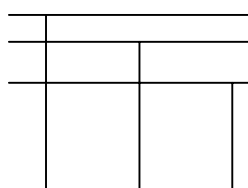




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35th EGAS CONFERENCE



BRUSSELS 15th – 18th JULY 2003
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E U R O P H Y S I C S C O N F E R E N C E



**35th Conference of the
European Group for Atomic Spectroscopy
Université Libre de Bruxelles,
Brussels (Belgium), July 15th-18th, 2003**

Abstracts

**Editors : H.-P. Garnir (ULg)
M. Godefroid (ULB)
P. Quinet (UMH, ULg)**

**Published by : European Physical Society
Series Editor : Prof. R.M. Pick, Paris
Managing Editor : P. Helfenstein, Mulhouse**

Volume

27B

35th EGAS CONFERENCE

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E U R O P H Y S I C S C O N F E R E N C E



**European
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 - **P2** : Instruments and techniques, Atomic and molecular collision processes, Quantum optics, Cold atoms and molecules, Laser spectroscopy and applications, Highly charged ions and X-ray spectroscopy, Plasma physics, Physics of clusters, others.

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ISBN : 2-914771-12-6

The 35th EGAS organizing committee gratefully acknowledges support by :



European Physical Society



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Faculté des Sciences et Département de Chimie



Fonds National de la Recherche Scientifique



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TIMETABLE OF THE 35th EGAS CONFERENCE

Tuesday July 15th		Wednesday July 16th		Thursday July 17th		Friday July 18th	
9.15 – 9.45	Opening	9.00 – 9.45	P. Bowe (INV5)	9.00 – 9.45	R. Cingolani (INV7)	9.00 – 9.45	P. Gill (INV11)
9.45 – 10.30	G. Rempe (INV1)	9.45 – 10.30	B. Sonntag (INV6)	9.45 – 10.30	A. Hibbert (INV8)	9.45 – 10.30	W. Quint (INV12)
10.30 – 11.00				Coffee Break			
11.00 – 11.45	C. Gabbanini (INV2)	11.00 – 11.45	Oral Sessions (S3-S4)	11.00 – 11.45	Oral Sessions (S7-S8)	11.00 – 11.45	Oral Sessions (S11-S12)
11.45 – 12.30	P. Indelicato (INV3)	11.45 – 12.30	Oral Sessions (S5-S6)	11.45 – 12.15	Oral Sessions (S9-S10)	11.45 – 12.30	Oral Sessions (S13-S14)
12.30 – 14.00				Lunch	12.15 : General Assembly*		
14.00 – 14.45	W.E. Ernst (INV4)			14.00 – 14.45	D. Schneble (INV9)	14.00 – 14.45	A. Jorissen (INV13)
14.45 – 15.30	Oral Sessions (S1-S2)		Social programme	14.45 – 15.30	I.B. Khriplovich (INV10)	14.45 – 15.30	M. Vrakking (INV14)
15.30 – 16.00				Coffee Break			
16.00 – 18.00	Poster Session(P 1)			16.00 – 18.00	Poster Session(P 2)	16.00 – 16.45	J.-F. Roch (INV15)
19.45 -	Reception at the Brussels City Hall			19.30 -	Conference Dinner	16.45 -	Goodbye Party

- Plenary sessions (INV1-15) and Oral sessions (S-odd: S1-S13): Auditoire “Lameere”.
- Oral sessions (S-even: S2-S14): Auditoire “Chavanne”.
- Poster sessions (P1-P2) + coffee breaks : “Grand Hall”.
- ★ EGAS General Assembly: Thursday July 17th – between 12.15 and 12.45 : Auditoire “Lameere”.

INVITED TALKS

Cavity quantum electrodynamics

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Cavity Quantum Electrodynamics is the only field of physics where experiments with individual atoms and photons can be performed at the fundamental quantum level. The combination of high-finesse optical cavities with laser-cooled atoms have resulted in a variety of spectacular advances. For example, an individual atom can be observed in real-time with unprecedented spatial and temporal resolution, it can be trapped inside the cavity either with a far-detuned or a near-resonant light field, its motion can be manipulated by means of feedback, and, most recently, its storage time can be extended by employing a novel cavity-mediated cooling mechanism.

A single atom in a high-finesse cavity also constitutes a key ingredient of a distributed quantum network with stationary atoms as quantum memories and flying photons as quantum messengers. A first experiment towards this goal has recently demonstrated that it is possible to emit a sequence of single-photon pulses on demand into a well-defined mode of the radiation field, and that the spectral properties of these photons can be determined by beating consecutively emitted photons on a beam splitter.

After a short introduction into cavity quantum electrodynamics, the talk will review some of the most recent achievements in this exciting field.

Ultra-cold Molecules

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While laser cooling of atoms and the manipulation of cold atomic samples based on radiative forces are widely used in the scientific community, the extension of such techniques to molecules is very difficult because typically in molecules there are no closed transitions for performing efficient cooling. The availability of cold molecular samples would open new perspectives in quantum optics, as well as in chemistry and metrology. Recent results on the formation of translationally cold molecules will be presented. While there will be a hint about some methods reliable on direct cooling of molecules, the focus will be on the conversion of laser-cooled atoms into molecules by photoassociation or other processes. The detection methods for the ultra-cold molecules will be presented together with a report on the trapping techniques. The treatment will be mainly focused on the results obtained by our group on rubidium dimers.

Exotic Atoms

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Exotic atoms are atoms that have captured a long-lived, heavy particle, like a muon, a pion, or an antiproton. During this capture process, many or all of the electrons of the initial atoms are ejected by Auger effect, in a way that resemble internal conversion in nuclei. For light elements, or heavy particles like the antiproton, the cascade can end up with an hydrogenlike ion, with only the exotic particle bound to the nucleus.

The spectroscopy of exotic atoms has been used as a tool for the study of particles and fundamental properties for a long time. Exotic atoms are also interesting objects as they enable to probe aspects of atomic structure that are quantitatively different from what can be studied in electronic or “normal” atoms. For example, all captured particles are much heavier than the electron, and thus closer to the nucleus, leading to a domination of vacuum polarization effects over self-energy contributions, in contrast to normal atoms. Pions are bosons, and thus obey the Klein-Gordon equation, while electrons, muons and antiprotons as spin 1/2 fermions, obey the Dirac equation. Yet antiprotons, which are not elementary particles, have a magnetic moment very different from the one of a Dirac particle. This leads to large corrections not present in other type of atoms.

In the last few years we have performed high-resolution X-ray spectroscopy of muonic, pionic and antiprotonic atoms. We have studied antiprotonic hydrogen and deuterium to improve knowledge of the strong interaction between nucleons and antinucleons at low energy [1]. We have measured the mass of the pion [2]. Currently we are studying pionic hydrogen. Improving the accuracy of the strong interaction shift and broadening measurements is essential for testing modern techniques in Quantum Chromodynamics at low energy like Chiral Perturbation theory.

In the last few years our collaboration has used improved experimental techniques that have lead to better resolution, improved signal to noise ratios, and cleaner production processes. These experimental techniques, the main results and recent theoretical developments will be reviewed.

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Alkali Clusters - Model Systems for the Study of Vibronic Interactions

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When electronic models for metals are discussed, alkali metals often serve as prototypes. Their appeal derives from their simple structure with a single s-electron in the outer shell. They continue to be the text book examples for the band theory of solids, and they provided the first paradigms of metal clusters, the finite size samples of electrical conductors.

Measurements of ionisation potentials and optical absorption spectra of alkali clusters gave rise to comparisons with work function and band structure of their bulk counterparts and inspired the development of an electronic shell model for metal clusters. An interesting question has been what minimum cluster size is required for declaring a sample a nanosized piece of metal. There will not be a single answer but it will depend on the considered property: electronic structure, nuclear geometry, phase transitions etc. approach bulk behavior in different ways.

We have been particularly interested in those details of the electronic and geometric structure that are results of the coupling of electronic and nuclear motion. Related phenomena in the solid state are electron-phonon interactions and find their expression in local lattice distortions and unconventional exciton-phonon states. In alkali clusters, many electronic states are doubly degenerate and thus subject to electron - nuclear vibration coupling. The corresponding energy potentials can be studied in alkali trimers at very high resolution with laser and microwave spectroscopic methods. Generating sodium clusters in a molecular beam experiment, we have investigated the electronic ground state and various excited states of Na_3 . Results range from electron spin densities at the three nuclei of the trimer in its ground state to the shape of an excited state potential consisting of three coupled surfaces that are the consequence of both pseudo Jahn-Teller and Jahn Teller interactions. High resolution spectroscopy reveals the full dynamics of these coupling mechanisms and provides the tools to disentangle the contributions of different effects causing geometric distortions and electronic energy splittings. The origin of a Berry phase in the electronic and nuclear wavefunctions and experimental tests for its existence will be discussed. Comparisons will be made with other authors' work on various metal trimers and higher clusters.

Production of Antihydrogen in ATHENA

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on behalf of the ATHENA collaboration:

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Genova^{8,9}, J. S. Hangst⁴, R. S. Hayano¹⁰, L. V. Jørgensen⁷, V. Lagomarsino^{1,5}, R. Landua³, D.
Lindelöf², E. Lodi Rizzini^{8,11}, M. Macrì¹, N. Madsen², G. Manuzio^{1,5}, P. Montagna^{8,9}, H.
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Antihydrogen, the antimatter counterpart of the hydrogen atom is of fundamental interest. A spectroscopic comparison of antihydrogen with hydrogen tests CPT symmetry with great precision and the availability of cold antihydrogen opens the way for studies of gravitational effects on antimatter. In 2002 the ATHENA experiment produced the first cold antihydrogen atoms by mixing trapped plasmas of positrons and antiprotons [1]. The neutral anti-atoms escape the trap and are detected by their unique annihilation signature.

In this talk the ATHENA experiment is described along with the developments that resulted in this success. Experiments aimed at understanding the physics of antihydrogen production will be presented. The prospects for probing the internal states of the antihydrogen atom and controlling antihydrogen production will be discussed.

References

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Spectroscopy with Free Electron Lasers

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Recent advances in linear accelerators, new developments in low-emittance electron guns, and the feasibility of ultra-precise long undulators open up the exciting possibility of building single pass Free Electron Laser (FEL) based on self-amplified spontaneous emission (SASE). These FELs promise to provide extremely intense, polarised ultra-short pulse radiation for the VUV and x-ray regimes. In addition their high peak and average brilliance, the tunability of the photon energy and the lateral coherence of the radiation will make the FELs to unique sources.

The principle of operation of SASE-FELs and the properties of the emitted radiation will be discussed. First results obtained on free atoms and clusters at the FEL tested at the Deutsches Elektronen-Synchrotron DESY will be presented. Non-linear interactions and ultra-fast processes are the focus of many studies on atoms, molecules, clusters, plasmas and surfaces proposed for the upcoming FELs. Outstanding examples will be presented to showcase the opportunities and challenges of this new area of research.

Nanoscale spectroscopy of artificial atoms and molecules

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We present an overview of recent experiments carried out at NNL aimed at analyzing the optical and electronic properties of single quantum dots with ultimate nanoscale spatial resolution.

A preliminar assessment of the quantum dot properties is accomplished by Near Field Scanning Luminescence at low temperature, showing the characteristic s-shell and p-shell band filling spectra of artificial atoms, with the addition of multi-particle complexes such as biexcitons and charged excitons.

A further enhancement of the resolution is achieved by low temperature Scanning Tunneling induced Luminescence, carried out in a ultra high vacuum STM systems. In this case a clear evidence of single quantum dot electroluminescence is provided, with lateral resolution of about 20 nm. The important role of carrier diffusion is demonstrated upon increasing the current injection, so that the transition from single dot to grand-ensamble STM induced luminescence is clearly evidenced.

Finally, wavefunction mapping of s- and p-like orbitals is demonstrated in a single dot, by means of Current-Voltage STM spectroscopy. The combination of these experiments provides a unambiguous identification of the quantum dot eigenstates and eigenvalues, which is then compared to numerical simulations.

Representative cases of strain induced InP based quantum dots and self assembled InGaAs quantum dots will be discussed.

Recent Progress in Atomic Structure Calculations

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We will discuss some of the difficulties in undertaking calculations of wave functions, and their use in the determination of accurate oscillator strengths.

Particular emphasis will be placed on transitions of astrophysical importance including recent work on Fe II, undertaken as part of the FERRUM Project in the study of Chi-Lupi, and also infrared transitions observed in Eta-Carinae.

Recent experiments with ultracold quantum-degenerate gases

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Quantum-degenerate atomic gases have brought quantum phenomena to a macroscopic scale and are now used for a host of scientific explorations, including new frontiers in condensed-matter physics and atom optics. In my talk I will present recent work on ultracold alkali gases at MIT with a focus on the collective scattering of light, the manipulation of Bose-Einstein condensates in microstructured magnetic potentials (atom chip), and studies of interacting degenerate Fermi gases.

Fundamental symmetries and atomic physics

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A general introduction, on an intuitive level, is presented to discrete symmetries of physical laws: P — parity, or mirror reflection, C — charge conjugation, T — time reversal, and CPT — product of all the three operations.

The discovery and measurement of parity-nonconserving neutral current effects in atoms was one of the crucial confirmations of the Standard Model, well before the discovery of the intermediate W- and Z-bosons. The accurate measurement of the weak nuclear charge in atomic cesium serves as a precision test of the Standard Model. The discovery of the nuclear anapole moment, a new P-odd electromagnetic multipole, in the cesium experiment not only is fascinating by itself, but gives a first-rate information on parity-nonconserving nuclear forces. New prospects in the field are discussed.

Permanent electric dipole moments violate the symmetry under both P and T. Upper limits on the dipole moments of elementary particles and atoms are presented and their physical implications discussed. The atomic experiments are demonstrated to be as informative in this respect as the neutron ones. The measurement of dipole moments has ruled out more theoretical models than any other experiment in the history of physics. Tremendous progress in the field can be expected from experiments at ion storage rings and linear electrostatic traps.

Trapped ion optical frequency standards

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Laser-cooled single trapped ions offer significant opportunities for future optical frequency standards on account of the ability to confine an isolated ion in a small volume under UHV conditions and without serious electromagnetic and collisional perturbation. For ions cooled to the Lamb-Dicke limit, where the extent of the motion of the ion is much less than the wavelength, the first order Doppler broadening is eliminated and second order Doppler shift can be made negligible. Under these conditions it is possible to observe weak optical absorptions such as quadrupole transitions, where the theoretical natural linewidth is ~ 1 Hz or below, with corresponding quality factors (Q) approaching 10^{15} . Already, cold ion linewidths in the range of a few Hz to a few hundred Hz have been observed for such clock transitions, with an experimental Q-factor in excess of 10^{14} being achieved in the best case. The Q of the transition contributes directly to the stability of a frequency standard and recent results for a narrow linewidth laser stabilised to the quadrupole transition in a single cold $^{199}\text{Hg}^+$ ion, have demonstrated an instability of below 7×10^{-15} at 1 second, which already surpasses the best microwave atomic clocks [1].

Research is underway at a number of laboratories worldwide to investigate the stability and accuracy of different trapped ion optical frequency standards, including those based on single cold ions of $^{199}\text{Hg}^+$, $^{115}\text{In}^+$, $^{177}\text{Yb}^+$ and $^{88}\text{Sr}^+$. With the high resolution cold ion lineshapes now available, it is possible to evaluate frequency systematics and uncertainties close to the Hz level, and make absolute frequency measurements of the standard using femtosecond optical comb technology [2]. This paper will review the current and future capabilities of a number of these trapped ion standards. In particular, the $^2S_{1/2} - ^2D_{5/2}$ quadrupole clock transition in a single $^{88}\text{Sr}^+$ ion [3] and the ultra-weak $^2S_{1/2} - ^2F_{7/2}$ octupole clock transition [4] will be discussed.

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The g-factor of the bound electron in H-like ions: a new determination of the electron mass

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A few years ago we started an experimental and theoretical program to investigate the magnetic moment anomaly (or g-factor) of the bound electron in highly charged ions [1].

The measurement of the g-factor of the electron bound in a hydrogen-like ion is a high-accuracy test of the theory of Quantum Electrodynamics (QED) in strong electromagnetic fields. We constructed a Penning-trap quantum jump spectrometer for highly charged ions and, for the first time, applied the continuous Stern-Gerlach effect to an atomic ion [2].

Quantum jumps between the two spin states (spin up and spin down) are induced by a microwave field at the spin precession frequency of the bound electron. With a novel double-trap technique we determined the g-factor of the bound electron in hydrogen-like carbon ($^{12}\text{C}^{5+}$) [3] and hydrogen-like oxygen ($^{16}\text{O}^{7+}$) [4] with an accuracy on the ppb level. We have performed bound-state QED calculations of the g-factor of the bound electron in hydrogen-like ions with different nuclear charge Z up to uranium ($^{238}\text{U}^{91+}$) in a non-perturbative treatment.

Recent theoretical progress made it possible to determine the electron's mass in atomic units with unprecedented accuracy from the measured g-factor of the electron in carbon ($^{12}\text{C}^{5+}$) [5,6,7].

In the future, we plan to extend our g-factor measurements to heavy hydrogen-like ions.

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Atomic and molecular spectroscopy for astrophysics

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This review highlights current (or future!) hot topics in astrophysics where atomic or molecular input data are essential. Reflecting the author's own interests, this review is biased towards topics relating to nucleosynthesis, stellar atmospheres and abundances, and cosmochemistry.

Progress in astrophysics has always been driven mainly by the development of new instrumentation. The current epoch is no exception. This paper therefore first reviews recent or forthcoming instruments which deliver data requiring appropriate atomic or molecular input for a proper exploitation. These instruments include the *Short and Long Wavelength Spectrometers* (SWS, LWS) on board the *Infrared Space Observatory* (ISO), the *Goddard High-Resolution Spectrometer* (GHRS) on board the *Hubble Space Telescope* (HST), the *Ultraviolet-Visible Echelle Spectrograph* (UVES) on the *Very Large Telescope* (VLT), the *Phoenix* spectrograph on the *Gemini* telescope, the *Cryogenic Infrared Echelle Spectrograph* (CRIRES) on the VLT, and the *Herschel* infrared satellite.

The rapid and tremendous increase in computing power has also driven progress through numerical modelling. Especially spectacular is the 3-D modelling of (convective) stellar photospheres which removes the need for the long-standing and *ad hoc* microturbulent parameter. Such simulations reveal as well that it may be necessary to lift the hypotheses of spatial homogeneity and time constancy traditionally adopted in the description of stellar atmospheres to derive chemical abundances. This is especially so in the presence of convection in the atmospheres of supergiant stars, and of "stellar meteorology" in ultracool stars like brown dwarves.

Finally, a few specific issues will be discussed. First, we give two examples where the solution of important astrophysical issues required atomic data for *blending* lines: (i) the Th II line at 401.9129 nm, used for dating the oldest stars in the Galaxy, is blended by a Co I line, which needs to be accurately modelled in order to derive reliable Th abundances, and hence, ages [1]; (ii) the Li I doublet at 670.776 and 670.791 nm is blended by a Ce II line at 670.899 nm, which totally dominates the blend in evolved, low-mass stars enriched in neutron-capture elements like Ce (the so-called post-AGB stars) [2]. Neglecting the Ce II line leads to a largely overestimated Li abundance for those stars, in complete disagreement with the predictions of stellar nucleosynthesis.

Secondly, accurate $\log gf$ values are of course needed for the lines of astrophysical interest themselves. Some among the spectrographs mentioned above opened the ultraviolet window, with its wealth of lines from heavy elements. Many, like Os, Pt, Pb, Bi, Th and U, are of importance for a better understanding of stellar nucleosynthesis [3,4,5]. Atomic spectroscopists have made valuable efforts to provide astrophysicists with the required input data, as I will review. Much remains to be done, however, in the infrared window (2 to 700 μm) which will be explored by infrared astronomical satellites.

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Slow photoelectron imaging

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Recent progress in photoelectron imaging techniques has enabled the extension of imaging techniques to the detection of photoelectrons with a kinetic energy of just a few milli-electronvolts. The photoionization dynamics of electrons that leave an ion with such low kinetic energies is very different from the photoionization dynamics of more energetic electrons, since the motion of slow electrons is not only determined by the external electric field, which drives the electrons towards the detector, but also by the Coulomb interaction with the ion that stays behind.

In my talk I will present results on three aspects of threshold photoionization leading to the production of slow photoelectrons. First, experiments will be presented on the photoionization of metastable Xe atoms using visible/ultraviolet light. These experiments illustrate that the far field photoelectron spatial distributions contain important information about the nature of the trajectory of the electron between the atom and the detector, and allow us to distinguish between direct and indirect photoionization processes. The latter correspond to photoionization events where the electrons interact one or more times with the remaining ion before the ionization takes place[1]. Second, experiments will be presented that reveal the formation of interference patterns in the far field, which arise from a quantum mechanical interference between several trajectories along which the electron can move from the atom to the detector, and which can be understood using a semi-classical path integral analysis [2].

Furthermore, experiments will be discussed where threshold photoionization of Xe Rydberg atoms by half-cycle THz pulses is studied. These experiments show that, while the half-cycle pulse ionizes the atom by means of a substantial acceleration of the electron, the final kinetic energy of the electrons is very low, as a result of the interaction of the ionized electron with the negative tail of the half-cycle pulse [3]. The half-cycle ionization in the THz experiment is relevant to the formation of attosecond pulses in high harmonic generation. Results on the experimental generation and detection of attosecond laser pulses will be presented at the meeting [4].

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Single photons from single emitters

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New types of light sources, which are able to emit photons one by one, have been realized over the past few years. The development of these single photon sources is mainly driven by possible applications in the field of quantum cryptography, and more generally for quantum information processing features.

Single photon emission can be easily obtained by controlling the fluorescence of a single emitter. Continuous wave fluorescence excitation provides antibunching in the emitted photons sequence, as a signature of the property to only emit one photon at a time. A short pulsed excitation can then produce single photons on demand, with an overall quantum efficiency up to a few

Convincing experiments that produce single photons on demand have been performed using individual organic molecules. Since single photons pulsed trains should have reduced intensity fluctuations compared to the shot noise limit, a non-classical signature of the photon statistics can be obtained by measuring the Mandel parameter $Q(T)$ for an observation period of duration T [3]. However, a significant drawback of molecular emission at room temperature is that the fluorescence of these emitters switches off irreversibly after a finite irradiation time. The photochemical mechanism responsible for this photobleaching process is still not well understood.

