00185 Rome Italy wernli@caspur.it
386.	Arlene	Wilson-Gordon	Department of Chemistry Bar-Ilan University Ramat Gan 52900 Israel gordon@mail.biu.ac.il

387.	Dirk	Witthaut	Technische Universitat Kaiserslautern Department of Physics Germany witthaut@physik.uni-kl.de
388.	Matthias	Wollenhaupt	Universität Kassel Institut für Physik und CINSaT Heinrich-Plett-Str. 40 D-34132 Kassel Germany wollenhaupt@physik.uni-kassel.de
389.	Joseph	Wood	Department of Physics and Astronomy University College London London UK joseph.wood@ucl.ac.uk
390.	Christof	Wunderlich	University of Siegen 57068 Siegen Germany wunderlich@physik.uni-siegen.de
391.	Manuel	Yáñez	Departamento de Química, C-9 Universidad Autónoma de Madrid Cantoblanco, 28049-Madrid Spain manuel.yanez@uam.es
392.	Vasilios	Yannopapas	Department of Materials Science University of Patras Rio, 26504 Greece vyannop@upatras.gr
393.	Farook	Yousif	Facultad de Ciencias Univesidad Autonoma del Estado de Morelos (UAEM) Cuernavaca, Morelos Mexico fbyousif@servm.fc.uaem.mx
394.	Sergey	Zemlyanoy	Joint Institute for Nuclear Research Dubna, Moscow Region 141980 Russia zemlya@jinr.ru
395.	Sylwia	Zielińska-Kaniasty	University of Technology and Life Sciences in Bydgoszcz Poland sziel@utp.edu.pl
396.	Nicola	Zurlo	Dipartimento di Chimica e Fisica per l’Ingegneria e i Materiali Università di Brescia 25133 Brescia Italy zurlo@bs.infn.it