One of the most efficient single-photon source realized so far relies on individual nitrogen-vacancy (NV) colour centers in diamond. These solid-state emitters share many similarities with individual organic molecules, with the strong advantage of a very high photostability even at room temperature. They can also be easily manipulated since they appear in both bulk and nanocrystals forms of diamond. Such a single photon source has recently been used for building a complete quantum cryptographic testbed [4]. On-going improvements should end up in a highly efficient, easy to use and reliable single-photon source, well suited for quantum key distribution schemes in open air.

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ORAL SESSION S1

DCM in hydrogen- and lithium-like simple atomic systems

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Systematic model calculations are performed for the magnetization distributions and the HFS in atomic and ionic states of helium and lithium in order to test the interplay of nuclear and atomic structure [1]. The results will contribute to the analysis of high-precision measurements of isotope shifts (IS) in lithium, which is currently underway at GSI and Isolde, CERN [2]. These measurements, in combination with accurate theoretical evaluations of the mass-shift contribution in the respective transition will yield the root-mean-square (rms) nuclear charge radii of unstable Li isotopes, particularly for the halo nucleus ^{11}Li . The presented calculations are performed using the Dynamic Correlation Model (DCM) to evaluate the mass shift of the three electron transitions. A hyperfine anomaly could additionally modify the field shift contributions between the different isotopes, thus casting new light on the (IS) theory.

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Relativistic theory of the recoil effect in atoms

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The nonrelativistic theory of the nuclear recoil effect for many-electron atoms was first formulated by Hughes and Eckart [1]. The nonrelativistic recoil operator is given by

$$H_M^{(\text{nr})} = \frac{1}{2M} \sum_{i,j} \vec{p}_i \cdot \vec{p}_j. \quad (1)$$

The full relativistic theory of the recoil effect can be formulated only within quantum electrodynamics (see [2] and references therein). In this paper we consider the present status of the relativistic calculations of the recoil effect in atoms. A special attention is focused on an approximate relativistic treatment of this effect for many-electron atoms. Within the lowest-order relativistic approximation ($\sim v^2/c^2$) and to first order in m/M , the recoil corrections can be derived by using the following recoil Hamiltonian ($\hbar = c = 1$)

$$H_M^{(\text{rel})} = \frac{1}{2M} \sum_{i,j} \left[\vec{p}_i \cdot \vec{p}_j - \frac{\alpha Z}{r_i} \left(\vec{\alpha}_i + \frac{(\vec{\alpha}_i \cdot \vec{r}_i) \vec{r}_i}{r_i^2} \right) \cdot \vec{p}_j \right], \quad (2)$$

where $\vec{\alpha}$ is a vector incorporating the Dirac matrices. The expectation value of $H_M^{(\text{rel})}$ on the Dirac wave function yields the recoil correction to the atomic energy level to first order in m/M (here the eigenvectors of the Dirac-Coulomb-Breit Hamiltonian are implied by the Dirac wave functions). It is shown that calculations based on averaging the nonrelativistic recoil operator (1) with the Dirac wave functions yield strongly incorrect results for the relativistic recoil corrections. This is caused by the fact that the relativistic contribution that results from averaging the nonrelativistic recoil operator (first term in equation (2)) with the Dirac wave functions is significantly cancelled by the contribution from the relativistic part of the recoil operator (second term in equation (2)). Numerical results confirming this statement are presented.

The work of V.M.S. was supported by the Alexander von Humboldt Stiftung.

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Perturbation theory for intercenter electron exchange and superexchange with degeneracy.

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The phenomena determined by the multi particle character of quantum interactions to become significant and topical.

A number of difficulties arise during an attempt to construct a theory in which the corrections to wave functions are anti-symmetrized with respect to the interchange of electrons. First, if the total Hamiltonian is symmetric with respect to interchange of identical particles, subdividing it into perturbed and unperturbed parts means that the latter is asymmetric because it is due to a particular distribution of label particles over the atoms. The zeroth wave function anti-symmetrized in inter-center permutations is not an eigenfunction of unperturbed part of the Hamiltonian and corrections calculated in the also asymmetric perturbation would contain nonphysical contributions. The second main problem is concerned with the so called overfilling catastrophe. The basis of antisymmetric unperturbed wave functions is nonorthogonal and then overfilled. To avoid this problems, a number theoretical techniques employ a basis in which the excited-state vectors are not orthogonal. The requirement of symmetrization is extended only to the own states of the ground energy level. The theory then proceeds by using the variational method at some stage of the calculations.

All variants of exchange perturbation theory (EPT) can be divided into two groups [1]. The first consists of theories nonsymmetric in the Hamiltonian. The second consists of approaches that make it possible to use the common Rayleigh-Schroedinger perturbation theory by setting up a special zeroth symmetric nonperturbate Hamiltonian for which the antisymmetric functions are eigenfunctions. The first group uses the fundamental basis of zeroth functions nonsymmetric in inter-center permutations, functions that are the eigenfunctions of the nonsymmetric Hamiltonian without perturbation. Antisymmetrization is done post factum at each interpolation step. An attempt to modify the Hamiltonian so that the perturbation operator becomes symmetric (it is known as the Sternheimer procedure) leads to non-Hermitian total Hamiltonian and actually limits the use of the method to two-electron systems.

In present work we use the idea of the method of symmetrizing the Hamiltonian and construct algorithm of EPT by using a special projection operators. These operators symmetrize the perturbation operator and unperturbed Hamiltonian and retain the hermiticity both of the total Hamiltonian and the unperturbed Hamiltonian with the perturbation separately. Also, the variant of ETP is developed to the case of degeneration in total spin. We have shown, that a special basis of antisymmetrical eigenfunctions owns to a completeness properties. We have considered a magnetic properties of different materials: MnF₂, the HTc- materials, cuprates La₂-xSrxCuO₄ and Ba₂Cu₃O₆.

Super-exchange contributions are presented usually in the form of a combination of two-center exchange integrals . Besides, one does not take into account the nonadditive three-center contributions, which cannot be considered as small corrections to the pairwise ones. This work reports on the derivation of the interaction energy analytically and analyzes in detail all possible three-center super-exchange contributions [2]. These contributions are shown to be of the same order of magnitude as the two-center ones.

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ORAL SESSION S2

Pressure broadening and shift of rubidium resonance lines by argon and helium

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Pressure broadening and shift of alkali resonance lines was widely investigated in the literature, e.g. [1,2,3]. However, no experimental data seem to exist on Rb resonance lines with resolved hyperfine structure. We present results of diode laser spectroscopy investigations of the pressure broadening and shift of rubidium $5s_{1/2}$ - $5p_{3/2}$ (780 nm) and $5s_{1/2}$ - $6p_{3/2}$ (420 nm) spectral lines by argon and helium buffer gases.

An external cavity diode laser, using diffraction grating feedback in a Littrow configuration, was used for absorption measurement in rubidium vapor. With a linewidth of the order of 1 MHz and continuous single-mode tuning range of over 20 GHz, the laser could be adjusted to fully scan the Rb $5s_{1/2}$ - $5p_{3/2}$ (780 nm) and $5s_{1/2}$ - $6p_{3/2}$ (420 nm) lines.

The absorption profiles consist of four distinct lines, two of them resulting from ^{85}Rb absorption and the other two from ^{87}Rb . Two lines from each rubidium isotope are a result of the hyperfine splitting of the ground $5s_{1/2}$ level, which are 3036 MHz for ^{85}Rb and 6835 MHz for ^{87}Rb . The hyperfine structure lines resulting from the splitting of the upper level are not resolved due to Doppler broadening, which is at room temperature approximately 500 MHz for 780 nm and 900 MHz for 420 nm. The measurements were performed on rubidium vapor generated in a heat-pipe oven. The oven was connected to a vacuum system and a buffer gas source. In addition to heat-pipe oven, a rubidium linear all-sapphire cell (no buffer gas) was used to provide the reference for pressure shift determination and for spectra calibration.

In order to determine the values of pressure broadening and line shifts, a Voigt profile function was fit to each absorption profile. For this purpose, a custom-written lineshape-fitting program was developed (based on the Voigt function calculation subroutine developed by R.J. Wells [4]), which performs a general non-linear least-squares fit of a Voigt profile.

As a result of fitting procedure, the shifts and Lorentzian widths of absorption lines were obtained. Plotting these values as a function of Ar and He buffer gas pressure, the pressure broadening and shift parameters were calculated.

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Vibration and orientation effects in ion-molecule collisions at intermediate energies

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Scattering experiments between charged particles and molecules have displayed novel many-body phenomena involving coherent interplay between electrons and nuclei. From the theoretical side, the development of *ab initio* theories have not followed the progress on the experimental side, partly because charged dynamical many-body problems becomes exponentially more complex with increasing number of nuclei. However, at low collision energies, $v_p < v_e$, theory has advanced based on the static molecular multi-center problem, followed by an expansion of the wavefunction on molecular state basis [1]. In the high energy limit it can be shown that the transfer probability become a sum of independent events from two atoms, which leads to an effective probability based on two impact parameters associated with each atom of the molecule [2]

At the conference we present an *ab initio* coherent three-center theory of ion-molecule scattering, applied for keV- $He^{2+} - H_2^+$ collisions [3]. Comparisons with recent experimental data [1] reveal strong dependences of the cross sections on the initial molecular vibrational distribution and suggest its possible indirect determination. The calculations demonstrate that ion induced oscillatory motion of the electronic probability density between the two molecular ions is a dominant feature of the dynamics of the capture process.

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Metastable level collision cross sections from an atomic lifetime measurement at a heavy-ion storage ring

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Collisions involving laser-excited neutral atoms have become an active field of atomic physics research. Very different techniques are required to arrange for excited states of multiply charged ions to be available for collisions. We have obtained such collision data in the course of an atomic lifetime experiment at a heavy-ion storage ring [1].

Li^+ ions of 7 MeV and Be^{2+} ions of 21.7 MeV, respectively, were produced by stripping in the high voltage terminal of a tandem accelerator and injected into the Heidelberg heavy-ion storage ring TSR. There they were left coasting for a while.

Most of the ions are expected to be in the ground state. The only long-lived low-lying levels in these ions are the $1s2s\ ^3\text{S}_1$ levels with predicted radiative lifetimes of 49 s and 1.8 s, respectively. The principal aim of the experiment was a measurement of these lifetimes. In order to study the beam storage behaviour, microchannel plate-based beam profile monitors were employed, detecting recoil ions produced in collisions of the circulating ion beam with the residual gas. The signal featured two decay components, one from ground state ions and one from excited ions that plausibly have a larger collision cross section. The decay constant of the latter signal represents the sum of radiative decay and ion loss rates.

Assuming the lifetime calculation to be reliable (Li^+) or varying the ultrahigh vacuum pressure ($p \approx 5 \cdot 10^{-11}$ mbar) by almost a factor of two (Be^{2+}), the ratio of the excited state cross section to the ground state cross section (at these ion beam energies, both are dominated by the electron-loss cross section) could be determined. In both cases the ratio was about 2 to 2.5. This is rather lower than the estimates obtained by Fiol and Olson [2] using the Born approximation or the non-classical trajectory Monte Carlo (nCTMC) approach for collisions with the dominant residual gas species, hydrogen.

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ORAL SESSION S3

Laser-dressed Lamb shift

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We show that the Lamb shift or self-energy of laser-dressed atomic states is different in an unexpected manner from the Lamb shift of bare atomic states which are usually observed in high-resolution spectroscopic experiments. Dressed states as introduced by Cohen-Tannoudji in 1975 describe the incoherent part of the atomic fluorescence spectrum (the many-photon processes). From a theoretical point of view, the diagonalization of the Hamiltonian that describes the atom-laser coupling leads to the dressed-state basis, and it is the Lamb shift (self-energy) of the dressed states which gives rise to unexpected surprises in the theoretical analysis.

Lifetime measurement of the metastable $3d^2D_{5/2}$ state in $^{40}\text{Ca}^+$ by observation of quantum jumps in a few-ion string

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The lifetime of the metastable $3d^2D_{5/2}$ state in $^{40}\text{Ca}^+$ is important as a test of atomic structure calculations[1]. Furthermore, this state is very relevant in such diverse fields as astronomy[2], optical frequency standards[3], and quantum information processing with trapped ions[4].

In recent years, many conflicting measurements and calculations of the lifetime of the metastable $3d^2D_{5/2}$ state in $^{40}\text{Ca}^+$ have been reported, and so far no agreement has been reached. In the most recent measurement by Barton *et al.*[5], many possible systematic effects are considered, and a lifetime of 1168 ± 7 ms is reported. The work seems to be convincing, however, the result has not been confirmed by other groups.

We have performed a series of measurements, observing quantum jumps in a few-ion string, where we measure the lifetime of the $3d^2D_{5/2}$ state. Our result is 1155^{+15}_{-19} ms, which is in agreement with the result of Barton *et al.* within one standard deviation.

Here we present the experiment together with the data analysis yielding our result for the lifetime.

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New laser-electron nuclear effects in an nuclear g transition spectra in atomic ion and their possible experimental observation in the laser plasma of multi-charged ions

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In last years a great attention is turned to problems of experimental and theoretical study of high temperature multi-charged ions plasma and developing the new diagnostics methods (c.f. [1-3]). Similar interest is also stimulated by importance of carrying out the approaches to determination of the characteristics for multi-charged ions plasma in thermonuclear reactors, searching new medium for X-ray range lasers [2]. A great progress in development of laser technique and accelerators experiments resulted to a new class of problems in the plasma physics and correspondingly diagnostics of their parameters. Here it should be noted a possibility of the cooperative dynamical phenomena [3,4] due the interaction between atoms, ions, molecule electron shells and nuclei nucleons. Attractive situation arises under transition to heavy multi-charged ions because of changing the energy and geometric parameters of electron shell. In result a character of interaction with a nucleus may strongly change and new channels of electron-nuclear processes are opened [3,4]. A principally new approach to problem of the multi charged ions plasma diagnostics is provided by using the new laser-electron-nuclear effects. In our paper a possibility of the experimental observation of set of the electron satellites in spectra of the electron-nuclear γ -transition of the nucleus in a multi-charged atomic ion is analyzed. It is proposed to use for observation of these effects the thermalized plasma of O-,F-like multi-charged ions. As example, the nuclear transition in the isotope Fe(57) with energy of the γ quantum 14,41 keV (the half decay period is $9.77 \cdot 10(-8)s$, the recoil energy $1.96 \cdot 10(-6)keV$) is considered for O-and F-like ions of Fe. It is shown that the electron-nuclear lines in spectra of emission or absorption can be experimentally observed in plasma of the O-and F-like multi-charged ions and it is very important that they are not overlapping by the Doppler broadening. Such a situation may be realized in the thermalized plasma of multi-charged ions. Let us give some numerical estimates. The values of the 1s,2s,2p-2p electron transitions for one-electron ions with $Z=10-50$ are as follows: $E[1s-2p(3/2)]$ in interval $[1.3?10(3); 2.3?10(4)]eV$, $E[2s-2p(3/2)] \approx E[2s-2p(3/2)]$ in interval $[0.1; 3.3?10(2)]eV$. The transition energies have an order of the Doppler shift value. Calculated relative intensities for the transitions: 1s-2s (monopole), 1s-2p(1/20, 2s-2p(3/2) (dipole), 2p(1/2)-2d(3/2) (quadruple) are lying in the interval $2 \cdot 10^{-5} - 7 \cdot 10^{-5}$.

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ORAL SESSION S4

Creation of Coherent Superposition States in Hydrogen-like atoms/ions via Multiphoton Excitation in Strong Laser Fields

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The current laser technology enables production of electromagnetic (EM) fields comparable and larger than internal atomic fields. Under these conditions the bound-bound and bound-free transitions in atomic systems have essentially multiphoton character. The increasing interest to the processes of intense laser and atom interaction is due in large part to the problem of high harmonic generation and short wave coherent radiation implementation via multiphoton bound-free transitions through free continuum spectrum. Over the past few years significant experimental progress has been made in coherent UV-X radiation generation by excitation of high harmonics in the mentioned systems.

On the other hand in strong laser fields one can expect for multiphoton resonant excitation (MRE) of atoms and by the appropriate laser pulses one can obtain various coherent superposition states, which can lead to cooperative processes such as superradiation, free-induction decay, photon-echo and etc. However, to obtain such superposition states is problematic if the energy gap between the states is large compared with optical transitions. Hence, the actual MRE of atoms needs a resulting dipole moment oscillating at corresponding resonant frequencies associated with the certain energy levels.

Regarding this problem recently we have investigated the possibility of implementation of coherent superposition states in three level atomic systems via MRE by strong laser radiation [1] and as an example we have considered a hydrogen like atomic system, where due to random degeneration upon an orbital moment atom has a mean dipole moment in the excited stationary states. However, the treatment was made in the scope of nonrelativistic theory for the atoms with a small nuclear charge, which can provide a coherent radiation up to the UV region. To reach a far X-ray region the problem needs the atoms or ions with a large nuclear charge [2] at which the problem becomes relativistic.

In the present work the MRE of Hydrogen-like atoms/ions with the large nuclear charge subjected to a strong laser field is studied in the scope of relativistic theory. The consideration is based on the Dirac equation which allows to take into account the fine structure of the atomic levels.

The time evolution of such systems is found using nonperturbative resonant approach. The analysis shows that quasi-energy levels close to the ground state arise. The probabilities of multiphoton transitions between these quasi-energy levels have a maximal values for the resonant transitions. As a result MRE problem is reduced to the usual Rabi problem with a generalized "Rabi frequency" [1], which has a nonlinear dependence on the amplitude of an EM field. Our calculations suggest that by the appropriate laser pulses when the rate of concurrent process of multiphoton ionization is small, one can achieve various superposition states by the MRE. It may serve as a scheme of superradiant laser based on MRE of atoms/ions and subsequent UV and X-ray superradiation from the coherent superposition states.

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New Absolute Frequency Measurement of the $1S - 2S$ Transition in Atomic Hydrogen: Preliminary Results

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During the last century spectroscopic experiments performed on the hydrogen atom have been used as critical tests of fundamental theories and have stimulated much progress of physics. An increasing accuracy of spectroscopic methods has not only allowed to improve the accuracy of the known theories and their consequences, but have also opened new horizons for further delicate tests.

The measurement of the absolute frequency of the $1S - 2S$ transition in atomic hydrogen with its natural linewidth of 1.3 Hz has attracted the attention of experimental physicists due to its important role for the definition of such fundamental values as the Rydberg constant and the Lamb shift [1], and for tests of QED. A recent breakthrough in absolute frequency measurements [2] has brought this experiment on a level of accuracy of 10^{-14} . The last measurement performed in the year 1999 has demonstrated a precision of 1.9 parts in 10^{14} [3]. Such a level of accuracy along with the 3-years time period passed since this measurement allows to discuss a possibility to observe the drift of fundamental constants in this laboratory experiment.

We report on preliminary results of a new measurement of the absolute frequency of the $1S - 2S$ transition in atomic hydrogen performed in February 2003. The hydrogen spectrometer used for these experiments is described in [4]. Important improvements have been introduced which significantly improve the signal-to-noise ratio and reduce the linewidth of the transition as well as the drift of the laser frequency. The unique transportable Pharaos Cs fountain with specified Allan standard deviation of 1.2×10^{-13} within one second and an accuracy of about 2×10^{-15} has been installed in Garching and served as primary frequency standard. With the help of an optical frequency comb generator based on a Ti:sapphire femtosecond laser [2], the frequency of the $1S - 2S$ transition has been phase coherently compared with the frequency of the Cs standard.

The data recorded during 12 days of measurement require a delicate processing for the elimination of systematic effects. Up to now we have treated 4 days, and the preliminary result of averaging is equal to 2 466 061 102 474 807(67) Hz. Assuming that the measurements performed in 1999 and 2003 years are equivalent, one can evaluate a possible drift of the $1S - 2S$ frequency as $-6.9(8.8) \times 10^{-15}$ Hz/year. The final analysis of the data will be made in the near future.

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Lifetime measurements with single ions and ion clouds

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In the past decade, the lifetime of the $3D_{5/2}$ state of the Ca^+ -ion has been measured a couple of times using either the technique of quantum jumps of a single cold ion confined in an rf trap, or spectroscopy of an energetic ion cloud in a trapping device. Over the years, measured values have become more precise and longer, reaching almost 1200ms [1]. The measurements of this level lifetime offer a test for the different model approaches being put forward by theoretical calculations [2]. Experimental applications of the Ca^+ -spectroscopy range from frequency metrology in the optical domain, via quantum computers to astrophysical interest in the dermination of stellar spectra.

Our experiment aims to propose the electric quadrupole transition $4S_{1/2}$ - $3D_{5/2}$ of a single trapped Ca^+ -ion at 729 nm as a frequency standard in the optical domain. The quality factor $\Delta\nu/\nu$ of the transition is inferior to 5×10^{-16} , orders of magnitude better than existing frequency standards. All the wavelengths necessary for the implementation of this frequency standard lie in the optical domain, easily accessible by solid-state lasers.

We confine ions in a modified Paul-Straubel trap, made from a molybdenum ring of 1.4 mm inner diameter and two far-off (5.5mm) grid electrodes of 11 mm diameter. The position of a single ion in this trap can be optimized by two copper tips serving as compensation electrodes. Typical pseudo-potential well depth is of the order of 3 eV. In this trap we have carried out lifetime measurements on a medium-size laser-cooled ion cloud (≈ 100 particles) using the technique of electron-shelving. In fact, direct optical pumping of a part of the cloud in the metastable $3D_{5/2}$ state, permits to measure the lifetime by direct observation of the return rate of the ions into the laser-cooling (fluorescing) cycle [3].

The miniature trap allows also to confine single particles and to laser-cool them to the Doppler limit, attaining temperatures in the mK regime. In this case, the use of the electron-shelving technique leads to the observation of quantum jumps. The presence of the ion in the metastable state can then be detected with almost 100% detection efficiency as the fluorescence in the laser-cooling cycle is switched off. The lifetime of the shelving state is given by the statistical distribution of the length of "dark" intervals.

Special care has been taken to avoid any systematic influence of experimental parameters such as output power and frequency detuning of the different lasers or collisions with the residual background gas. Measurements of the lifetime using an ion cloud and single ions will be presented at the conference.

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ORAL SESSION S5

Cesium atoms feel the human heart beat

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Many physiological processes in the human body involve the flow of electrical currents, which generate time-varying magnetic fields. The beating human heart produces the strongest of such biomagnetic fields, which barely reaches a peak amplitude of 100 pT above the chest, less than a millionth of the geomagnetic field and orders of magnitude weaker than typical magnetic noise fields. The cardio-magnetic field can be recorded as a time trace of the magnetic flux density component perpendicular to the chest. This magnetocardiogram (MCG) closely resembles the well-known electrocardiogram (ECG).

So far mainly superconducting quantum interference devices (SQUID) were used for the detection of biomagnetic fields. SQUID detectors designed for this purpose are commercially available, but are very expensive, in particular multi-channel devices, and their operation requires the use of cryogenic cooling liquids. These facts significantly contribute to the slow acceptance of MCG diagnostics, despite the proven advantages of this non-invasive technique in a growing number of applications.

Our team at University of Fribourg has developed a room-temperature magnetometer based on an optical-radio-frequency double resonance technique (M_x -mode) using optically pumped cesium vapor in a 6 cm³ buffer gas cell at room temperature. The device has the sensitivity, the spatial resolution and the bandwidth necessary to record human magnetocardiograms (MCG). Environmental magnetic noise is suppressed by the combined use of a weak magnetic shield, a gradiometric arrangement of two identical sensors and data averaging over 100 heartbeats. By stepping the gradiometer across the chest on an array of 6 x 6 grid points two-dimensional maps of the cardiomagnetic field can be recorded with a quality comparable to SQUID data [1]. Such maps can be recorded with a time resolution of 10 ms during the heart beat cycle, and display of the maps in the form of movies reveals the heart beat dynamics [2] from which relevant medical diagnostic information can be inferred.

We will present a status report on the development of the device and outline future developments such as the implementation of a second-order gradiometer that will allow us to operate the sensor in an unshielded environment and the development of sensor arrays for reducing the data acquisition time.

We believe that OPM sensors will make biomagnetic diagnostics and therapy control more convenient and cost-effective and that the OPM technique will significantly contribute to the future acceptance of non-invasive MCG diagnostics as a standard medical technique.

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Fourier-transform spectroscopy of NaRb

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The heteronuclear alkali dimers attract interest of both experimental and theoretical researchers involved in collision dynamics, photoassociative spectroscopy, laser cooling and trapping of alkali atoms. A special interest is put on the study of the ground states and especially near the asymptotic region, since the precise knowledge of the long-range interactions between two different types of alkali atoms is necessary for understanding and realization of such cold collision processes as sympathetic cooling, formation of two species BEC and ultracold heteronuclear molecules. Experimental information on the ground singlet and triplet states of the NaRb molecule is still limited [1-3]. Therefore the goal of the present investigation was to study the ground $X^1\Sigma^+$ and $a^3\Sigma^+$ electronic states of the NaRb molecule with the help of the Fourier-transform spectroscopy.

In the present experiment high-resolution Fourier-transform spectra of the NaRb molecule from laser induced fluorescence (LIF) were obtained. NaRb molecules were formed in a heat pipe oven. LIF was excited by an Ar⁺ laser, dye laser (R6G) and a single-mode frequency doubled cw Nd:YAG laser. This allowed us observing the $B^1\Pi \rightarrow X^1\Sigma^+$, $D^1\Pi \rightarrow X^1\Sigma^+$ and $C^1\Sigma^+ \rightarrow X^1\Sigma^+$ band systems. Also transitions to the triplet $a^3\Sigma^+$ state were observed with partially resolved hyperfine structure by exciting the strongly mixed $B^1\Pi - c^3\Sigma^+ - b^3\Pi$ complex.

The data field for the $X^1\Sigma^+$ state includes about 6000 transitions and covers a range of rotational quantum numbers from $J'' = 1$ to 200 and a range of vibrational quantum numbers from $v'' = 0$ to 76. The classical turning point of the last observed bound level is about 7.8 cm⁻¹ below the molecular asymptote. Experimental information about the $a^3\Sigma^+$ state consists of app. 500 transitions with $v'' = 0 \div 17$ and $N'' = 1 \div 78$. The typical uncertainty of the recorded transition frequency is 0.003 cm⁻¹. Direct fit of the potential energy curve (PEC) to the observed differences between ground-state levels is realised [4, 5]. Experimental data for both isotopomers of NaRb are described by a single PEC. For the ground $X^1\Sigma^+$ state the fitted potential describes the experimental differences with a standard deviation of 0.0032 cm⁻¹ and a normalized standard deviation of 0.77. The work on the $a^3\Sigma^+$ state is still in progress.

The long-range interactions between a Na and a Rb atoms are described by combined analysis of the spectroscopically determined PEC and the most recent theoretical values of the dispersion coefficients [6, 7].

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Fourier transform absorption spectroscopy of water vapour in the visible spectral region

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This work presents measurements of the water vapour line parameters from the near ultra-violet to the near infrared ($26000\text{--}9250\text{ cm}^{-1}$ spectral region) [1-3]. The measurements were obtained by combining a high-resolution Fourier transform spectrometer with a long-path absorption cell, thus allowing the observation of very weak, previously unobserved, lines. More than 16000 lines have been studied. Their positions and intensities have been determined, and for many lines, self- and air-broadening coefficients, as well as pressure-induced shifts were obtained. A preliminary analysis of the dependence of the broadenings and shifts with vibrational and rotational quantum numbers is given. The complete list of empirical parameters is compared to the HITRAN molecular spectroscopic database [4], most frequently used in atmospheric calculations. It is shown that these empirical parameters provide an improved dataset for water vapour in the visible spectral region, especially with regard to the determination of the atmospheric water column from FT-visible solar absorption spectra [5].

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ORAL SESSION S6

Determination of Hyperfine-Induced Transition Rates from Observations of a Planetary Nebula

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We have made observations of the planetary nebula NGC3918 with the STIS instrument on the Hubble Space Telescope to reveal the first unambiguous detection of a hyperfine induced transition $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ in the beryllium-like emission line spectrum of N IV at 1487.89 Å [1]. A nebular model allows us to confirm a transition rate $4 \times 10^{-4}\ \text{sec}^{-1} \pm 33\%$ for this line. The measurement represents an independent confirmation of the transition rate of hyperfine induced lines in low ionization stages, and provides support for the techniques used to compute these transitions for the determination of very low densities and isotope shifts in other astrophysical objects.

In spite of being a $J = 0 \rightarrow J = 0$ transition, the hyperfine induced line becomes allowed through a change of the nuclear spin direction. Basically the hyperfine interaction induces a mixing of $J = 1$ states in the upper $J = 0$. A theoretical description of this requires a large-scale and careful treatment of both correlation and relativistic contributions, and their effects on fine structure, hyperfine structure and transition rates. A recent calculation [2] based on the MCHF method is supported by the present results.

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Time-resolved laser spectroscopy studies on excited state lifetimes of Sm II

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Time-resolved laser-induced fluorescence spectroscopy is a reliable method for studying the radiative lifetimes of atoms and ions. In the present work, radiative lifetime measurements were performed with this technique for 47 levels in Sm II. Free Sm II ions were produced in a laser-induced plasma, in which metastable states of atoms or ions could be populated and serve as a starting point for subsequent laser excitation. Stimulated Brillouin scattering (SBS) techniques in water were employed to produce laser pulses as short as 1 ns for the excitation of short-lived levels, and Stimulated Stokes Raman Scattering techniques were used to extend the tunable range of the exciting dye laser. Special care was taken to avoid possible systematic effects on the lifetime measurements. The experimental results have allowed to test new theoretical calculations with the relativistic Hartree-Fock method taking configuration interactions and core-polarization effects into account, and a good agreement has been found for this ion. A set of calculated oscillator strengths and transition probabilities were obtained by combining the experimental values and theoretical branching fractions. These results will be useful to evaluate abundance values of astrophysical interest for Samarium.

Multi-electron atoms and ions in a strong laser field: Multi-photon resonances and stochastic effects

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A quantum-electrodynamical (QED) density functional theory (DFT) method is used for studying the interaction of the atoms and ions in a plasma with the intense laser field in a presence of a DC electric field. Method bases on a description of atom 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 with the use of the DFT Dirac-Kohn-Sham scheme and the Gell-Mann and Low adiabatic formalism. We have studied the cases of the single, multi-mode, coherent, stochastic laser pulse shape. An account for the stochastic fluctuations in a field effect is of a great importance. Results of the calculation for the multi-photon resonance and multi-photon ionization profile in the H, Na, Cs atoms are presented. Our method is compared with other DFT approaches to atoms in strong laser pulses (c.f.[3,4]). It is also studied the phenomenon when an energy spectrum liberated in the high intensity multi-photon ionization exhibits succession of peaks separated by photon energy (above threshold ionization). Efficiency of method is demonstrated by DFT and QED perturbation theory calculations for the two-photon ionization cross-sections and photo-electron angular distribution for extended photon energy range (including above-threshold ionization) in magnesium. Comparison with the eigen-channel R-matrix calculation of Luc-Koenig et al [5] 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 ($n=40, m=2$; $E \cdot 10^8$ V/cm) and ground state, when it's possible the radiation of photons with very high energy (short-wave laser amplification). Besides approach developed is applied to calculation of probability for two-photon electron detachment from negative atomic ion of Na (process: $\text{Na}^- + n\omega \rightarrow \text{Na} + e^-, n=2$) by circularly-polarized light. An approach developed is also generalized on a case of additional account of the external DC electric field.

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ORAL SESSION S7

High-resolution spectroscopy on neutral calcium using Coulomb crystals

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We have studied the isotope-shifts and hyperfine splitting of the $4s^2\ ^1S_0 \rightarrow 4s5p\ ^1P_1$ transition in neutral calcium using a frequency doubled CW laser system tuned to the transition wavelength at $\lambda = 272\text{nm}$. The excitation of the upper state is detected by monitoring the ions produced by photoionization via the $4s5p\ ^1P_1$ state. The spectroscopic laser beam at $\lambda = 272\text{nm}$ crosses a well-collimated effusive thermal beam of calcium atoms at right angles in the center of a linear Paul trap. This geometry is chosen in order to obtain small Doppler shifts of the transition under study as well as to have a large capture efficiency of the ions produced. Since the atomic beam is derived from an oven containing natural metallic calcium, all the isotopes ^{40}Ca (96.9%), ^{42}Ca (0.647%), ^{43}Ca (0.135%), ^{44}Ca (2.086%), ^{46}Ca (0.004%) and ^{48}Ca (0.187%) are present. The detection of the produced ions is done first by trapping them in the linear Paul trap and then independent of the specific ion isotope produced, by converting almost all the trapped ions into $^{40}\text{Ca}^+$ through near-resonant electron transfer collisions with atoms in the atomic beam containing 96.9% ^{40}Ca atoms. Finally, the number of trapped ions is counted with a near-100% efficiency by monitoring the fluorescence from the $^{40}\text{Ca}^+$ ions when laser cooled into a Coulomb crystal.

From the isotope-shift data retrieved using this new method, we have derived the specific mass shift constant, $M_{SMS} = 243 \pm 3 \pm 9\text{ GHz}\cdot\text{amu}$, and the field shift constant, $F = 179 \pm 39 \pm 2\text{ MHz/fm}^2$, of the $4s^2\ ^1S_0 \rightarrow 4s5p\ ^1P_1$ transition. For the hyperfine splitting of ^{43}Ca in the $4s5p\ ^1P_1$ state a magnetic dipole coupling constant of $A = 39.8 \pm 0.8 \pm 0.4\text{ MHz}$ and the electric quadrupole constant of $B = -0.3 \pm 3 \pm 0.003\text{ MHz}$ are found. The uncertainties stated above are the statistical and the systematic respectively.

In the experiments described above near-resonant electron transfer was used as a tool for counting the number of trapped ions. Although this method conveniently simplifies the data treatment, it is not essential as long as Coulomb crystals with at least one fluorescing species can be made. From the shape and size of the fluorescing part of the crystal, the amount of ions in the remaining (non-fluorescing) part can be deduced. For this reason, we believe that the Coulomb crystal method can be extended even to atomic elements of which the ions can not be laser cooled simply by simultaneously having a laser cooled species, like $^{40}\text{Ca}^+$, present to create partly detectable Coulomb crystals.

A DFG-based spectrometer for detection and spectroscopy of atmospheric-relevant molecular species

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The need to cover the spectral region where laser sources were not available has significantly driven, in recent years, the research in nonlinear Optics.

The recent availability of engineered nonlinear media such as *periodically poled* crystals, has represented a fundamental step towards the realization of new tunable sources, based on frequency conversion phenomena. The high conversion efficiency exhibited by such media has in fact allowed the the generation of relatively high power levels, also using as primary sources low-power solid-state lasers in single pass geometry. In particular, by *Difference Frequency Generation* (DFG) it becomes possible to produce mid-IR radiation starting from near-IR laser sources. There is a relevant interest in developing tunable and narrow-band sources in the mid-IR region. Indeed, in the 3-12 μm region lie strong fundamental vibrational bands of most of the chemical species of atmospheric interest. Transitions belonging to these bands are two or more orders of magnitude stronger than transitions in *overtone* or *combination* bands which, since they fall in near-IR region, are instead accessible by traditional diode-laser systems. It is well known that in the mid-IR region are available several radiation sources (lead-salt diode lasers, OPOs) but all suffer for practical drawbacks, as necessity of cryogenic cooling or complex frequency locking systems, which limit their effective use to *laboratory applications*. In particular, in the spectral region around 3 μm it is possible to find very strong vibrational bands of several molecular species, such as H_2O , N_2O , OH , HCN and C_2H_2 , which are particularly interesting for environmental questions. For this reason, the development of DFG-based system operation in this spectral window assumes a particular importance.

In this work, we present a DFG-based spectrometer which, mixing in a periodically-poled Lithium Niobate crystal the radiation emitted by a Nd-Yag laser and an extended cavity diode laser, produces tunable, narrow-linewidth radiation around 3 μm [1], [2]. The developed system constitutes the first radiation source operating in this region with, at the same time, an high spectral purity, a large tunability range and, not last in importance for all practical applications, a considerable handiness. We characterized the performances of this system as trace-gases sensor; in particular, we show the test performed for C_2H_2 molecule, both in a pure and in an N_2 -broadened sample. In the first case we evaluated a minimum detectable pressure of only 0.4 nbar; in the second one, we obtained a minimum detectable concentration of 4 ppb (1 in 10^9 parts) at a total pressure of 350 Torr.

The very high sensitivity of this apparatus was also used for an accurate determination of the concentration of the H_2^{18}O and H_2^{17}O water molecule isotopes in a distilled water sample. The developed spectroscopic technique for the determination of isotope abundance ratio presents several important advantages over the traditional isotope-ratio mass spectrometer (IRMS) method: smaller sample sizes and direct measurements of the isotope ratios, avoiding time consuming and necessity of sample preparation. The obtained results are quite promising for the application of our spectrometer both for biomedicine applications and paleoclimatology studies.

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The peculiarities of coherent population trapping resonances for different geometries of experiment and initial conditions

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The effect of coherent population trapping (CPT) has been discovered in 1976 [1] and now is widely used in modern atomic and laser physics. This effect has found important applications in ultrahigh-resolution spectroscopy, lasing without inversion, laser cooling, in atom optics and interferometry and so on. Many references on this theme can be found in [2].

The most of publications concern the results of theoretical and experimental investigations of CPT on hyperfine levels of different atoms. We consider peculiarities of this effect on magnetic sublevels of fine structure levels, for example, for Thallium (Tl) atoms. The system of levels taken into account consists of eight levels. By considering spontaneous decay onto the levels of thermostat we have found the solutions of Schrodinger equation in resonant approximation and so we have found the populations of magnetic sublevels.

We have considered different geometries of experiment. Among them there are the cases for which the polarization vectors of both components of radiation fields are parallel to each other and parallel or perpendicular to magnetic field, polarization vectors are perpendicular to each other (one of them is parallel to magnetic field). Also the orientation of magnetic field may be parallel or perpendicular to wave vector of radiation field.

Also we have considered different initial populations of magnetic sublevels. In contrary to trivial initial populations of sublevels of the ground state of considered atom we have considered the initial population of another metastable fine structure level of Tl atom. This situation can take place for atomic photofragments produced in the photodissociation of diatomic molecules [3].

We have shown how the geometries of experiment and varying of initial conditions influence the form and number of CPT resonances.

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ORAL SESSION S8

The Structure of Small Mercury Clusters

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The simulation of mercury clusters or the bulk is a notoriously difficult problem in computational physics. First, the Hg-Hg interaction is relatively weak ($370\text{--}400\text{ cm}^{-1}$) and in the range of typical Van der Waals interactions such as Ar_2 (85 cm^{-1}), Kr_2 (127 cm^{-1}) or Xe_2 (186 cm^{-1}). While classical two-body potentials for the Group 18 atoms give lattice constants, bulk moduli, and cohesive energies close to the experimental values, a recently derived relativistic coupled cluster two-body potential for mercury in our group leads to lattice constants $a = b = 3.47(3.46)\text{ \AA}$, $c = 8.49(6.66)\text{ \AA}$ and a cohesive energy of $E_{coh} = 0.42(0.79)\text{ eV}$ for the rhombohedral lattice (experimental values are given in parenthesis). For mercury this implies a rather slow convergence of the n -body expansion of the interaction potential and therefore a slow convergence of the Van der Waals expansion. DFT methods are shown to be inadequate for an accurate description of the weakly bound mercury dimer, and so *ab initio* relativistic MP2 and CCSD(T) methods are used to obtain accurate structures of the smallest clusters. An analysis of the frequencies of vibration shows that the Lennard-Jones type structures are indeed minima on the potential surface.

Photoabsorption Spectrum of Li_3O : Experiment and Theory

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Hypermetallic or hypervalent molecules or clusters are stable species in which the octet-rule in the chemical bonding is formally violated [1]. E.g., Li_3O and Li_6C are thermodynamically stable compared to their corresponding octet-molecules Li_2O and Li_4C . We studied these molecules in our group before by measuring the ionization potentials (IP) of Li_NO and Li_NC clusters in combination with quantum chemical calculations on the structures and IP's of these species [2]. Recent experiments and calculations have shown that the ground state potential energy surface of the hypervalent Li_3O cluster is very flat [3].

Here we report the measurement of the photoabsorption spectrum of Li_3O using the technique of resonance enhanced two-photon ionization spectroscopy (RE2PI) together with a calculation of the absorption spectrum. A geometry optimization for Li_3O is performed at the CCSD(T)/6-311+G(d) level of theory, vertical excitation energies are calculated, and the flatness of the potential energy surface is analyzed.

The RE2PI experiment on Li_3O shows at least 4 broad absorption bands in the energy range between 0.7 and 2.75 eV. Ab initio calculations predict Li_3O to have a D_{3h} ground state structure. The observed RE2PI spectrum is in good agreement with vertical excitation energies obtained with the CASPT2 method. The broadness of the observed features is related to the flatness of the ground state potential energy surface. A large deformation of the cluster is allowed in its different vibrational modes at room temperature. By calculating the excitation spectra at the turning points of the different vibrational modes, the width of the absorption bands could be estimated. The calculated transitions reproduce as well the position as the width of the measured bands.

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Thermionic emission in carbon cluster anions and neutral C_{60} studied by time-resolved photoelectron imaging

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Atomic clusters are model systems to study the decay of energy-rich microscopic species where the excitation energy exceeds the threshold for the emission of an electron. If a single-photon is sufficient to induce ionization or detachment, the emission of electrons by a finite-size system maybe separated into direct processes, giving rise to characteristic structures in the photoelectron kinetic energy spectrum on one hand, and delayed processes, revealing the internal energy redistribution, on the other hand. This phenomenon of delayed ionization [1] has been observed mainly from metal [2] or carbon [3] clusters. It is described as thermionic emission when the excitation energy is equipartitioned between the nuclear and electronic degrees of freedom. On the other hand, if multiphoton excitation is required to induce ionization and if the internal energy redistribution timescales are much shorter than the laser pulse duration (general case in nanosecond excitation), only thermionic emission may be observed, at potentially very long timescales.

The first situation is illustrated by our recent results in time-resolved studies of photodetachment of small carbon cluster anions. Combination of velocity-map imaging with a gating of the position-sensitive-detector has allowed us to record photoelectron spectra during a finite time-window (typically 50 ns) at a variable delay after excitation. The spectra exhibit a clear distinction between direct and delayed electron emission. Namely, the broad structure corresponding to direct transition from the ground state of the anion to the ground state of the neutral totally disappears in the delayed spectrum. On the other hand, after a few tens of nanoseconds, only the low energy part of the spectrum remains. This low energy part corresponds to pure thermionic emission and may be described in the framework of the detailed-balance theory with an energy distribution characterized by a well-defined temperature. Spectra recorded at various cluster sizes between $n = 10$ and $n = 22$ will be presented at the conference.

Owing to its relatively high ionization potential (7.6 eV) and to its large number of degrees of freedom, many photons are required in order to induce thermionic emission in C_{60} . The internal energy distribution is thus very broad, leading to a power law for the time-evolution of electron emission. This leads also to a decrease of the effective temperature observed in the delayed electron spectrum as a function of the time-delay. Our experimental results are the first direct measurements of such dynamical processes. This phenomenon is described in the framework of the detailed-balance theory, including the competition with ejection of fragments C_2 .

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ORAL SESSION S9

Ultralong Range Potentials In Cold Collisions Involving Rydberg Atoms

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Recently cooling and trapping techniques were applied to experiments involving Rydberg atoms. Thermal Rydberg atoms have been studied in depth both theoretically and experimentally, but at low temperature the magnitude of their properties make them excellent candidates for collisions. In this work we measure the time evolution of the population resulting from energy transfer collisions as a function of the energy difference between the entrance and exit collisional channels using a sample of cold Rydberg atoms produced in a rubidium magneto-optical trap. The $34S_{1/2}$ population, produced by collisions between atoms in $33P_{1/2}$ state, is monitored as a function of time through the pulsed-field ionization technique. The experimental results are compared with a recent published model based on a two-body interaction considering an attractive potential [1]; which is calculated according a recent letter by C. Boisseau et al. [2]. The agreement is remarkable, which suggests the existence of such ultralong range potential proposed by C. Boisseau et al..

The details about our experimental setup and detection technique are described elsewhere [1]. Briefly, the cold Rb atoms are excited by a pulsed dye laser (1mJ/pulse, 4 ns, repetition rate 20 Hz, $\lambda \sim 480\text{nm}$) pumped by the third harmonic of a Nd:YAG laser, from the $5P_{3/2}$ state. The Rydberg states are detected by pulsed field ionization. By varying the delay between the optical excitation and the high voltage pulse, we are allowed to observe the time evolution of the $34S_{1/2}$ state population. This collision process is studied as a function of the energy difference between the entrance and exit collisional channel, the energy difference is tuned by applying a static electric field using the Stark effect. The time evolution of the $34S_{1/2}$ state population is dominated by spontaneous decay and by the ultralong range potential. Our model suggests that atoms separated as much as $100.000a_0$ can contribute for this collisional process. By modeling our results we can extract the potential parameters and compared them with the ones calculated by C. Boisseau et al..The agreement is remarkable, suggeting the existence of such potentials. This work has received financial support from Fapesp and CNPq - Brazilian Agencies.

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Rotational decoherence of non-polar molecules in off-resonant laser fields

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Recent advances in trapping [1,2] and photoassociating [3,4] cold molecules, progressively give access to the quantum-statistical properties and dynamics of molecular gases. The question therefore arises as to how the quantum molecular state can be manipulated by nonlinear optical interactions or how some of its properties can be revealed from optical spectra. For this purpose it is necessary to go beyond standard calculations of nonlinear optics, in order to treat not only the optical-field dynamics, but to focus on the dynamics of the molecular system.

As a first step towards such considerations we study, as a generic model for various applications, the rotational dynamics of molecules that interact with off-resonant laser fields. For dimers having no permanent dipole moment and being infrared inactive, the rotational dynamics is expected to be to large extent undamped. However, the molecular polarizability supports two-photon transitions and we show that these may in fact lead to decoherence and damping in the rotational dynamics.

For the case of non-polar molecules interacting with weak, off-resonant laser fields, we have derived the equations of motion for the reduced molecular rotational dynamics [5]. Such a description is justified for vibrationally cold molecules, for interaction times that are only limited by the vibrational heating, that may eventually lead to resonant vibronic transitions. Besides Rayleigh scattering, stimulated and spontaneous Raman scattering processes occur that coherently drive the molecular rotation and lead to quantum decoherence, respectively.

For illustration of the decoherence effects the optical Kerr effect is considered, for which the rotational equations of motion are solved by means of quantum trajectories. We show the decoherence effects by use of a Wigner function of the molecular rotation and indicate the progressive loss of purity of the rotational quantum state. Such a situation is also related to the configuration of optical dipole traps for molecules [1,2]. The rotational heating predicted by our theory may lead in such a case to finite trap times of molecules and in the case of dipole trapped molecular Bose-Einstein condensates it may pose a limit to the lifetime of the condensate.

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ORAL SESSION S10

Analysis of field isotope shifts in visible and near-UV transition lines of Sm I

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Isotope shifts of atoms have been measured and analyzed in so many studies because of their precise information about the nuclear properties of the atoms involved, leading to such applications as multi-photon ionization, ultra-high trace analysis, and so on. In particular field shift contribution of the isotope shifts is closely related to the electric charge distribution of nucleus and thought to be an important factor for testing various quantum mechanical *ab initio* calculations.

The Sm (Samarium), one of rare earth elements, has very complex energy level structure of 4f open shell and many spectral lines caused by the transitions between electronic configurations of $4f^n(5d+6s)^m6p$. Most of the isotope shifts of Sm I (neutral Samarium) in the wavelength region of 550-620 nm were measured with CW tunable dye lasers. Recently tunable CW diode lasers in IR, blue, and Near-UV wavelengths have become commercially available and are widely used for high resolution spectroscopy owing to their advantages such as narrow linewidth, wide tunability, and compactness in size. Jin *et al.*[1] measured the isotope shifts of Sm I in the transitions of 636.74 nm, 672.59 nm, and 686.09 nm by using atomic-beam diode laser spectroscopy.

Previously we have reported high resolution Doppler-free spectra of Sm I in the wavelength region of 635-690 nm measured with a single-mode diode laser in a long atomic vapor cell[2]. Later we measured the isotope shifts of Sm I in the wavelength region of 399 nm by means of Doppler-free saturation absorption spectroscopy with a Near-UV diode laser.

Here we report results of analysis of the field shift of the measured isotope shifts in the wavelength regions of 672 nm and 399 nm. The measured field shift of 672 nm transition line from $4f^66s^2\ ^7F_0$ to $4f^66s6p\ ^9F_1$ is negative whereas that of 399 nm transition line from $4f^66s^2\ ^7F_5$ to $4f^55d6s^2\ ^7F_4$ is positive. We calculated the electronic charge density at the origin of nucleus by Multi-Configuration Dirac-Fock method. The calculated change of the electronic charge density at the origin in atomic unit (a_0^{-3}) is -187 for the $6s-6p$ transition and 458 for the $4f-5d$ transition. In this calculation the charge densities of non- s electrons at the origin are not negligible because of the relativistic effect. The positive field shift for the $4f-5d$ transition can be explained by large decrease in screening of the $6s$ and inner shell electrons as a result of the $4f-5d$ transition. Hence we obtained the ratio of field shifts of the two transitions, $F_{4f-5d}/F_{6s-6p} \simeq \Delta|\psi(0)|_{4f-5d}^2/\Delta|\psi(0)|_{6s-6p}^2 = -2.4$. This value roughly matches with the experimental value of $\simeq -1.0$, and is more accurate than that of non-relativistic Hartree-Fock calculation by Wilson[3]. Wilson obtained the field shift ratio of -3.0 for $4f-5d$ transition vs $6s-6p$ transition by considering only configuration averages without LS-term dependence.

The possibility of configuration mixing between two configurations of upper levels, $4f^66s6p$ and $4f^55d6s^2$, is under investigation in an attempt to account for a discrepancy between the experiment and the *ab initio* calculation.

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Two-colour Frequency Mixing Spectroscopy of E2/M1 amplitude ratio in Atoms

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A three-wave resonance frequency mixing process is considered in a gas of free atoms in their ground state $|0\rangle$ in a field of two incident waves, which stimulate generation of a third wave. In view of applications to *In* and *Tl* atoms, we assume the *E2-M1* transition $|0\rangle \leftrightarrow |1\rangle$ to be in resonance with the wave of frequency $\omega_1 = E_1 - E_0 - \varepsilon$. The *E1* transitions $|0\rangle \leftrightarrow |2\rangle$ and $|1\rangle \leftrightarrow |2\rangle$ are in resonance with the waves of frequency $\omega' = E_2 - E_0 - \varepsilon'$ and $\omega_2 = \omega' - \omega_1$, where the resonance detuning $|\varepsilon| \ll \omega_1$ and $|\varepsilon'| \ll \omega'$.

The amplitude of scattering the (i) difference- or (ii) sum-frequency photons look identical to one another, and may be written as resolutions in irreducible tensor products $\mathbf{T}_p$ of polarization and wave vectors $\mathbf{e}, \mathbf{n}$:

$$U = \frac{A}{2\varepsilon\varepsilon'} \sum_{p\lambda} C_{J_0 M_0 p \lambda}^{J_0 M'_0} \sqrt{2p+1} \mathbf{T}_p, \quad (1)$$

where $A = \alpha F_1 F_2 F' \langle 1|r|2\rangle \langle 2|r|0\rangle / 8$ is the field-amplitude-dependent factor, including also the radial part of the dipole transition matrix elements. The Clebsh-Gordan coefficient $C_{J_0 M_0 p \lambda}^{J_0 M'_0}$ determines the dependence of amplitude on orientation of the total momentum $\mathbf{J}$ (on the magnetic quantum number M_0). In coherent scattering, $M_0 = M'_0$, after averaging over polarization states of atoms (over M_0), the amplitude is

$$U_{coh} = \frac{A}{2\varepsilon\varepsilon'} \mathbf{T}_0 = \frac{Ai}{54\varepsilon\varepsilon'} \left\{ (1+Q)(\mathbf{n}_1 \cdot \mathbf{e}_2)(\mathbf{e}'^* \cdot \mathbf{e}_1) - (1-Q)(\mathbf{e}_1 \cdot \mathbf{e}_2)(\mathbf{e}'^* \cdot \mathbf{n}_1) \right\}. \quad (2)$$

The quantity $Q = 3\omega_1 \langle 0|r^2|1\rangle / 5$ determines the ratio of *E2* and *M1* amplitudes.

For $J_0 = 0$ only coherent scattering is possible as the amplitude (1) reduces to (2), vanishing for collinear waves $\mathbf{n}_1 = \mathbf{n}_2 = \mathbf{n}'$. In contrast, for atoms in states with $J_0 \neq 0$ the amplitude (1) includes terms with $p \neq 0$ which describe forward scattering of sum- or difference-frequency photons. The corresponding cross section is

$$d\sigma|_{\mathbf{n}_1=\mathbf{n}_2=\mathbf{n}'} \sim \sum_{M_0 M'_0} \frac{|U|^2}{2J_0+1} = \left| \frac{A}{2\varepsilon\varepsilon'} \right|^2 \sum_{p=1}^{2J_0} (\mathbf{T}_p \cdot \mathbf{T}_p^*). \quad (3)$$

For $J_0 = 1/2$ this quantity includes only one term with $p = 1$, where the vector

$$\begin{aligned} \mathbf{T}_1 = & \frac{1}{54} \left\{ (1+Q) \left[(\mathbf{e}'^* \cdot [\mathbf{e}_2 \times \mathbf{n}_1]) \mathbf{e}_1 - (\mathbf{e}'^* \cdot \mathbf{e}_2) [\mathbf{e}_1 \times \mathbf{n}_1] \right] \right. \\ & \left. - (3-Q) \left[(\mathbf{e}'^* \cdot [\mathbf{e}_1 \times \mathbf{n}_1]) \mathbf{e}_2 - (\mathbf{e}'^* \cdot \mathbf{e}_1) [\mathbf{e}_2 \times \mathbf{n}_1] \right] \right\} \end{aligned} \quad (4)$$

determines the amplitude of incoherent collinear scattering of the sum-frequency photons. $\mathbf{T}_1$ also depends on Q , providing possibility of measuring the quadrupole matrix element in frequency-mixing experiments. In one-electron model potential approximation we obtained $Q = 0.352$ for *Tl*, $Q = 0.100$ for *In* atoms, well consistent with recent experimental data [1].

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ORAL SESSION S11

Interactions of Short Laser Pulses with Atoms: Resonance and Interference Effects

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The dynamics of the ionization of atoms submitted to intense electromagnetic fields is a subject of wide interest and active research. Several important effects including enhancement of the ionization rate are partly explained by the rescattering process (multiphoton inverse Bremsstahlung) [1,2]. Different modifications of rescattering mechanisms were considered with the help of the semiclassical approach [3] and the DWA method [4].

Here the theory of ionization and excitation of atoms by the short laser pulses is developed on the basis of the close-coupling approach for solving the time-dependent Schroedinger equation [5,6]. Studies of the interactions of atoms with intense electromagnetic fields require the use all the continuous states of the system, without discretization of the continuum. The infinite set of integro-differential equations is solved using the analytic properties of the kernels [7,8]. The systematic investigations have been done in the case of femtosecond laser pulses with linear and circular polarization, for the different values of the laser frequency, intensity and duration times. Interactions of the intermediate discrete states with the continuum (bound-free transitions) are found to be very important for structures of the energy spectra of the ejected electrons. It is shown that these bound-free transitions give the larger contributions than the rescattering process (free-free transitions) at the medium energies of the ejected electrons. The resonance and interference structures in populations of the discrete and continuum atomic states are displayed as functions of the laser pulse parameters.

It is shown that there exist the laser pulse parameters at which the metastable 2s-state in the hydrogen-like atom is populated much more than other excited states. This effect gives a tool for creating the metastable beams in the laser-atom experiments.

Ionization and excitation from the 2s-state were also considered.

The support from the INTAS (N 99-1326) and RFBR (N 02-16274) is acknowledged.

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A study of electron-negative ion interactions in a storage ring

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We will present results from experimental studies of negative ions using the heavy ion storage ring CRYRING at the Manne Siegbahn Laboratory in Stockholm.

Reliable measurements of cross sections for electron impact detachment from negative ions have been very limited until rather recently. This is especially true in the case of multiple detachment processes. The advent of magnetic ion storage rings has changed this situation dramatically. It is now possible to investigate electron impact detachment from atomic or molecular negative ions over a wide range of collision energies using a merged beam technique. This method has decided advantages over crossed beam geometries in that it allows the electron and ion beams to interact over a long beam path and it permits one to access the threshold region with ease. A number of studies using the storage ring technology have been performed by Andersen and collaborators[1,2].

At CRYRING negative ions are produced in a cesium sputter source. The resulting ion beam was injected into the ring where it was accelerated to an energy in the MeV range. A beam of electrons produced in an electron gun was merged with the ion beam over a path of about 85 cm. The electrons served to both reduce the momentum spread of the ions by phase space cooling and to act as collision partners in the study of detachment processes. A wide range of collisions energy was available by merely changing the energy of the electrons. The products of the detachment collisions (neutral and positive fragments) were monitored by the use of moveable surface barrier detectors

The presentation will include the results of a recent investigation of electron-impact detachment from the H^- ion over an energy range 0-400 eV. In the experiment we measured the absolute cross sections for both single and double detachment under identical conditions. The single detachment cross section has been most recently measured by Andersen et al [2] over an energy range 0-20 eV. The most recent measurement of the double detachment cross section was that of Peart *et al* [3]. The present measurement allows us to accurately determine the ratio of the single-to-double cross sections over a wide energy range that includes the region near the double detachment threshold. This region was difficult to access in a previous measurement [3] that involved a crossed beam geometry.

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Differential Cross Sections for Radiative Collisions



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The absorption differential cross sections (DCS) $d\sigma(E, \omega, \vec{e}, \Omega)/d\Omega$ for the collisions between *He* and *Ne* atoms in a weak laser field with a frequency ω detuned from the frequency ω_0 of forbidden atomic transition $He(1^1S - 2^1S)$ and with a polarization $\vec{e}$ have been theoretically investigated at the thermal collision energy $E = 220\text{cm}^{-1}$.

This process is due to the mixture of $1s2s$ and $1s2p$ configurations of *He* atoms owing to interatomic interaction (see, e.g., [1]). It can be described in terms of the dipole interaction between two quasimolecular states of 0^+ symmetry correlated with the ground 1^1S and metastable 2^1S atomic states.

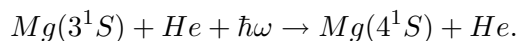
This work represents, as far as we know, the first detailed analysis of the dependences of DCS on parameters $\omega, \vec{e}, \Omega$ for the radiative collisions, associated with the forbidden atomic transitions. The main theoretical distinction of such processes from the optical collisions consists in strong (usually exponential) dependence of the transition dipole moment $d(R)$ on internuclear distance. It can result in essential disagreement with well-known Franck-Condon approximation (see [2]).

We developed the uniform quasiclassical method (see [2,3]) and applied it to calculation of DCS. This method had been used earlier for investigation of the collisionally induced spectral profiles of the forbidden atomic lines [2]. It gives the results which are very close to the exact quantum mechanical calculations. On the other hand, this method makes it possible to give a simple semiclassical interpretation of the results obtained.

The scheme of our calculations is following: starting from the previously evaluated repulsive potential energy curves and transition dipole moment [1] we calculated the S matrix elements $S_{l \rightarrow l+1}$ and $S_{l \rightarrow l-1}$ in the framework of distorted waves approximation. The uniform quasiclassical approach [2,3] based on the uniform Langer's approximation for the radial quasimolecular wave functions was used to calculate the overlapping integrals. Further, the scattering amplitudes were obtained by exact quantum summation over the Legendre polynomials.

The DCS have been calculated both for the range of positive detunings $\Delta\omega$, when the Franck-Condon approximation is admissible for the qualitative analysis, and for the negative detunings, when the Franck-Condon approximation becomes inapplicable. The results obtained demonstrate oscillatory structure, which for the positive detunings can be interpreted as a Stueckelberg interference. This structure strongly depends on the polarization of light.

Additionally, the preliminary results have been obtained for DCS of the collisions



Financial support from the Russian Ministry of Education under grant PD02-1.2-377 is gratefully acknowledged.

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ORAL SESSION S12

Light Shift in Optical Frequency Standards

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Alkaline-earth atoms are widely used in a number of important applications including atomic clocks, laser cooling of atoms at temperatures close to the recoil limit, low-temperature Bose-Einstein condensation experiments, etc. This paper is motivated by emerging experiments on cooling and trapping of alkaline-earth atoms, in particular, on sideband cooling and spectroscopy neutral atoms in the Lamb-Dicke confinement [1].

In the present paper we estimate the light shift on the optical clock on $^3P_0 - ^1S_0$ transition in Sr in the framework of the measurements with atomic trap [1]. In the presence of the dipole-trapping laser field the observed transition frequency is written as

$$\nu = \nu^{(0)} - \frac{1}{4}\Delta\alpha(\omega_t, \mathbf{e})F^2 - \frac{1}{64}\Delta\gamma(\omega_t, \mathbf{e})F^4 - \dots, \quad (1)$$

where $\nu^{(0)}$ is the transition energy for the unperturbed atomic states, α and γ are ac polarizability and ac hyperpolarizability, respectively. Evidently, that the level of the experimental accuracy can be increased significantly by using any specific trapping laser frequency and the type of polarization vector which can enable an exact cancellation of the second-order terms (ac polarizabilities of the upper and lower levels [1]).

The goal of this paper is a theoretical analysis of the field-induced terms up to the order of F^4 as the function of the laser frequency and polarization. After the time averaging and angular integration, applying angular momentum theory, the ac susceptibilities may be resolved into irreducible parts. Accurate calculations of the matrix elements for the components of the susceptibilities are based on the use multiconfiguration Dirac-Fock (GRASP code [2]) program. The key point is that it is consistent to use precise wave functions for the evaluation of dipole matrix elements, together with the experimental value of transition energy.

For a comparison purpose, the components of the polarizability and hyperpolarizability tensor for the upper and lower levels calculated in the single-electron model potential approximation will be presented and corresponding estimates for the zero-shift frequency ω_t will also be given.

As a result, the crossing point for the both $5s5p\ ^3P_0$ and $5s^2\ ^1S_0$ states is realized at the laser wavelength of about 790 nm with linear polarization and intensity $100mW/\pi(17\mu m)^2$. In order to evaluate this point, we note that the fourth-order Stark contribution is not large enough ($\leq 10^{-3}Hz$) for the trapping laser with this intensity.

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One dimensional evaporative cooling in a hybrid magnetic and optical trap.

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Bose-Einstein condensation (BEC) in a atomic cesium gas prepared in a “low field seeker” Zeeman sublevel and confined in a magnetic trap has been thwarted by a high cross section of inelastic spin-flip collisions. We will discuss a hybrid magnetic and optical trap that overcomes this problem by trapping the atoms in the true hyperfine ground state, the “high field seeker” Zeeman sublevel, $F = m_F = 3$. Although this trap allows only one dimensional (1D) evaporative cooling, we show that achieving BEC conditions with such a trap should be possible. We present simulations of 1D evaporative cooling, which shows that the BEC transition could be reached within 5-7 seconds.

Superfluid – Mott insulator phase transition in two-component Bose-Einstein condensate in an optical lattice with the Raman scheme of the atomic transition

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We have theoretically investigated the superfluid – Mott insulator phase transition in a two-component Bose-Einstein condensate of neutral atoms, possessing an excited electronic state and two Zeeman-degenerate internal ground states characterized by the magnetic quantum number $m = \pm 1$, in an optical lattice. The optical lattice is created by two counterpropagating linear polarized laser beams with the angle ϕ between the polarization vectors (lin-angle-lin configuration), which are detuned by an amount Δ from the internal atomic transition. The phase diagram of the system has been obtained and the critical values of the parameters have been worked out.

We have shown that in the case of blue detuning ($\Delta > 0$) there exists only the superfluid phase and the Mott phase can not be reached for any values of the laser light intensity and ϕ . In the case of red detuning ($\Delta < 0$) the Mott phase can be obtained, besides the critical laser intensity is a strongly increasing function of ϕ . As ϕ tends to $\pi/2$ the critical intensity goes to infinity, which makes the observation of the Mott phase in this case practically impossible. This property of the critical laser intensity provides a useful tool of switching between Mott and superfluid phases just varying the angle between the polarization vectors of the laser beams.

ORAL SESSION S13

Coherent backscattering of light in a narrow resonance atomic system of alkali atoms

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Light interaction with ultracold atomic ensemble confined to magneto-optical trap and isolated from environment is an example of the physical problem, which can be profoundly studied both experimentally and theoretically. Moreover it has a good potential and perspectives in extending the quantum properties of matter, normally associated with microscopic systems, on the macroscopic objects. This can be illustrated by example of coherent back scattering phenomenon, which is a convenient indicator of difference in classical and quantum description of light scattering in a dense atomic medium. It makes the problem more challenging that in such an isolated sample of matter all the internal relaxation processes are deeply suppressed and it becomes possible to organize the non-classical states of matter, such as coherent states, squeezed or entangled states, in the spin subsystem of atomic sample. Considered together with general interest to light localization problem, existing in AMO community, the above arguments motivate growing interest to the studies of coherent back scattering phenomenon.

In our presentation we are going to report a combined theoretical and experimental study of the spectral and polarization dependence of near resonant radiation coherently backscattered from an ultracold gas of ⁸⁵Rb atoms. Measurements in a $\pm 6\text{MHz}$ range about the $5s^2S_{1/2} \rightarrow 5p^2P_{3/2}$ $F = 3 \rightarrow F' = 4$ hyperfine transition are compared with simulations based on a realistic model of the atomic density distribution. In the simulations, the influence of finite spectral bandwidth, magnetization of the vapor, heating of the atoms in the vapor, and other nonresonant hyperfine transitions are considered. Good agreement is found between the simulations and measurements. Our theoretical approach was based on complete quantum description of light-matter interaction and in our numerical simulation we follow to Monte-Carlo method. We tried to self-consistently describe the experimental conditions and to consider density distribution and polarization state of atoms and temperature conditions closely to how they were modified in our experiment. The radiation field frequency was selected to be in the vicinity of the $F = 3 \rightarrow F' = 4$ hyperfine transition, and to have polarization states and a weak-field intensity corresponding to the experimental realization. The effects of sample size, and the spatial and polarization dependence of the coherent backscattering cone were considered in detail. Some aspects of the spectral variation of the coherent backscattering enhancement factor were also considered, including the surprisingly-strong influence of the far-off-resonance $F = 3 \rightarrow F' = 3$ and $F = 3 \rightarrow F' = 2$ hyperfine transitions.

Benchmarking of x-ray spectra of He-like argon and titanium on tokamak plasmas

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X-ray spectroscopy of He-like ions is a powerful tool to determine basic plasma parameters such as ion temperature and plasma motion, electron temperature and plasma composition. It has been used from the beginning of high temperature plasma physics and is now being applied in all major fusion experiments. X-ray spectroscopy has also been used successfully for the investigation of solar flares, and x-ray telescopes measure x-ray emission from astrophysical objects with low resolution. The next generation of x-ray satellite experiments will provide sufficient spectral resolution to obtain high quality spectra from faint x-ray objects.

An accurate determination of plasma parameters from the analysis of experimental spectra requires a precise theoretical description of the He-like spectra, which in turn has to be benchmarked on well diagnosed plasmas. In this work, we compare theoretical descriptions of He-like spectra of intermediate- z ions (Ar, Ti) based on new atomic calculations with experiments on thermonuclear plasmas. Different theoretical approaches have been used and both internal consistency of the spectra, as well as the coincidence with the other diagnostics has been confirmed.

$K\alpha$ spectra from He-like ions of intermediate- z elements consist of transitions in the He-like system, as well as satellite lines from doubly excited Li-like ions. The He-like spectrum is composed of the resonance line in the singlet system as well as inter-combination and forbidden transitions between the triplet and the singlet system. The doubly excited Li-like satellite lines are either populated by dielectronic recombination of He-like ions or by collisional inner-shell excitation of Li-like ions.

Both the intensity ratios between the triplet and singlet lines, as well as doubly excited Li-like satellites populated by dielectronic recombination depend on the electron temperature, while the satellites populated by collisional excitation provide information on the charge state distribution. Therefore, a full modelling of the experimental spectra is a sensitive check to the internal consistencies of theoretical data. The spectra of He-like argon and titanium have been measured on the tokamak experiments TEXTOR and TORE SUPRA. If available, the wavelengths of the different lines have been checked with the results from EBIT measurements. Best fit between experimental data and theoretical modeling has been obtained on the basis of wavelengths calculated by the MZ code and excitation and auto ionization rates based on the ADAS package (R-Matrix and AUTOSTRUCTURE). Cascades from higher levels both in the He-like system and the Li-like system as well as charge exchange recombination from H-like ions have been taken into account.

Deviations of experimental spectra from theoretical predictions are below 5 %, except for the inter-combination line, where up to 10 % are found, both for argon and titanium. The plasma parameters are obtained with accuracies better than 10 % and promise reliable data even for astrophysical objects, where the spectra are the only source of information.

Modeling the Plasma Chemistry using UV/Vis- and Mass-Spectrometry Data

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Goal of the project is a solvent free painting shop. The environmental technologies laboratory is developing processes of plasma etching and polymerization. Polymerized thin films are first order corrosion protection and primer for painting.

Using pure acetylene we get very nice thin films which were not bonded very well. But using air as bulk gas it is possible to polymerize in an acetylene plasma well bonded thin films which are stable first order corrosion protections and well primers.

Nitrogen is necessary to generate well bonded thin films. UV/Vis spectroscopy shows nitrogen oxide radicals in emission spectra of pure nitrogen and air. But nitrogen oxide is fully suppressed in presence of acetylene. IR spectroscopy shows only C=O, CH₂ and CH₃ groups but no nitrogen species.

With the aid of UV/Vis spectra and the chemistry of ozone formation it is possible to define reactive traps and steps, molecule depletion and processes of proton scavenging and proton loss. Using a numerical model it is possible to evaluate these processes and to calculate theoretical mass spectra. The adjustment of theoretical mass spectra to real measurements leads to specific channels of polymerization which are driven by a couple of radicals especially the acetyl radical.

The estimated theoretical mass spectra show these specific channels of chemical processes. It is possible to quantify these channels. This quantification represents the mass flow through this chemical system. With respect to these chemical processes it is possible to have an idea of pollutant production processes. The results are presented in several talks and papers. [1...3].

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ORAL SESSION S14

Spectroscopy of a single atom placed near nanobodies

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The influence of nanobodies of different shapes (sphere, cylinder, cone, spheroid) and made of different materials (dielectric, metal, 'left-handed') on decay rate of an atom is considered. The results of calculations performed within the framework of quantum and classical electrodynamics are presented both in analytic and graphical forms and can be readily used for planning experiments and analysis of experimental data. The results obtained show that one can use nanobodies to control effectively the decay rate of spontaneous emission. For example, the decay rate of an excited atom with dipole orientation, which is normal to surface of nanospheroid or nanocylinder, can be enhanced by factor 10 - 100 in comparison with free space rate. More substantial enhancement of decay rate occurs for special (negative) values of permittivity. It corresponds to excitation of surface plasmons inside nanobody. On the other hand, the decay of an excited atom whose transition dipole moment is directed tangentially to the nanobody surface substantially slows down. The probability of nonradiative decay of the excited state is shown to increase substantially in the presence of nanobodies possessing losses.

The results obtained allow us to simulate the observation of an individual molecule with the aid of an apertureless scanning microscope with a needle tip modeled by a prolate nanospheroid wherein plasmon resonances can be excited. We consider that the process of excitation of the object molecule and the process of emission of light by it are separated both in time and frequency. It means that the molecule excitation process is off resonance with the nanoscope needle, whereas the emission band of the molecule falls within the resonance region of the microscope needle. With this formulation, the problem is reduced to the determination of the rate of the radiative loss suffered by the preexcited molecule in the presence of the nanotip possessing resonance properties due to the plasmons excited therein. Our results show that it is possible to achieve space resolution about 2-3 nm. More over it is possible to determine the orientation of dipole through dip in scan image.

Single and double ionization of Mg in the vicinity of the doubly excited $3p^2\ ^1S_0$ state

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Single and double ionization of Mg was observed experimentally in the spectral range 595 - 583 nm where the doubly excited autoionizing $3p^2\ ^1S_0$ state may be excited from the ground state via four-photon absorption. Excitation and ionization of a Mg atomic beam was achieved by a Nd-YAG pumped dye laser delivering 5 ns pulses, with a maximum power density $\sim 3 \times 10^{11}$ W/cm² under our focusing conditions. The ions produced were recorded by a time-of-flight (TOF) mass spectrometer. All three $^{24,25,26}\text{Mg}^{q+}$ ($q=1,2$) isotopes were clearly observed.

By recording the ionic signals as a function of laser pulse energy, for a number of specific wavelengths within the spectral range under study, the orders of nonlinearity K_{1+} and K_{2+} for Mg^{1+} and Mg^{2+} respectively, were determined. K_{1+} is always found very close to 4 (as expected for a four-photon ionization process) while K_{2+} ranges between 4.5 and 5.5. For the maximum available laser intensities, saturation is clearly evident for Mg^{1+} but barely evident for Mg^{2+} . Moreover, the Mg^{2+} signal appears at the onset of Mg^{1+} signal saturation. This fact strongly suggests that doubly charged ions are formed sequentially.

The Mg^{1+} spectrum consists of a single broad resonance attributed to the doubly excited autoionizing $3p^2\ ^1S_0$ state. As observed in previous experiments using psec pulses [1], the resonance is found considerably down-AC-Stark-shifted with respect to its undisturbed energy position. This shift is due to the strong one-photon coupling between the $3p^2\ ^1S_0$ state and the higher lying $3p3d\ ^1P_1$ level. Our Mg^{1+} spectra exhibit two broad features around 592 nm and 587 nm, respectively. The former lies close to the position of the shifted $3p^2\ ^1S_0$ resonance. The latter feature is tentatively attributed to the four-photon resonant, six-photon ionization of the $3p_{1/2,3/2}\ \text{Mg}^{1+}$ excited states via the $5f_j$ ionic levels. This scenario requires the presence of considerable population in the $3p_{1/2,3/2}\ \text{Mg}^{1+}$ levels, which in turn implies the absorption of two additional photons above the $3s\ \text{Mg}^{1+}$ threshold, in excess of the minimum number of four required to ionize ground state Mg atoms. Such an above threshold absorption process is in accordance with previous results, which however have been obtained with psec pulses and intensities higher by more than an order of magnitude[1]. On the other hand, the only earlier experiment in Mg in which above threshold absorption has been observed with pulses of duration and intensity comparable to ours, was performed at a different and fixed wavelength (532 nm) [2].

In order to verify the production of Mg^{1+} ions in the $3p_{1/2,3/2}$ levels, a complementary experiment based on fluorescence detection was performed in a heat-pipe cell. The only lines detected within the range 200-350 nm, were those corresponding to the $3p_{3/2} \rightarrow 3s_{1/2}$ and $3p_{1/2} \rightarrow 3s_{1/2}\ \text{Mg}^{1+}$ transitions. Moreover, the total fluorescence signal was found to peak roughly around the shifted position of the $3p^2\ ^1S_0$ resonance.

The preliminary results of a density matrix calculation employing ab-initio atomic parameters are in fair agreement with the experimental data.

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Exploring electron-electron correlation with attosecond pulses

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We study two-photon double ionisation of helium in its ground state at sufficiently low laser intensities so that three and more photon absorptions are negligible. In the regime where sequential ionization dominates, the two-photon double ionisation energy spectrum exhibits a well defined double peak structure directly related to the electron-electron correlation in the ground state. We demonstrate that when helium is exposed to subfemtosecond or attosecond pulses, both peaks move and their displacement is a signature of the time needed by the He^+ orbital to relax after the ejection of the first electron. The displacement of the peaks is strongly enhanced when the pulse is chirped. These results rest on the numerical solution of the corresponding time-dependent Schrödinger equation.

POSTER SESSION P1

Fine and Hyperfine-Structure Calculations of Even Configurations in ScI

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The parametric analysis of the fine structure has been performed for five even configurations $3d^3$, $3d4s5s$, $3d5s^2$, $3d4s4d$ and $3d^25s$. The $3d5s^2$ configuration has any experimental energy value. Our parametric study has been made in multi-configurational fits following the Slater-integral approach using the programme code of Cowan [1] in SL-coupling scheme. The results of the parametric analysis of the fine structure and g values of even configurations for $3d^3$, $3d4s5s$, $3d4s4d$, $3d^25s$ will be presented.

Besides the usual fine structure parameters, i.e. average energies of the configuration E_{av} , direct Coulomb interaction parameters F^k , indirect Coulomb interaction parameters G^k , spin-orbit interaction parameters ζ^k , configuration interaction parameters R^k and effective Coulomb interaction parameters, i.e. α , β had to be included to fit the experimental energies with satisfactory accuracy. Fits with different conditions, i.e. choice of the parameters and the coupling ratios will be compared.

The best fitted energy values of the least squares fit will be listed in table together with the experimental values, leading eigenvector components and percentage distributions over the configurations. The comparison between experimental and calculated energies shows good agreement. In order to emphasize the good fit, the experimental g factors are compared with the calculated factors.

We have also investigated the hyperfine structure of even configuration $3d^24s$ after the analysis of the fine structure. The magnetic dipole hyperfine structure constants A of $3d^24s$ configuration will be presented and compared with the values found in the literature [2], [3], [4]. Our calculations are based on our new measurements as well as all other available experimental hyperfine data. Taking into account all this information, we will be able to give predictions of the value of the magnetic dipole hyperfine structure constants A for all levels of the $3d^24s$ configuration. The number of experimental B values are much smaller than the number of experimental A values, because in some references no B constants are given.

The angular coefficients of these parameters $\alpha^{k_s k_l n_l}$ have been calculated on the basis of the wave functions from our fine structure calculations using the CHFS programme [5]. The experimental and the best fitted A values as well as their differences will be listed in table.

Our experimental study is presented in the other poster.

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New relativistic approach to calculation of the autoionization resonances for heavy atoms in a presence of electric field

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We propose a new approach to construction of the optimal schemes of the laser photoionization method for further applying to problem of the isotopes and nuclear isomers separation. The most effective scheme is based on a selective resonance excitation of atoms by laser radiation into states near ionization boundary and further autoionization decay of excited states under action of external electric field [1-3]. In this situation there are needed the correct data about the Stark and autoionization resonances for different atoms, especially, for atoms and ions of heavy elements. In our paper a new relativistic approach to calculation of the Stark resonances energies and widths in heavy atoms is developed. It is based on the finite-differences solution of the Dirac equation and model potential formalism. There are presented the numerical data for the Stark resonances widths and shifts in the H, Na, U atoms. We also develop a new consistent relativistic method for numerical calculation of the atomic autoionization under the external electric field action. We have carried out calculation of the autoionization resonances widths and shifts for atoms of Tm and U in the external electric field. We have discovered and analyzed the unusual features of their behaviour in a field, in particular, an effect of a drastic broadening of the autoionization resonances widths in a quite weak external field. We considered two main channels for the autoionization resonances decay. One is the traditional Beutler-Fano channel (BFD). Another one is a new Letokhov-Ivanov re-orientational decay (ROD). The availability of two pairs of near-lying ionization limits (with vacancy states $4f(7/2)$ and $4f(5/2)$ in the Tm atom provides the indicated types of autoionization resonances decay [1-3]. Any two states of different parity can be mixed by the external electric field. The mixing leads to redistribution of the autoionization widths. In the case of degenerate or near-degenerate resonances this effect becomes observable even at a moderately weak field. As example, we consider the $f(7/2)6s(3)25s[5/2]$ state, decaying due to the quadruple interaction and $f(7/2)6s(3)25p1/2[5/2]$ undergoing to the monopole ROD. We carried out the detailed calculation of the energies E , autoionization widths G of the $4f(7/2)6s(3)ns,np$ Tm states ($n=20-35$) for different values of the electric field strength e . Let us give some data (e in V/cm; E and G in cm^{-1}). For state $4f(7/2)6s(1/2)[3]25s[5/2]$: $e=0$, $E=49854.7$, $G=1.861(-05)$; $e=50$, $G=1.847(-4)$; $e=150$, $G=1.330(-3)$. For state $4f(7/2)6s(1/2)[3]25p(1/2)[5/2]$: $e=0$, $E=49865.3$, $G=1.196(-1)$; $e=50$, $G=1.194(-1)$; $e=150$, $G=1.182(-1)$. One can see a strong change of the autoionization resonances width occurs at a moderately weak electric field and this effect is found more strong, than it was predicted earlier within non-relativistic calculation [2]. Detailed spectroscopic information about Stark and autoionization resonances is needed to optimize the selective atomic photoionization schemes for further application to problem of the isotopes and nuclear isomers separation [1].

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A systematic method for investigating Rydberg series

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A systematic method for calculations of Rydberg series has been developed and tested for ^1G , ^3G , ^1H , ^3H , ^1I , ^3I , ^1K , ^3K , ^1L and ^3L series in Cl VI. States for n up to 9 has been studied with this Multi Configuration Hartree-Fock (MCHF) method. From these calculations a theoretical spectrum for the allowed transitions has been constructed. Parts of this has been compared with theoretical spectra produced from Hartree-Fock calculations and it has been studied how the correlated calculations, where perturbers are of greatest significance, change the spectrum. Very good agreement has been found with an experimental beam-foil spectrum.

MCHF and HF calculations have also been done for ^1G , ^3G , ^1H and ^3H Rydberg series in Ar VII and S V for states with n up to 9. Theoretical spectra have been produced and we have compared the MCHF spectra with the HF spectra. By comparing how the spectra changes due to the perturbers along the isoelectronic sequence we show that in many cases it is not possible to interpolate the structure of an ion by isoelectronic comparison.

Reciprocal form factors and atomic shell structure

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The reciprocal form factor $B(\mathbf{r})$, i.e. the Fourier transform of the momentum density $\gamma(\mathbf{p})$, is studied for atoms with nuclear charge $Z = 1 - 92$. In doing so, atomic wavefunctions based on different sets of Slater-type orbitals are employed. The main results are summarized below:

- Attending to the number of local extrema of $B(r)$, the neutral atoms with $Z = 1 - 92$ are classified into three groups: (I) monotonic decrease from the origin for $Z = 1 - 4, 11 - 12, 19 - 30, 37 - 41, 55 - 77, 87 - 92$ (52 atoms), (II) a negative minimum for $Z = 5 - 10, 13 - 18, 31 - 36, 49 - 54, 81 - 86$ (30 atoms), and (III) a pair minimum-maximum for the other 10 atoms, the minimum being negative for $Z = 46, 78$ and positive for $Z = 42 - 45, 47 - 48, 79 - 80$.
- The quantum number l of the outermost electron determines the structural character of $B(r)$ as follows:
 - s and f shells ($l = 0, 3$) always belong to type I.
 - Exact correspondence among p shells ($l = 1$) and type II $B(r)$.
 - d shells ($l = 2$) concern one of types I or III. The whole shell $3d$ as well as shells $4d$ and $5d$ for low occupation number display type I functions.
 - A negative minimum for shells $4d$ and $5d$ of type III (i.e. with high occupation number) appears in the case of the anomalous shell filling $(n+1)s^0nd^{10}$.
- The location of the minimum shows up a linear dependence on $1/Z$ within each subshell.
- The connection between the present classification of $B(r)$ and the well-known similar one for the momentum density $\gamma(p)$ is also analyzed.
- Extensions of the present study to other systems concern:
 - Anions and cations.
 - Comparison with excited states of one-electron atoms.
 - Arbitrary dimensionality (e.g. D -dimensional hydrogen atom).

High resolution spectroscopy of Mn I, V I and V II and transition probabilities for Mn I.

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Spectra taken with the Goddard High Resolution Spectrograph (GHRS) and now STIS (Space Telescope Imaging Spectrograph) on the Hubble Space Telescope have, in some cases, revealed how limited our present knowledge of laboratory atomic spectra is, see Leckrone et al. [1]. The need for an improvement in the accuracy and range of the laboratory data is quite apparent and has been called for in the literature, including Grevesse & Sauval [2]. Fourier Transform Spectroscopy (FTS) is ideal for making large-scale improvements to the atomic data due to its combination of high resolution and large free spectral range.

The previous research carried out on the neutral spectrum of manganese falls into two groups: Line measurements, which are extensive but often of poor accuracy, and high resolution, but small spectral region measurements of hyperfine structure (hfs). The most recent compilation of fine structure for Mn I levels was that of Sugar & Corliss [3] in 1985. This compilation takes much of its data from work carried out in the 1940's and 1950's and pre-dates the development of high resolution Vacuum UV FTS. There have been no broad spectral studies on Mn I since this date. The accuracy of the current wavelength data is approximately 1pm whereas wavelengths are now needed to an accuracy of 1 part in 10^7 or 0.0002 Å at 2000 Å for state-of-the-art high resolution astronomical studies.

We report on the measurements of the spectrum of manganese. The work was carried out at Imperial College, with further measurements taken in the IR at NIST². The effective spectral range of the measurements now extends from 55000 Å to 1400 Å, at a wavelength resolution of at least 1 part in 10^7 , with all lines resolved to their Doppler width. The accurate wavelengths have been used to improve the accuracy of the known energy levels by at least an order of magnitude and new levels predicted from theory have been found for the first time. The hyperfine splitting factors have been found for 42 levels in Mn I. We are continuing this analysis of the hfs splitting factors for Mn I levels with the aim of finding hfs splitting constants for the majority of the known levels of Mn I. Intensity calibration of our spectra has led to accurate relative line intensities and new branching ratios have been calculated. Furthermore, lifetime measurements on 12 levels in Mn I have been made at the Lund Laser Centre³; $3d^5(^6S)4s4p(^1P) y^6P_{7/2, 5/2, 3/2}$, $3d^54s(^7S)5p w^6P_{7/2, 5/2, 3/2}$, $3d^6(^5D)4p z^6D_{7/2, 5/2, 3/2}$ and $3d^6(^5D)4p x^6P_{7/2, 5/2, 3/2}$. The lifetime measurements have been combined with branching ratios to give new oscillator strengths for transitions in the UV, visible and IR.

We are currently carrying out term analysis for V I and V II using high resolution FT spectra recorded with the IC FT spectrometer in the visible-UV and the Kitt Peak FT spectrometer in the IR. The accuracy of the V I and V II line wavenumbers has improved by at least an order of magnitude. These wavenumbers have been used to rework the known energy levels of V I, improving level accuracy, and new levels have been found. The analysis of V II is also ongoing.

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The Kramers formulas in parabolic coordinates

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The presence of an external electric field acting on an atom in plasma or produced by external sources necessitates considering radiative transitions in parabolic quantum numbers, in contrast to the spherical basis for a free atom. The transformation from the spherical basis to the parabolic one is known to be determined by the transformation of the wave functions with the Clebsch-Gordan coefficients:

$$\Psi(n, n_1, n_2, m) = \sum_l C(n, n_1, n_2, m) \Psi(n, l) \quad (1)$$

where n_1 and n_2 are the parabolic quantum numbers; m is the magnetic quantum number; and $C(n, n_1, n_2, l, m)$ are the Clebsch-Gordan coefficients. Below, we use the "electric" quantum number $k = n_1 - n_2$ that defines the level energy shift in an electric field.

The direct calculations the transition probabilities between Rydberg states with the wave functions (1) are cumbersome. We will use the quasi-classical and purely classical approximations. In these approximations, the transition probabilities in the spherical and parabolic bases are related by the squares of the Clebsch-Gordan coefficients:

$$C^2(n, k|l, m) = 2l[l^2 - l_{\min}^2](l_{\max}^2 - l^2)^{-1/2}/\pi, \quad (2)$$

where

$$\begin{aligned} l_{\min}^2 &= [(n-1)^2 + m^2 - k^2]/2 - \{[(n-1)^2 + m^2 - k^2]^2 - 4(n-1)^2 m^2\}^{1/2}/2, \\ l_{\max}^2 &= [(n-1)^2 + m^2 - k^2]/2 + \{[(n-1)^2 + m^2 - k^2]^2 - 4(n-1)^2 m^2\}^{1/2}/2, \end{aligned} \quad (3)$$

The quantities $l_{\max}$ and $l_{\min}$ define the relationship between the parabolic and spherical variables.

It is of interest to establish the explicit form of the classical radiative transition probabilities in parabolic coordinates. To this end, we transform the standard Kramers formulas for the radiative decay probability $A(n, l)$ in the spherical basis by using the quasi-classical representation of the Clebsch-Gordan coefficients (2) according to the relation

$$B(k, m) = \int_{l_{\min}}^{l_{\max}} A(n, l) [C(n, k|l, m)]^2 dl \quad (4)$$

Directly calculating the integrals in (4) yields

$$B(k, m \neq 0) = \frac{4Z^4}{\pi\sqrt{3}c^3} \frac{1}{n^3(n-1)|m|}, \quad (5)$$

$$B(k, m = 0) = \frac{4Z^4}{\pi\sqrt{3}c^3} \frac{2}{n^3\sqrt{(n-1)^2 - k^2}}. \quad (6)$$

(c is the speed of light). Formulas (5) and (6) are the "parabolic analogs" of the Kramers formulas in the spherical basis. Note that for $m \neq 0$, these probabilities do not depend on the electric quantum number k .

This work was supported in part by a grant from the Russian Ministry of Industry, Science and Technology and in part by the grant 01-02-16305 from the RFBR.

Wave packets in critical region of potential energy surfaces

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Dynamics of wave packets around critical points of potential energy surfaces such as conical intersections or bifurcation points is studied using a reduced dimensionality method. We select an active subspace of degrees of freedom for which an ab initio minimum energy surface (MES) can be computed. Dynamics is carried out directly with the internal coordinates used to describe the geometry in the Z-matrix. The spectator coordinates are taken into account by the constrained Hamiltonian technique [1]. They can be simply frozen or adiabatically adapted to the movement in the active space. The code Tnum [2] generates numerically but exactly the coefficients of the differential operators occurring in the kinetic energy or flux operators, for any generalized coordinates.

- Bifurcation around a Valley Ridge Inflexion point, VRI The intramolecular energy exchange is analyzed around a VRI region where a valley along a reaction path becomes an unstable ridge and opens the way to bifurcation of wave packets. [3] The benchmark case is the H transfer in the methoxy radical. The behavior of the wave packets is studied in terms of non adiabatic energy transfer between the symmetry conserving reaction coordinate and the symmetry breaking torsional mode. The VRI region is characterized by large non adiabatic couplings among these modes. The main factor influencing the possibility to travel on the unstable ridge or to early bifurcate is the shape of the wave packet in the entrance valley. This suggests how to prepare wave packets in order to influence the branching ratio between enantiomers.
- Non adiabatic Tunneling around avoided intersection and conical crossing. Different time or energy resolved properties such as fluxes in critical region, cumulative reaction probability and rate constant are computed from active 2 or 3-dimensional subspace by time dependent and time independent wave packet methods. Examples in cyclopropylidene or bromoacetone are in progress.

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Valence ab initio calculations of the potential energy curves for the Ca- and Sr-rare gas van der waals molecules

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Adiabatic potential curves for the ground state and low-lying excited $1(3)P$ and $1(3)D$ states of the calcium (strontium) atom interacting with rare gas (RG) atoms have been obtained in the ΛS coupling scheme from valence ab initio complete-active-space multiconfiguration self-consistent-field (CASSCF)/complete-active-space multireference second-order perturbation theory (CASPT2) calculations. In the calculations, the Ca (Sr) atom is considered as 2-valence electron system whereas the Ca^{2+} , Sr^{2+} and RG^{8+} atomic cores are represented by scalar-relativistic energy-consistent pseudopotentials. Core polarization and core-valence correlation have been accounted for by adding a core polarization potential (CPP) to the hamiltonian. In addition, the closed-shell single-reference coupled-cluster approach with single and double excitations including a perturbative estimate of triple excitations (CCSD(T)) has been used to obtain more accurate ground-state potential curves for Ca-RG and Sr-RG species. The transition dipole moments from the ground state to the excited 1Σ and 1Π states correlating with the $1D$ and $1P$ excited terms of Ca and Sr have been evaluated as a function of R . Fine structure of the molecular terms has also been studied using a semi-empirical two-electron spin-orbit pseudopotential for the Ca (Sr) atom.

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Investigation of Dynamic of Processes at Highly Excited States of Ca atoms due to the multiphoton ionization.

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The three-photon ionization in Ca from $4s^2\ ^1S_0$ ground state is studied. The two-photon process is a near-resonance process with one of the following bound states: $4s4d\ ^1D_2$, $4p^2\ ^3P_2$, $4s6s\ ^1S_0$, $4p^2\ ^1D_2$ and $4p^2\ ^1S_0$ while the third photon reach either directly the continuum or one of the autoionizing states [1]. The dynamics of the multiphoton excitation processes is discussed and decay times of the Ca autoionizing states for different quantum numbers has been determined [2,3]. We also discussed two possible ways of the two electron excitation which is connected to the problem of a classification of highly excited states. One must thus take into account the channels including a double ionization, an ionization of one electron accompanied by an excitation of another one or an excitation of two electrons. In the latter two cases the excited states may be autoionizing states, which decay leading to the ionization.

The analysis of the autoionizing line shape using the proper Fano profiles [3] has been done by deconvolution of this profile using the least-squares algorithm for nonlinear parameters given by Marquardt [4]. From this analysis we have obtained the corresponding values of the asymmetry q parameters and of time decay of the high lying Ca states. If the coupling between the bound intermediate state and the higher (autoionizing) state is not very large the contribution of the autoionizing channel in such a process decreases. Taking into account that if the bound-high autoionizing state transition is farther from the resonance the contribution of the autoionizing channel decreases, the direct three-photon ionization channel starts to be dominant. Ionization channel and the Fano asymmetry parameter q decreases. In our case the Fano parameter is of order of 10–30, so we can say that both channels take play a role in that transitions, but the direct ionization channel can be dominant. Such a measurements give important experimental information on the autoionization spectrum profiles and the sequence of excitation in such processes.

The values of the time decays τ of the autoionization states are determined. Those states which belong just to the ionization limit have the decay time of 30 ps while the decay time of the higher states compare to the ionization limit (in energy scale) are of 6–3 ps. The determination of the decay of the highly excited states can inform about recognizing that there are transitions to the autoionizing states or bound-continuum transitions. We can simple conclude that the higher state are stronger coupled with the continuum and the channel of direct ionization could be dominant.

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Hyperfine interaction operator in coupled tensorial form of second quantization

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High resolution of contemporary spectroscopic methods allows the studies of hyperfine structure and isotope shifts of energy levels of many atoms and their ions. However, the relevant theoretical studies due to the complexity of the problem were so far restricted to light atoms having simple structure of electronic shells. This abstract is aimed at filling up the gap between theory and experiments.

The general tensorial form of the hyperfine interaction operator in the formalism of second quantization is presented. For example, the magnetic multipole interaction [1]

$$T^{(k)} \equiv T_{magnetic}^{(k)} = \left(\nabla^{(1)} \left\{ r^{-k-1} C_q^{(k)} \right\} \cdot \left(\frac{2}{k} L^{(1)} - 2S^{(1)} \right) \right) \quad (1)$$

has schematically the tensorial form

$$T_{magnetic}^{(k)} \equiv H_{magnetic}^{(k \ 1 \ k)} + H_{magnetic}^{(k+1 \ 0 \ k)}. \quad (2)$$

Such formulation is suitable for evaluation of diagonal and non-diagonal matrix elements in a uniform way according to an approach [2]. It is based on a combination of second quantization in the coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin), and a generalized graphical technique. It allows one to make use of the most of the advantages of Racah algebra. One of the basic features of this approach is the use of the tables of standard quantities and their symmetry properties in quasispin space, without which the process of obtaining the matrix elements of magnetic multipole and electric multipole interactions operator between any electronic configurations is much more complicated.

The general expressions for the operators describing hyperfine interactions obtained allow us to efficiently evaluate this interaction for any atom or ion of periodical table, atoms with open f^N shell included.

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An exact method for the calculation of ion partition functions in the superconfiguration approach

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In hot dense plasmas under local thermodynamic equilibrium, atomic physics calculations using a detailed configuration accounting method may become computationally prohibitive due to the huge number of configurations relevant to the emission process. The super-transition-array method or STA [1] is a rather powerful approach that permits to model these situations in a statistical framework by gathering the numerous configurations into a reduced number of superconfigurations. A superconfiguration consists of supershells, i.e. groups of ordinary shells, which are populated in all possible ways consistent with the Pauli principle. Average atomic variables (like energy and width of the transition arrays, shell occupations, *etc*) are deduced through the computation of partition functions of the supershells treated in the grand canonical ensemble. In the STA method, the partition functions are calculated using recursion relations which involve summing alternate large negative and positive numbers. This results in a strong numerical instability that can severely limit the range of applicability of the STA model, in particular in the low temperature regime. Moreover, this prevents an arbitrary choice of the supershells definition in the STA model. Wilson *et al* [2] have proposed to extend the domain of validity of the STA theory by using an integral representation of the partition functions. A numerical approximation is then obtained by evaluating the integral at the saddle point [3], i.e. in the average atom conditions.

We propose an exact method [4] to calculate the partition functions of superconfigurations without any restriction on the thermodynamic conditions and on the definition of the supershells. This represents a considerable progress for the applicability of the STA theory. This method is based on the derivation of new recursion relations free of the numerical problems encountered with the previous recursion relations. The formalism introduces a normalization factor in the calculation of the partition functions, and an origin for the energies of the shells inside a supershell that arise from a variational principle in a grand canonical ensemble. Examples where only one superconfiguration (i.e. one sole supershell) is assigned to each ion charge state of the plasma will be presented.

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Energy levels, radiative corrections and hyperfine structure of the superheavy ions for different nucleus models: QED calculation

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A great interest to this topic has been, in particular, stimulated by inaugurating the heavy-ion synchrotron storage cooler ring combination SIS/ESR at GSI. With this facility, which allows to produce, store and cool fully stripped heavy ions beams up to U^{92+} [1], new ways are opened in the field of atomic and nuclear spectroscopy and nucleus structure studying from this side. Paper is devoted to calculation of the energy levels, radiative corrections and hyper fine structure parameters for superheavy element ions with account of the definite nucleus structure modelling. One of the main purposes is establishment a quantitative link between quality of the nucleus structure modelling and accuracy of calculating energy and spectroscopic properties of super heavy ions. A new, highly exact, ab initio approach [2] to relativistic calculation of the spectra for multi-electron superheavy ions with an account of relativistic, correlation, nuclear, radiative effects on the basis of gauge-invariant quantum electrodynamical perturbation theory is used. Zeroth approximation is generated by the effective ab initio model functional, constructed on the basis of the comprehensive gauge invariance procedure (c.f.[1-3]). The wave functions zeroth basis is found from the Dirac equation with potential which includes the core ab initio 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) [1,4,7]. The correlation corrections of the high orders are taken into account within the Green functions method (with the use of the Feynman diagram's technique. There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction, mass operator iterations). The magnetic inter-electron interaction is accounted in the lowest (on parameter), 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. It's developed new scheme for calculation of the self-energy and vacuum polarization contributions into Lamb shift. It's carried out the relativistic calculation of spectra of the nlj ($n=2,3,4$) states for Li-like ions with nuclear charge $Z=20-100$ with account of the correlation, nuclear, radiative effects for different models of the charge distribution in the nucleus (hollow shell charge one, uniform one, Fermi model). It is fulfilled a detailed analysis of relation between cited corrections and shown a principal role of radiative corrections for ions with high Z . The nuclear size effect is accounted in the electric and polarization potentials. We carried out calculations :1). $1s^2 2lj, 3lj, 4lj$ energy levels, hyperfine structure intervals for superheavy Li-like ions in interval $Z=55-100$; 2). energy spectra of the super heavy elements atoms $Z=112, 114$. Comparison with results of some calculations by other methods [3-7] is presented.

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Two-Loop Bound-State Self-Energy

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Recent analytic and numerical calculations have significantly advanced our understanding of the historically problematic two-loop bound-state self energy shifts. Analytic calculations of logarithmic corrections have been carried out for excited S states up to the sixth power in $Z\alpha$ where Z is the nuclear charge number and α is the fine-structure constant. Intermediate expressions with about 200000 terms are encountered in the evaluations which depend on the extensive use of computer algebra. An extrapolation of the $Z\alpha$ -expansion from low to high Z suggests a large and negative value for the remaining nonlogarithmic correction given by the so-called B_{60} -coefficient when compared to the numerical calculations by Yerokhin, Shabaev and Indelicato. We also discuss the physical interpretation of the squared decay rates that contribute to the two-loop bound-state energy shifts of excited states.

Theoretical evaluation of the $^{7,9}\text{Be}^- 2s2p^2 \ ^4\text{P}_{1/2,3/2,5/2}$ hyperfine structure parameters and Be $2s2p \ ^3\text{P}^o$ electron affinity

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The hyperfine structures of $^{7,9}\text{Be}^- 2s2p^2 \ ^4\text{P}_{1/2,3/2,5/2}$ are investigated theoretically using the multiconfiguration Hartree-Fock and configuration interaction methods. The effects of the hyperfine mixing between the fine-structure J -levels are discussed. The feasibility of some atomic spectroscopy experiments, allowing determination of the ^7Be quadrupole moment from observed hyperfine structure of the $^7\text{Be}^-$ negative ion and from the present electronic parameters, is investigated. The Be $2s2p \ ^3\text{P}^o$ electron affinity is monitored as a function of the orbital and configuration spaces to assess the reliability of the wavefunctions of the neutral atom and the negative ion. The theoretical values nicely converges toward the most recent theoretical and experimental results.

Valence ab initio calculations on the molecular structure of the Ca_2 and Sr_2 dimers

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The electronic structure of the Ca_2 and Sr_2 molecules has been investigated by use of a two-valence-electron semi-empirical pseudopotential (PP(2)) and applying the internally contracted multireference CI method (ICMRCI) with complete active space SCF (CASSCF) reference wavefunctions. Core-valence correlation effects have been accounted for by adding a core-polarization potential (CPP) to the hamiltonian. The ground-state properties of the Ca_2 , Sr_2 , Ca_2^+ and Sr_2^+ dimers have also been studied at the single-reference coupled-cluster level with single and double excitations including a perturbative treatment of triple excitations (CCSD(T) RCCSD(T)). Good agreement with experiment has been obtained for the ground-state potential curve and the only experimentally known $\text{A}^1\Sigma_u^+$ excited state of Ca_2 and Sr_2 . The spectroscopic parameters D_e and R_e deduced from the calculated potential curves for other states are also reported. In addition, spin-orbit coupling between the singlet and triplet molecular states correlating with the $(4p)^1\text{P}$ and $(4p)^3\text{P}$ Ca terms and, respectively, $(5p)^1\text{P}$ and $(5p)^3\text{P}$ Sr terms has been investigated using a semi-empirical 2-electron spin-orbit pseudopotential.

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A new *ab initio* method for the calculation of molecular vibration-rotation spectra. Application to water, ozone and methane.

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The method presented here is implemented for the Watson Hamiltonian in which the Born-Oppenheimer potential and the Coriolis matrix are both expanded in series of the mass-weighted cartesian normal coordinates up to finite orders [1]. The $J = 0$ vibrational problem is first solved by means of the vibrational mean-field configuration interaction method (VMFCI). This original variational approach consists in a series of successive symmetry adapted contractions including a mean-field treatment at each step. The efficiency of such a scheme for describing intra- and inter-mode couplings is illustrated on molecules H_2O , O_3 and CH_4 , for which vibrational calculations have been performed using accurate *ab initio* potentials from the literature.

Rotational spectra are calculated in a second step, using the variationally converged $J = 0$ solutions as zeroth order basis sets of a perturbation theory treatment. The advantage of such a partition is to provide a faster convergence than in the traditional approaches based on the harmonic oscillator/rigid rotor zeroth order model. The method is illustrated on the $v = 0$ rotational spectrum of methane (energies and intensities) calculated at different temperatures [2] and compared with the HITRAN [3] atmospheric database results.

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Ab initio calculations and Fourier transform emission spectroscopy on *NbCl*

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Ab initio calculations and Fourier transform spectroscopy experiments have been carried out in order to characterize for the first time the electronic structure of the molecule *NbCl*, which as most transition metal diatomic halides presents an astrophysical interest.

On the theoretical side, the potential energy curves of all the electronic states lying below 15000 cm^{-1} from the ground state (9 quintet, 16 triplet and 3 singlet states) have been calculated by means of a large scale CASSCF/MRCI approach [1] based on quasi-relativistic pseudopotentials and related basis sets [2]. The corresponding spectroscopic properties and the electric dipole transition moments within the different spin systems are predicted.

On the experimental side, the emission spectrum of *NbCl* has been recorded in the $3000 - 20000\text{ cm}^{-1}$ region. Two groups of bands (5 in the $6700 - 7000\text{ cm}^{-1}$ region and 9 in the $9800 - 11000\text{ cm}^{-1}$ region) are assigned to two different electronic transitions. These observations are interpreted by means of the *ab initio* predictions and the results are compared to those recently obtained for the isovalent *VCl* chloride [3].

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Electronic structure of the radical cations of isolated and stacked pairs of DNA bases from Møller-Plesset and density functional theory calculations.

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Electron abstraction from DNA bases is an important elementary step in processes of biological interest like charge transport within double helical DNA and radiation damage to DNA. In this work we investigate the ground and first excited states of the cations of isolated and stacked bases by means of MP2 and DFT calculations. The excited states, which could contribute to some of the reactive processes of interest, are characterized for the first time.

The vertical and adiabatic ionization potentials of the isolated DNA bases have been first calculated. Results of restricted and unrestricted DFT calculations using different functionals and of MP2 calculations are compared. A systematic study of the basis set effect is also presented, showing that the augmented 6-31G**(0.1 or 0.2) basis set, successfully used in the calculation of interaction energies of stacked base pairs [1], also gives ionization potential values in good agreement with experiment [2]. A comparison with other theoretical results from the literature is presented [3,4].

Electron abstraction from stacked pairs of DNA bases is then considered, with the Guanine-Guanine stack as a first binary target system.

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Electron re-arrangement induced by nuclear transmutation and stochastic autoionization of radioactive atoms

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A nuclear transmutation (i.e., change in the nuclear charge) induced by nuclear reactions or radioactivity are often accompanied by a redistribution of the electrons around the final transmuted nucleus (c.f.[1]). Electrons originally in the ground state of the target atom can be excited either in the bound spectrum or to the continuum of energy. Therefore, calculations of the population distribution of the atomic states of the daughter atom require a complete description of both the bound spectrum and the continuum of energy. The electronic rearrangement resulting from the β decay of ^6He has been calculated in the framework of the sudden approximation using the operator perturbation theory basis set [2]. We have calculated the excitation probabilities to the final discrete states of $^6\text{Li}^+$ (including to the doubly excited autoionization states) as well as the total probabilities for single and double ionization. We compare in table our results with the pioneering work of Winther and results of Wauters-Vaeck, obtained on the basis of calculation within the sudden approximation with the use of numerical B-spline [1]. It is analyzed an account of the electronic correlation and its contribution into value of (the probability that an atomic K vacancy is created. Let us present some data regarding the transition probabilities (P,in the β decay: final Li^+ state $1s2up\ 1upS$, according to Winter data $P=67.0$, according to Wauters-Vaeck data $P=70.85$ and data of present paper $P=69.93$; final Li^+ state $1s2s\ 1upS$, according to Winter $P=16.6$, according to Wauters-Vaeck $P=14.94$ and present paper $P=14.35$. In second part of paper it is considered a problem of stochastic autoionization of the radioactive atoms and proposed a new quantum-electrodynamics approach for description of such phenomena [3].

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Hyperspherical approach to four-electron atomic systems

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Since the advent of quantum mechanics, the description of a many-electron atom is based mostly on the independent electron model. Within this model, a many-electron atomic state is designated by a collection of quantum numbers from the individual electrons. However, theoretical and experimental investigations of doubly excited states and triply excited states of atoms in the past few decades have revealed that the independent electron model is inadequate. For such multiply excited states, the motions of the electrons are highly correlated and they are better described as analogous to the rotation and vibration of a polyatomic molecule. Thus doubly excited states of a two-electron atom can be described qualitatively in terms of the ro-vibrational motion of a linear XY_2 molecule where X stands for the nucleus and Y for the electron. Similarly, triply excited states of an atom can be described in terms of the ro-vibrational motion of an XY_3 molecule. These qualitative descriptions are supported by analyzing the actual calculated wavefunctions, and doubly and triply excited states have been classified in terms of new quantum numbers which describe the collective normal modes of their joint motion in the hyperspherical adiabatic viewpoint [1-3]. In this work, we present a new development on the understanding of electron correlations in four-electron atomic systems, where one can expect much richer electron correlation effects, using the hyperspherical approach.

In the hyperspherical method, the total wavefunction for a four-electron atom is expanded as

$$\psi_{\mu n} = \sum_{\mu} F_{\mu}^n(R) \Phi_{\mu}(\Omega; R), \quad (1)$$

where $R = \sqrt{r_1^2 + r_2^2 + r_3^2 + r_4^2}$ is the hyperradius, which characterizes the size of the system and Ω denotes a set of hyperangles which measure the relative positions among the four electrons from the nucleus. $F_{\mu}^n(R)$ is the hyperradial function which measures the size of the state; $\Phi_{\mu}(\Omega; R)$ is the hyperspherical adiabatic channel function, which contains all the information about electron correlations for states within channel μ . The hyperspherical channel function $\Phi_{\mu}(\Omega; R)$ and its associated hyperspherical adiabatic potential $U_{\mu}(R)$ are obtained by solving the adiabatic eigenvalue problem at each R ,

$$[H_{\text{ad}}(\Omega; R) - U_{\mu}(R)] \Phi_{\mu}(\Omega; R) = 0. \quad (2)$$

We solved this eigenvalue problem for $\text{Be}^{(1,3,5)S^e}$ within the s^4 configurations, using direct products of discrete variable representation (DVR) functions as a basis set. We found that the adiabatic potential curves are clearly separated into four groups of the singly, doubly, triply, and quadruply excited states of the atom. We also analyzed the channel functions to identify the multiply excited states with the number of nodes in the hyperangles.

Further details of the analysis will be presented at the seminar.

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Isotope shift in the electron affinity of beryllium

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The isotope shift in the electron affinity is defined as the difference of the electron affinities between two isotopes. It is well known that electron correlation effects play an important role in the calculation of electron affinity and of the level specific mass shift. The comparison of theory and experiments through the isotope shift in the electron affinity is therefore of particular interest for probing correlation effects that affect both properties.

Experimentally, the electron affinities of atomic hydrogen and deuterium have been determined by tunable-laser threshold photodetachment spectroscopy [1] confirming the predicted shift in theory. The isotope shift in the electron affinity between ³⁵Cl and ³⁷Cl has been measured by the same technique but the many-body calculations are less successful due to the extreme difficulty of a theoretical treatment [2]. Progress has been achieved recently for isotope shifts in the electron affinity of oxygen for which electron affinities have been measured for the three isotopes ^{16,17,18}O using photodetachment microscopy [3]. The theoretical results are for this system in good agreement with observation revealing an “anomalous” isotope shift, corresponding to a smaller electron affinity for the heavier isotope [4].

Atomic spectroscopy experiments on unstable beryllium isotopes are performed these days thanks to the ISOLDE facility at CERN and the feasibility of some experiments allowing the determination of the nuclear quadrupole moment of ⁷Be from the observed hyperfine structure of the negative ion ⁷Be⁻ ($2s2p^2\ ^4P_J$) has been investigated [5]. In the present work we report the first *ab initio* calculations of the isotope shift in the electron affinity of Be ($2s2p\ ^3P^o$) for various isotopic pairs involving ^{11,10,9,8,7}Be isotopes. We have studied the convergence of the specific mass shift parameters for both the neutral atom and negative ion, evaluated from elaborate multiconfiguration Hartree-Fock/configuration interaction wave functions that provide a theoretical value of the electron affinity in good agreement with both other theory and experiment [5]. The quality of the wave functions is also assessed by the good agreement between theoretical isotope shifts for the $2s2p\ ^3P^o - 2s^2\ ^1S$ transition using another correlation model [6]. The isotope shift in the electron affinity of ¹¹⁻⁹Be is estimated to be -2.168 GHz of which -2.940 GHz are due to the specific mass shift. As for the oxygen case [3], but oppositely to chlorine [2], the isotope shift in the beryllium electron affinity is “anomalous”.

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Thermodynamics of dense plasmas in the superconfiguration approach : application to photo-absorption and equation-of-state calculations

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We investigate a self-consistent approach for the modeling of dense plasma thermodynamics. The plasma is supposed to be in local thermodynamic equilibrium and each ion is represented by a set of superconfigurations describing its ground state and excited states. As a configuration is defined by shells occupied by an integer number of bound electrons, a superconfiguration is defined by supershells, which are groups of shells close in energy[1]. In each superconfiguration the nucleus is totally screened by bound and free electrons in a Wigner-Seitz sphere (ion-sphere model). The minimisation of the plasma total free energy with respect to ionic volumes leads to the equality of the boundary electronic pressure of all ions, which means that all the ions have the same electronic environment. Bound electrons are treated quantum-mechanically while free electrons are described by the Thomas-Fermi model at finite temperature, i.e. in the quasi-classical approximation. The electronic pressure is calculated together with the ionic volumes in a self-consistent way. Comparisons between ionic distributions and photo-absorption spectra obtained with this new approach and with the previous one[2] in which all ions have the same volume (and different boundary pressures) will be presented.

The improvement in thermodynamic consistency brought by the diversity of ionic volumes (in other words the "redefinition" of ions) encouraged us to apply this approach to equation-of-state calculation. However, although the ion-sphere model provides an accurate description of strongly correlated plasmas ($\Gamma \geq 1$), the confinement of an ion in a finite volume may still lead, in our model and when the matter density is sufficiently high, to unacceptable discontinuities in the thermodynamic functions when a bound level disappears (pressure ionisation). We show that boundary values of the wave-functions play a crucial role in the continuity of pressure and in the expression of the Virial theorem from which our pressure formula is derived. Moreover, discontinuities in thermodynamic functions are due to the fact that it is difficult to obtain a variational formulation of the problem[3]. We thus finally present a condition which should make variational the ion-sphere model when bound electrons are treated quantum-mechanically and free electrons quasi-classically, and discuss its impact on the expression of electronic pressure.

Although density effects are not very important at matter densities encountered up-to-now in photo-absorption experiments, interactions between bound and free electrons become important at higher densities. The approach presented here appears to be promising for the interpretation of photo-absorption and equation-of-state experiments which will be undertaken with lasers of the future generation.

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Non-linear Susceptibilities of an Excited Helium Atom

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Theoretical treatments of high-resolution measurements of the energy level structure for helium atom in an external field F require numerical values of susceptibilities up to the fourth order in F . The “resonance part” of the fourth-order susceptibility (hyperpolarizability γ_{n^3P}) describing the deviation from the quadratic law for the Stark effect on triplet sublevels of atomic helium is determined by the tensor part of polarizability $\alpha_{n^3P}^t$ [1] and gives a satisfactory agreement with experimentally observed data in the low field limit. In the vicinity of the anticrossing effect for the n^3P_J fine-structure sublevels with the total momentum $J = 0$ and $J = 2$ and the magnetic quantum number $M = 0$, the “resonance” approximation comes out of the boundaries for the experimental errors.

In our paper [2] the fourth-order terms of diagonal matrix elements for the atom-field interaction, described by the hyperpolarizability tensor of the triplet state, have been taken into account. In a close vicinity to the anticrossing field $F \approx F_a$, the contribution of these terms to the fine-structure level splitting $\delta(F) = E_{n^3P_0}(F) - E_{n^3P_2}(F)$ amounts to $\sim 3\%$ of the second-order corrections. In this field region the fourth-order corrections to the off-diagonal matrix elements may also be significant, although rigorously speaking, their contribution to $\delta(F)$ is of the order of F^6 . However, one order of smallness disappears since $\delta(F_a) \approx \alpha_{n^3P} F_a^2$ and hence $\alpha_{n^3P} \gamma_{n^3P} F_a^6 / \delta(F_a) \approx \gamma_{n^3P} F_a^4$.

A thorough theoretical analysis of the fourth-order terms in non-diagonal matrix elements demonstrates, that their contribution almost equals that of diagonal elements. So, in the vicinity of anticrossing the total contribution of the 4-th-order terms to $\delta(F_a)$ for $n = 2, 3, 4, 5$ states amounts correspondingly to 0.1%, 5%, 10%, 15% of the second-order correction.

In this paper we modify and extend our previous results in several ways: (i) we give a general formulation of the higher-order perturbation theory for close levels which have non-zero energy separation $\delta(0) \neq 0$ in the field $F = 0$; (ii) analytical expressions are derived for the 4-th-order corrections in a two-level system; (iii) numerical and analytical results for the electric field F_a , components of dipole polarizabilities and hyperpolarizabilities and the energy separations at the anticrossing point, $\delta(F_a)$ are presented. Analytical calculations were accompanied by numerical diagonalization of the atom-field interaction energy in the basis of bound states with the principal quantum number $n \leq 7$.

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Calculation of Landé g-factors in doubly ionized lanthanides

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A fundamental limitation that is met in studies of stellar magnetic fields is the lack of accurate values of the Landé factor g . Values of this parameter have been determined from laboratory, most of which can be found in extensive compilations of atomic data such as those published at the National Institute of Standards and Technology (NIST) in Washington (see e.g. Ref. [1]). The accuracy of these experimental values is generally rather good, and sufficient for astrophysical applications. However, the available experimental data are far from being complete, and the Landé factors of many levels of astrophysically interesting ions have never been determined in laboratory. This is particularly the case for doubly ionized lanthanides ($Z=57-71$) for which, among the ~ 1500 experimentally known energy levels, only about 30% of g -factors have been estimated so far.

Theoretically, the Landé factor can be calculated in intermediate coupling by:

$$g_{\gamma J} = \sum_{\alpha LS} g_{LSJ} |\langle \alpha LSJ | \gamma J \rangle|^2 \quad (1)$$

where g_{LSJ} is the g -factor of a level αJ belonging to a pure LS -coupling term and where the summation is over the same set of quantum numbers as for the wavefunction $|\gamma JM\rangle$ of the M sublevel of a level labelled γJ and expressed in terms of LS basis states $|\alpha LSJM\rangle$ by the following formula:

$$|\gamma JM\rangle = \sum_{\alpha LS} |\alpha LSJM\rangle \langle \alpha LSJ | \gamma J \rangle \quad (2)$$

In the present work, the wavefunctions in intermediate coupling for the doubly ionized lanthanides from La III to Lu III were generated by the pseudo-relativistic Hartree-Fock method (HFR) using the computer codes written by Cowan [2] in which we have included core-polarization effects (HFR+CP) by means of a pseudo-potential according to the procedure described in Ref.[3]. This potential depends on two parameters, i.e. the electric dipole polarizability of the ionic core, α_d , and the cut-off radius, r_c , which can be seen as a measure of the size of the core. In our calculations, this latter parameter corresponds to the HFR expectation value of $\langle r \rangle$ for the outermost core orbitals ($5p^6$). In addition, this HFR+CP method was combined with a well-established semi-empirical least-squares optimization of the radial parameters (average energies, Slater integrals, spin-orbit parameters) minimizing the discrepancies between the calculated energy levels and the available experimental values.

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The 2p and 3d structure of antiprotonic hydrogen and deuterium.

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High resolution X-ray spectroscopy of antiprotonic hydrogen and deuterium has been performed at LEAR just before its shutdown in 1997 [1-3]. The idea of these experiments was to determine with high accuracy strong-interaction shifts and broadenings of the 3d-2p transition energy. Because the experimental resolution and precision are of the order of a few meV, it is necessary to perform very accurate calculations of the QED transition energy. In the case of antiprotonic hydrogen and deuterium, we have three majors specifications: 1) due to the large proton mass, the QED corrections are dominated by vacuum polarisation. 2) the fine and hyperfine structures are the same order of magnitude. 3) one must include the anomalous magnetic moment sometime called "g-2 correction". The antiproton is not an elementary Dirac particle. As such its gyromagnetic ratio $g_{\text{antiproton}} = -5.585694772(126)$ [4] is very different from the gyromagnetic moment as predicted to be 2 by the Dirac equation for an elementary particle. We have calculated this complete g-2 correction: both diagonal and non-diagonal for both the electric and magnetic contributions. This is of the same order of magnitude as the vacuum polarisation, fine and hyperfine structures.

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Dalgarno-Lewis method for static polarizabilities and hyper-polarizabilities for various electronic states of alkali atoms

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Values for the static electric polarizabilities and hyperpolarizabilities for the ground state and various excited states of alkali atoms, obtained by a novel computational approach, are presented. Our approach is consisted of a discrete variable representation (DVR) formulation with the use of an analytic model potential and is applied in solving problems of nondegenerate perturbation theory with the use of the method of Dalgarno and Lewis. Our methodology is exceptionally simple. Comparison of our results with existing experimental data and other theoretical values are presented.

Identification of 4-4 transitions in Ni-like spectra Ag XX and Cd XXI produced in a capillary discharge plasma column

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Spectra of nickel-like silver and cadmium ions have been produced with a high current capillary discharge (peak amplitude up to 200 kA and 10 to 90 percents rise time of 10 to 15 ns) provided by a high power density pulse generator [1]. The radiation axially emitted by the plasma was focused into the slit of a 2.217m grazing incidence spectrograph equipped with a 2400 lines per mm grating. The detector consisted of micro-channel plates and a CCD array with a time resolution of 5ns. Time resolved spectroscopy was carried out in the range 10 to 20 nm and impurities F and O provided standards for wavelength calibration. Strong lines of the Cu-like spectra Ag XIX and Cd XX were found within 0.004nm of the published values [2,3].

The first configurations $3d^9nl$ of Ni-like ions have been studied by means of the chain of programs at Laboratoire Aimé Cotton [4] which follows the Racah-Slater method explained in Cowan[5]. Experimental energy levels of all ions in the sequence were used in *generalized least-squares fits* for deriving the dependance of radial parameters versus Z. Indeed the "scaling factors" $SF(P)=P_{fit} / P_{HFR}$ were used as parameters and the energies were weighted as $1/(Z-27)$ in order to compensate the rising experimental uncertainties on the levels as Z increases. This led to reliable predictions of 4p-4d and 4d-4f transition energies and about 50 lines have been identified in Ag XX and Cd XXI, *i.e.* ten times more than in the earlier analysis of these spectra [6]

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Optical properties of rare earth double tungstates in α -KY(WO₄)₂ structure.

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The single crystals of potassium erbium and potassium holmium double tungstates with structure related to the α -KY(WO₄)₂ type are particularly promising optical materials. The applications are mainly determined by their laser properties.

The rare earth double tungstate single crystals are grown with use of the Top Seeded Solution Grown (TSSG) technique and crystallizes with C_{2h}⁶(C2/c) symmetry. The chain-layered crystallographic structure is a reason of strong anisotropy of many physical properties. The rare earth double tungstates are biaxial and pleochroic.

The paper presents the results of spectroscopic investigations of the KEr(WO₄)₂ and KHo(WO₄)₂. Using spectroscopy methods, the orientation of optical axes and refractive indexes, were found. The investigations of absorption spectrum were performed in a wide spectral range (6000—35000 cm⁻¹) at temperature from 1.5 K up to 300 K. The trichroism those crystals were confirmed experimentally.

The luminescence properties of erbium and holmium double tungstates are investigated at temperature from 3.5 K up to 300 K. All luminescence transition from excited state give insight into the Stark level structure of the ground level ⁴I_{15/2} for KEr(WO₄)₂ and ⁵I₈ for KHo(WO₄)₂.

The temperature dependence of optical absorption for KHo(WO₄)₂ was investigated.

The Hamiltonian of erbium ions and holmium ions in low-symmetric crystal fields is constructed with fifteen crystal field parameters calculated within the framework of the point charge model.

Experimental demonstration of light shift suppression in optically pumped Rb-cell atomic clocks

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The light shift (LS) constitutes a major concern for the medium- and long-term stability of laser-pumped vapor-cell atomic clocks and optical magnetometers. This is caused by the strong dependence of the light shift on the laser frequency close to the center of the atomic transition, characterized by the β -parameter ($\Delta f_{\text{clock}}/\Delta f_{\text{laser}}$). In our previous theoretical work [1] we proposed a simple method to reduce the value of β by frequency modulation of a single-frequency diode laser at a modulation frequency close to the HWHM of the atomic line. Our calculations have shown that if the intensity of the first sidebands is significantly higher than that of the carrier, fluctuations of the laser frequency will cause significantly less LS than for the case of a single-frequency excitation.

Here we present the experimental verification of such suppression of the β -parameter of the light shift in an optically pumped Rb vapour-cell atomic clock by using a modulated DBR-laser. The experiments were conducted at Observatoire de Neuchâtel in the frame of the development of advanced high-performance Rb atomic clocks.

It is well known that optically pumped clocks suffer from a β which is 1-2 orders of magnitude larger than that of frequency standards based on Coherent Population Trapping (CPT). Our experiments with an optically pumped clock show that the light shift of the clock transition can be reduced by a factor of at least 55, which means a value of β comparable to those typical for CPT frequency standards. These results open up the possibility to improve the medium- and long-term stability of laser pumped vapor-cell clocks at the level of 10^{-13} to 10^{-14} (Allan deviation) for sampling times of 1000 to 20,000 seconds.

Another consequence of the demonstrated light shift suppression is the reduced sensitivity of a given instrument (here the clock) to laser frequency fluctuations, while preserving the overall instrument performance. This is of advantage in instruments for practical applications, where the most simple and comparably low-performance laser stabilization schemes are preferable.

Acknowledgment

We thank Temex Neuchâtel Time for providing a lamp-removed Rb frequency standard. This work was supported by the Swiss National Science Foundation (SCOPES 7BUPJ062412). GM, CA thank the European Space Agency (ESA contract 15280/01/NL/US). DS, CA, TK, SC thank the Bulgarian National Scientific Council (F-1005/00).

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Oscillator strengths for some E1, E2, M1, M2 transitions of the Zn-like multi-charged ions (Z=31-92) calculated within relativistic energy approach

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In paper there are presented the results of calculating the energies, oscillator strengths and probabilities of transitions of the electric and magnetic type between low lying levels $4s^1S_0$, $4s4p^{1,3}S_J$, $4s4d^{1,3}S_J$, in multicharged ions of isoelectronic sequence ZnI with nuclear charge $Z=31-92$. Calculation is carried out on the basis of the energy approach - QED perturbation theory (S-matrix Gell-Mann and Low formalism) with using in the zeroth approximation (it defines basis of relativistic wave functions) gauge invariant one-quasi-particle representation [1-4]. It is fulfilled a comparison of obtained results with available experimental, compillated and theoretical ((Hartree-Fock-Dirac calculation) data for some ions and transitions. A part of results is obtained in paper at first with high accuracy and can be used in a different applications, including, non-linear optics, laser physics etc.

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A polarisation effect in molecular photodetachment microscopy

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Photodetachment microscopy[1] consists in recording the electron interferogram that appears when a negative ion emits an electron via photodetachment in the presence of an electric field. The observed interferogram is very sensitive to the initial kinetic energy of the electron, which gives an interferometric way of measuring the energy excess carried by the photon in the photodetachment process. This has been used for several electron affinity measurements, the accuracy of which is as good, if not better, than the accuracy of the usual laser-photodetachment-at-threshold technique[2,3].

However the model used to analyse the electron interference pattern is the free-electron approximation, which supposes that the excited electron undergoes no perturbation by the residual neutral core. This approximation becomes questionable when one deals with a molecular anion, the neutral residue of which is a polar molecule.

Photodetachment microscopy experiments have been carried out on OH^- , which has the advantage of well-separated vibrational and rotational detachment thresholds. No perturbation of the electron interferograms appears, which can be attributed to the fact that energy eigenstates of OH are actually parity eigenstates, due to Λ -doubling, and parity eigenstates have no permanent electric dipole. LoSurdo-Stark mixing of adjacent eigenstates, leading to the onset of a permanent electric dipole, would require an electric field 100 times greater than the applied one[4].

However, taking the known rotational spectroscopy of both OH and OH^- into account, one can use the threshold detachment energies to make several independent measurements of the electron affinity of OH. An anomaly appears in all cases where the neutral atom happens to be left in the upper state of a Λ -doublet. We suggest that this may be due to polarisation of the neutral molecule by the outgoing electron.

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Theoretical and Experimental Study of Soft X-ray Photoionization of Kr-Like Ions: 4s-Subshell Photoabsorption of Y^{3+}

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As archetypal systems for the study of the atomic photoelectric effect, rare gas atoms, with their closed shell electronic configurations, have been the subject of innumerable experimental and theoretical investigations during the past four decades [1]. However, the situation for ions is far less complete due to the experimental difficulties and the concomitant paucity of measurements. Two techniques, one using a pair of synchronized laser plasmas (known as DLP) [2] and the other involving merged ion and synchrotron beams [3] are now routinely providing relative and absolute photoionization data on ions and so this situation is rapidly improving. Using the DLP technique we have already studied the 3s-subshell photoabsorption spectra of the Ar-like isoelectronic sequence [4] and more recently 4s-subshell excitation in the Kr-like ions Rb^+ and Sr^{2+} [5].

Due to experimental difficulties it was not previously possible for us to make convincing measurements of the Kr-like Y spectrum. However, with a new, more flexible target alignment/laser focusing optics arrangement in place we can now report here the extension of this latter work to the fourth member of the sequence Y^{3+} using the DLP technique. The triply ionized yttrium ions were isolated in a laser produced plasma and their XUV absorption spectrum measured at DCU. The spectrum already compares well with a theoretical photoionization cross section computed within the framework of Configuration Interaction Pauli Fock Calculations. The calculations also predict that the first member of the Rydberg series (4s – 5p) drops below the 4p-threshold and that the q - values for the other series members become quite large in contrast to earlier isoelectronic sequence members [5].

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The influence of the magnetic field on the efficiency of the optical pumping in $S_{1/2} - P_{1/2}$ system

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Recently a method giving population inversion on transition involving the ground state of atoms was proposed [1]. Such an inversion was obtained experimentally in the medium of sodium optically active atoms and helium buffer atoms. At first low-intensity circularly polarized and resonant to the D_1 transition prepulse orients the atoms in the ground state. Then much more intensive similar pulse but with the orthogonal circular polarization transfers the population to the first excited state. The high pressure buffer gas is the source of the fine structure mixing collisions which redistribute this population among the sublevels of the P multiplet. Since one of the sublevels of the ground state is nearly empty there appear population inversions between this sublevel and some of the sublevels of the P multiplet. In effect the lasing at the frequency corresponding to the sodium D_2 transition in the presence of the pump radiation resonant to the D_1 line was observed.

It is obvious that the efficiency of such an antistokes lasing scheme which converts the pump D_1 radiation into the D_2 amplified light strongly depends on the efficiency of the optical pumping by the prepulse. This process is influenced by two factors: collisions with the buffer gas atoms and laboratory magnetic field. Since the cross section for the deorientation in the ground state of the alkali-metal atom is very small the first factor can be neglected. It is well known from the practice and theory of the optical pumping that the deorientation caused by the transverse, in relation to the light beam, laboratory magnetic field can be at least partially compensated by the longitudinal magnetic field. Such a method was used in the considered experiment. It was found that there exist the threshold helium pressure and threshold longitudinal field induction at which amplified radiation on D_2 frequency can be observed.

The described experimental scheme exploits the effect of the optical pumping. However, the key role is played by the collisions with the buffer gas atoms which cause the population transfer between the fine structure components.

We present theoretical description of the excitation of the $J = 1/2 - J = 1/2, 3/2$ sodium atom by the light tuned to or slightly detuned from the $J = 1/2 - J = 1/2$ transition in the presence of the static magnetic field with an arbitrary direction. Since we assume high buffer gas pressure we can neglect the hyperfine structure. To simplify the description we assume that the level with $J = 3/2$ is populated only due to the collisions with the buffer gas atoms. Moreover we neglect the motion of the sodium atoms which leads to redistribution of the atomic transition frequencies due to the Doppler effect.

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The MCHF/MCDHF Data Collection

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The **MCHF/MCDHF Collection** is a database of theoretical results for atoms and ions that includes energy levels, lifetimes, transition probabilities, and some Zeeman factors. Calculations are “spectrum” calculations [1] in that wavefunctions are obtained for all levels up to a certain level in the spectrum, in the LSJ or jj approximation. From these wavefunctions, transition probabilities for all transitions between the levels and the lifetimes of most levels have been determined. Included are all E1 transitions and selected E2, M1, M2 transitions between lower levels.

The collection consists of iso-electronic sequences, up to as high as $Z=30$. At the moment, these include Li-like to Si-like, with several other sequences in progress. Some MCDHF data is for selected ions of an iso-electronic sequences with Mg-like going as high as $Z=92$ (uranium). A few spectra have been determined using the non-orthogonal spline Breit-Pauli CI program [2]. In C I, levels up to $2s^22p9d\ ^1P^o$ have been determined.

The database provides an internet accessible system for storage, retrieval, and analysis of large amounts of transition data. It may be found at <http://atoms.vuse.vanderbilt.edu>. Data may be viewed either through the periodic table for a selected spectrum and property or through a search capability for one or more elements of an iso-electronic sequence. NIST (National Institute of Standards and Technology) energy levels have been included in the database so that, for every transition, the computed and observed (if available) energy can be compared. A particularly useful feature has been the ability to easily compare and evaluate results such as *ab initio* and “energy adjusted” data (to see the effect of errors in the energy) or results from different methods.

The poster will describe the objectives of the database in more detail, present some tables and figures that illustrate the accuracy of the data, and compare some present results with other theory and experiment. Special attention will be given to the spectrum of Ca I where the effect of correlation in the core and relativistic effects through Breit-Pauli improve the earlier work of Hansen *et al* [3].

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Extension of the analysis of the second spectrum of Bi

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The spectrum of Bi II was remeasured in the wavelength range 6200 – 740 Å, using a hollow cathode light source. An extension of the analysis of the level structure was started based upon the work of Stachowska[2] and preliminary results were given in Stachowska, Dembczyński & Meijer[3]. Joshi and Mazzoni[4], using flash photolysis, established the levels in the *6pnd* series up to *d* = 14. More recently interest for this spectrum was revived from astrophysical side, while Dolk et al.[5] improved the accuracy using Fourier spectroscopy, but in the latter work not all data available at the time [2,3] were used. We have furthermore obtained additional data in the VUV[3].

In Poznan the hyperfine structure of 150 lines was measured in the visible and ultra-violet wavelength regions with a 2m PGS-2 plane grating spectrograph equipped with a 1300 lines/mm grating used in first to fourth order. The light source used was a hollow cathode, made from a hollow copper cylinder, lined with metallic bismuth.

At the former Zeeman-laboratory of the University of Amsterdam a 6.5 m normal incidence vacuum spectrograph was used with a 1200 lines/mm grating in the wavelength range 2300-1100 Å and with a 2400 lines/mm grating in the range 1200-700 Å. A practical resolving power from 100 000 to 200 000 was obtained, depending on wavelength. In this case we used a pulsed hollow cathode discharge with currents between 200 and 1600 A, duration up to 1 ms. The cathode used for these exposures consisted of a carbon or aluminum cylinder on the inside covered by Bi by sputtering. The plates were evaluated on the automatic comparator Zelacom. In the vacuum ultra-violet we attributed 417 lines to Bi II, of which 58 are newly classified.

We classified in total 8 new odd levels and confirmed all but six levels from previous authors. We also measured 80 newly classified lines. Our level classifications are supported by parametric least square fits, in a many configuration approximation. These fitting procedures have been performed for fine and hyperfine structures of the level systems of both parities. The results of these calculations provide information on predicted energy values as well as hfs-splittings of the high lying levels not yet observed.

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Numerical study of the dynamics of a two-electron system in a strong field: methodological considerations

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We describe a new approach of spectral type for numerically integrating the time-dependent Schrödinger equation associated to the interaction of a two active electron system (H^- , He...) with a strong and ultrashort linearly polarized electromagnetic field. The method is based on the expansion of the full wavefunction of the system in a basis of products of Coulomb Sturmian functions for the radial coordinates of the electrons and bipolar harmonics for their angular coordinates. The time propagation is carried out in the atomic basis and the interaction picture by means of a Runge-Kutta type formula. A complex rotation of the Hamiltonian is used to generate both the position and the width of the autoionizing states. When used for the time propagation, this complex rotation takes account of the usual problem of the reflection of the probability density due to the truncation of the basis.

The extraction of a quantitative information from the (numerical) wavefunction is a difficult problem which, in the cases of both the single and double ionisation probability, is still unsolved. This is because a finite basis describes the continuum states over finite distances. In that case, the numerically built positive energy states contain necessarily both single and double continuum components in addition to the fact that the two-electron single and double continuum states may be degenerate in energy. In order to isolate either the single or the double continuum component of the wavefunction we use the J-matrix method [1]. This method allows to generate within our Sturmian basis an accurate expression (with a proper asymptotic behaviour) of the single continuum wavefunctions. The double continuum component is then obtained by subtracting from the total wavefunction its projection on the accurate single continua. Switching to momentum space allows to extract the energy distribution of both ejected electrons.

The above method will be described in details and results for single and double ionisation probability will be presented and compared to experimental data and results obtained with other methods.

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Hyperfine structure studies in the framework of the Racah program

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Hyperfine experiments are now carried out routinely, leading to a large amount of valuable data for theoretical investigation and for comparison with *ab-initio* calculations of atomic properties.

The leading contribution to the hyperfine splitting of the atomic (fine-structure) levels is due to the magnetic dipole and electric quadrupole interaction between the nuclear spin moment and the electrons. Using first order perturbation theory in a non relativistic scheme, the interaction matrices A for the magnetic dipole and B for the electric quadrupole can be calculated for one open shell configurations in either LS - or jj -coupling. Procedures express the matrices as a linear combination of exact spin-angular parts using Racah's algebra and (variables) effective single electron parameters. These effective parameters are products of nuclear properties (magnetic dipole moment or electric quadrupole moment) and radial integrals (proportional to r^{-3}). Experimental data on hyperfine structure give the A - and B - factors, allowing a least square fit to the effective parameters leading to better wave functions. *Ab initio* calculations of the parameters allow a direct comparison with experimental data. Moreover, comparison of the various parameters gives further insight into the atomic interactions, i.e. into the relativistic effects and/or configuration interactions and, hence, allow for to draw conclusions about the nuclear magnetic dipole moment μ and the electric quadrupole moment Q .

With the present extension to the RACAH program [1,2] we implemented procedures for hyperfine structure calculations based on the effective operator approach developed by Sandars and Beck [3]. The evaluation of matrix elements of hyperfine structure operators is based on [4].

In practise, a single MAPLE line return the matrix element of the magnetic-dipole or electric-quadrupole hyperfine structure constant in terms of the one electron splitting parameters. Both, expression in the LS - and jj -coupling scheme can be derived and expressed in terms of radial integrals with the associated nuclear properties. Least-square-fit to experimental deduced hyperfine constants is implemented. Additional MAPLE procedures allow the calculation of the energy splitting and the transition strength. A simulation of the spectral lines between two hyper fine levels can be plotted.

Together with the shell notation introduced earlier [2] one now has a useful tool to perform hyperfine structure analysis of spectra without concerning about tedious RACAH algebraic manipulations.

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Lifetime measurements in highly ionized Xe

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Spectra and lifetimes of highly ionized Xe (III-VIII) have been recorded using the beam-foil technique. The light, analysed by a 1 m Seya-Namioka spectrometer, was detected by a thin back-illuminated, liquid nitrogen cooled, CCD working under vacuum. The efficiency of the whole apparatus extends from 40 to 200 nm and the CCD detection allows fast recording of spectra by chunks of 20 nm. In practice, images are recorded every 10 nm and a specially written computer code reconstructs the whole spectrum by adding the successive images.

Lifetimes have been measured by recording the decay of light observed when the excitation foil is moved upstream along the ion beam axis. Thanks to the CCD detector, many lines could be recorded simultaneously. The lifetimes have been deduced from the fitting of the whole decay curves (including the growing-in part at the beginning of the curve).

In Xe V, the experimental results will be compared with theoretical values obtained with a partly relativistic approach.

Autoionizing Rydberg series $n_c p_{1/2}^5 n \ell' [K']_J (\ell' = 1, 3)$ of the rare gas atoms: comparison between theory and experiment

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In a combined theoretical and experimental effort we have studied even autoionizing Rydberg states $Rg(n_c p_{1/2}^5 n \ell' [K']_J) (\ell' = 1, 3)$ of the rare gas atoms $Rg = \text{Ne, Ar, Kr, and Xe}$. Experimentally, we used both ion and ZEKE-PFI spectroscopy involving single photon excitation of members of the np' and nf' resonance series from the metastable $Rg(n_c p_{1/2}^5 - ns^3 P_2)$ level [1] to determine the energies (quantum defects) as well as the widths or lifetimes of these resonances. Theoretically, the quantum defects and the reduced widths of the resonances were calculated within the configuration interaction Pauli-Fock approach including core polarization (CIPF CP) [2,3]. The most significant many-electron effects influencing the decay dynamics are the polarization of the atomic core by the Rydberg electron and photoelectron, the correlational decrease of the Coulomb interaction and the interaction between Rydberg states. From a theoretically-guided analysis of the measured complex resonance profiles we clarify the role of the different contributing resonance components and we derive reduced resonance widths which are compared with the theoretical predictions and results from previous experimental work [1-6].

This work has been supported by the Deutsche Forschungsgemeinschaft through the grant 436 RUS 17/13/01 and 436 RUS 17/1/02 and by grants from the Israeli Science Fund and from the James Franck programme in Laser Matter Interaction.

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Collisional-radiative model DESNA for atomic spectra calculations of non-LTE plasmas in a wide range of plasma parameters.

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Calculated absorption and emission spectra of plasma are required for many applications connected with emitting multicharged ion plasma for interpretation of experimental data and some other tasks. Earlier we presented a collisional-radiative model for the calculation of ionization composition and excited level populations [1]. The main purpose of this report is to present a new simple and exact enough model DESNA developed on the base of previous model.

The DESNA model is intended to calculate such optical characteristics of nonequilibrium plasma as emission and absorption spectra, mean opacities, and radiation energy losses. The name DESNA shows a main peculiarities and properties of this model. In the model we used detailed configuration accounting (meaning of letter **D**) including the splitting into configurations and terms. The excited level populations are calculated by solving a system of equations of level kinetics (**E**). Calculations of atomic spectra are carried out for steady-state (**S**) plasma with the given temperature and density. Since we consider both the collisional and radiative processes, the state of plasma is nonequilibrium (no local thermodynamic equilibrium or coronal equilibrium, letter **N**). This allows us to calculate the spectra in a wide range of plasma temperatures (1 eV - 10 keV) and densities (10^{-6} - 10 g/cm³). The rates of recombination and ionization in the model are calculated by commonly used approximations. The needed for the calculations atomic data (**A**) on the energy levels and spontaneous radiative transition probabilities (or oscillator strengths) were extracted from freely available in the internet databases, mainly TOPBASE, NIST Atomic Spectra Database, CHIANTI. Full list of such databases is given in [2]. By numerical codes based on the DESNA model we have calculate the properties of plasma of a complicated composition. At present time in model included atomic data for multicharged ions such as H, Be, C, N, O, F, Mg, Al, Si, Ar and it is possible to produce the optical properties for arbitrary mixtures. On the base of DESNA model have been done interpretation of numbers of the experiments on the interaction of laser pulses with targets from different materials [3].

In this paper we shall present a description of physical-mathematical model DESNA. Some results of comparison of spectra with published calculation results of other models and with experimental data will be described, as well as the plans on the development of DESNA model.

This work is partially supported by grants ISTC 2165 and RFBR 02-01-00185.

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The influence of plasma nonequilibrium ionization state on spectra and mean opacities of the multicharged ion plasmas.

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The results of a theoretical investigation of the importance of radiative processes under a formation of atomic spectra of multicharged ion plasma are reported. An approximation of nonequilibrium ionization state of plasma (or plasma in collisional-radiative equilibrium, CRE) correlates more precisely with conditions of real experiments, in comparison with the LTE approximation. For example, in plasma of laser targets at various stages of interaction process, the plasma can be found both in the equilibrium state (LTE or coronal equilibrium) and in the intermediate CRE state when it is essential to consider the whole collection of elementary processes. Calculations of plasma optical coefficients were carried out by means of a collisional-radiative model DESNA [1] and the programs on its base. The model produces satisfactory results in a wide range of changing electron temperatures $T_e=1\text{ eV}\div 10\text{ keV}$ and ion concentrations $N_i=10^{14}\div 10^{24}\text{ cm}^{-3}$, including both the equilibrium ionization state of plasma and the nonequilibrium conditions.

It is shown, that under certain conditions the equilibrium approximations turn out to be inapplicable, and for the calculation tasks and interpretation of experimental data it is necessary to consider both the collisional and radiative processes. In particular, the influence of photorecombination and spontaneous radiative transitions on the results of calculations of spectral emissivity was investigated for modeling of experimental spectra obtained at interaction of powerful ultrashort laser pulses on targets of various compositions. Moreover, the comparison of results was carried out for a series of model situations when the Rosseland and Planck mean opacities were calculated for two cases: 1) LTE approximation and 2) the common case when equilibrium is absent. Also the questions connected with the influence upon spectra of photoionization and photoexcitation processes are discussed. The role of such processes becomes essential in the presence of strong radiation fields.

This work is partially supported by grants ISTC 2165 and RFBR 01-02-17336.

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Stark effect in atomic helium in high electric field up to 1500 kV/cm.

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In the spectral range between 480 nm and 630 nm the Stark effect of the transitions $n^1Q - 2^1S$, $n^1Q - 2^1P$ and $n^3Q - 2^3P$ ($n = 3 \div 9$, $Q = S, P, \dots$) has been studied using electric field up to 1500 kV/cm.

The experimental arrangement was similar to that used by L. Windholz and co-workers in numerous Stark effect investigations [1]. The spectra have been measured perpendicular to direction of the electric field, using a stigmatic three prism spectrograph. The spectra were recorded on the spectroscopic plates. The shifts of the Stark components were measured against unshifted lines, which were recorded on the same plate as exposure without field. For this measurements a modified Abbe comparator coupled with a computer processing set was used.

At low electric field the Stark components of atomic lines are resolved and their individual positions can be precisely determined by spectroscopic photometry. Problem arise at very high electric field when the Stark splitting becomes greater than the fine structure of atom and additionally occur anticrossings of the Stark components. Then the identification of components with respect to the magnetic quantum number is extremely difficult. For such cases the computer technique become very useful. The theoretical description of the Stark splitting should take into account large number of interacting levels corresponding to different shells with different main quantum numbers n . In our computer program we considered electric field interaction between levels with $n = 1 \div 8$. The agreement between performed calculations and experimentally determined position for transitions $n^1Q - 2^1S$, $n^1Q - 2^1P$ and $n^3Q - 2^3P$ ($Q = S, P, \dots$) for $n = 3 \div 5$ are satisfactory [2].

This work has been supported by the University of Gdańsk grant BW 5200-5-0120-3 and the KBN Committee grant 127/E-335/S/2002/2003 for Scientific and Technical Cooperation between Poland and Austria.

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Hyperfine structure for neutral manganese lines of astrophysical interest

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The hyperfine structure of 40 levels of neutral manganese has been studied by mean of Fourier transform emission spectroscopy. In the wavelength region 2000 to 20 000 cm⁻¹ we have recorded new spectra with the Bruker IFS120 Fourier transform spectrometer of the University of Liège using several different detectors and beamsplitters (resolution 0.03 cm⁻¹). In addition, we have analyzed a spectrum previously recorded at the National Solar Observatory on Kitt Peak (USA).

The light source was a home-made 99,5% pure manganese hollow-cathode lamp filled with a gas mixture of 14% helium, 29% argon and 57% neon at a total pressure of 2-3 mbar. Most of the spectra were recorded with a current between 200 and 900 mA.

From the observation of the Mn I HFS patterns of more than 70 transitions, it was possible to derive the magnetic dipole constants for 40 levels. Among these, we have been able to deduce new magnetic dipole constants for 18 levels and to revise previous results for 22 additional levels. For analyzing the data, we followed the same fitting procedure as for V I [1].

At the meeting, we will describe the experimental device and present our results.

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Studies of metastable lifetimes in Ti^+ , Ar^+ and Fe^+ in a ion storage ring

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Most ions and atoms have levels which are not allowed to decay radiatively by electric dipole transitions (E1). These states are denoted metastable. The metastable states can usually decay radiatively by magnetic dipole (M1) or electric quadrupole transitions (E2), emitting so-called forbidden lines. The probabilities for such transitions may vary over a wide range. At the ion storage ring CRYRING at the Manne Siegbahn Laboratory in Stockholm [1], we have developed a Laser Probing Technique (LPT) for studies of metastable levels in single-charged ions [2,3]. For lifetime measurements in complex atomic systems it is necessary to have a highly selective technique since these systems can have a number of close lying metastable levels. With the LPT, which combines laser excitation and an ion storage ring, such high selectivity is obtained. To estimate the contribution from the collisional destruction rate, which is pressure dependent, the lifetime measurement are made at different pressure points.

The LPT method described above have been used for measurements of the extremely long lifetime of the $3d^2(^3P)4s\ b\ ^4P_{5/2}$ level in Ti II. This is the longest lifetime ever measured in a storage ring. Due to the fact that this level had a extremely long lifetime, the data analysis of the recorded data required special caution. The repopulation of this level gave extra significant contribution to the measured decay curve. Substraction of the repopulation curve from the decay curve changed the lifetime by more than 30%. The pressure was changed to estimate the collisional destruction rate. The pressure points plotted versus the decay rate shows a good linearity within error bars. The fitted repopulation curves were subtracted from the lifetimes curves and the resulting curves were fitted by a single exponential function. The radiative lifetime were estimated to 28 ± 10 s for this level.

The lifetime of the $3d\ ^4F_{9/2}$ level at Ar II was measured with the same method. The plot with pressure points versus decay rate shows a good linearity within error bars. When the fitted repopulation curves were subtracted from the lifetime curves and the resulting curves fitted further by a single exponential function, the lifetime of this level was found to be 5 s.

Similar measurements have also been performed on the $4d\ ^4D_{7/2}$ level in Kr II. These measurements are presently being analyzed.

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Electronic correlation effects in endohedral Mg (Mg@C₆₀)

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We have studied theoretically the atomic structure of endohedral Mg (Mg@C₆₀) with particular emphasis on doubly excited bound and autoionizing (AI) states. We model Mg@C₆₀ as a system of two active electrons outside a frozen, doubly-charged ionic core, confined by a spherically symmetric potential well of finite depth. The parameters of the confining well (radial distance from origin, depth, width) provide a reasonable description of the C₆₀ cage. They have been determined in order to reproduce the experimentally measured photoionization cross-section of C₆₀.

We employed a suitable B-spline basis set within a CI approach to calculate the two-electron states of the confined system. This approach had in the past yielded excellent results for the Mg atom. It has proven equally efficient in the calculation of the spectrum and transition matrix elements of the confined system. Specifically, we have been able to calculate the bound states of S, P and D symmetry as well as the corresponding AI states lying above the first ionization threshold. In addition, we have calculated bound-bound transition matrix elements, as well as the photoionization cross section in a limited energy range above the first ionization threshold.

The most important conclusions of our study can be summarized as follows:

(1) one or two doubly-excited perturbers appear in each regular singly-excited Rydberg series of bound states. They are composed of two-electron configurations built with those one-electron orbitals mostly affected by the confining potential

(2) the low-lying part of the AI spectrum for each symmetry analysed, is perturbed by states novel to the confined system, whose configuration expansion is again dominated by the one-electron orbitals mostly affected by the confining potential;

(3) the AI widths of these novel AI states vary over a wide range of values

(4) the AI widths of AI states whose counterparts can be found in the Mg atom are also moderately affected

(5) the dipole couplings between bound states are moderately modified compared to the corresponding ones in Mg, while the variation is significant in the couplings to the doubly-excited perturbers

(6) the photoionization cross section in a limited energy range (a few eV) above the ionization threshold is structured by the AI resonances in a way markedly different from the corresponding Mg atom cross-section.

In conclusion, our study has revealed that electronic correlation is subtly affected by the confining potential. Novel features modify both the bound and the AI spectrum while the interaction with laser fields can clearly identify these novel features. Further study is under way in order to explore the effects of non-spherically symmetric confining potentials and of asymmetric confinement.

Acknowledgement

This research has been supported by a Marie Curie Fellowship of the European Community programme **Improving Human Research Potential and the Socio-economic Knowledge Base** under contract number **HPMF-CT-2002-01592**

Radiative lifetimes of excited states of ZnI and ZnII

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In the present work radiative lifetimes of 12 levels of ZnI belonging to the $4sns$ ($n=4-7$) series and 5 levels of ZnII belonging to the $3d^{10}4p$, $3d^{10}5s$, and $3d^{10}4d$ configurations have been investigated.

The lifetimes were measured using time-resolved laser-induced fluorescence technique.

Free atoms and ions were obtained by laser ablation using a Nd:YAG laser with 10ns pulse duration. The laser system for excitation of ZnI, ZnII states consists of two tunable dye lasers. The first one has a pulse duration of about 1.2ns which was achieved by compressing the dye laser pulse using Stimulated Brillouin scattering. The second laser has a pulse duration of 8 ns. The UV radiation was obtained by doubling and tripling the laser frequency and, for different states, we used also Stokes and anti-Stokes components of the 2ω , 3ω frequencies. All three lasers were synchronized. The excitation was delayed from the ablation pulse in order to avoid recombination processes.

The resonance ZnII $4p\ ^2P_{1/2, 3/2}$ states were excited in a single step (1ns) from the ground ZnII $^2S_{1/2}$ state. The ZnII $4d\ ^2D_{3/2, 5/2}$ and $5s\ ^2S_{1/2}$ states were populated by two-step excitation via the resonance ZnII $4p\ ^2P_{1/2, 3/2}$ states.

The $4d\ ^3D_3$ and $5d\ ^3D_3$ levels of ZnI were excited in a single excitation step from the metastable $4p\ ^3P_2$ ZnI level, which is populated in the laser ablation. The $nd\ ^3D_{1, 2}$ ($n=4-7$) and $ns\ ^3S_1$ ($n=6-8$) levels were excited by two-step excitation via the $4p\ ^3P_1$ level.

The spectral lines were registered using a grating monochromator, a Hamamatsu R3809U-58 photomultiplier and a fast digital oscilloscope (Tektronix Model DSA 602). The decay curves were averaged over 1000 laser pulses and were stored in a personal computer.

The experimental results have been compared with theoretical lifetime values calculated with a relativistic Hartree-Fock approach taking core polarization effects into account.

The results obtained allow to consider the dependence of the radiative lifetimes of the investigated excited states upon the effective principle quantum number.

The present results are compared with the available theoretical and experimental data available in the literature.

Acknowledgments

This work was supported by the European Community, under the Programme "Access to Research Infrastructures", Contract HPRI-CT 1999-000 41. Some of us (G. Malcheva, K. Blagoev and V. Pentchev) are grateful to the colleagues from the Lund Laser Center for their kind hospitality and support.

Transition probabilities in AgII spectrum

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In this work experimental transition probabilities for lines arising from $4d^8 5s^2$, $4d^9 6s$ and $4d^9 5d$ configurations of AgII have been determined for $4d^8 5s^2 - 4d^9 6p$, $4d^9 6s - 4d^9 6p$, $4d^9 5d - 4d^9 6p$ transitions.

A plasma produced by laser ablation was employed as a source of AgII spectrum. A focused Nd:YAG laser beam was used to generate the plasma on the surface of a silver target in argon atmosphere. A Nd:YAG laser generates 240 mJ pulses (7ns duration) at 10640Å. The light emitted by the laser produced plasmas was focused on the input slit of grating monochromator which has resolution 0.3Å. A time-resolved optical multichannel analyzer system allowed the detection and digital analysis of each spectrum. Spectral response calibration of the experimental system was made using a deuterium lamp in the wavelength range from 2000 to 4000Å, and a tungsten lamp in the range from 3500 to 6000Å.

The obtained spectra were treated by a program which allows to separate overlapping lines and to define their relative intensities. The obtained results are preliminary. The transition probabilities were obtained using measured branching ratio and experimental [1] and theoretical [2] data for radiative lifetimes of the corresponding states: $4d^8 5s^2$ [3], $4d^9 6s$ [1,2], $4d^9 5d$ [1,2].

Acknowledgments

K. Blagoev and G. Malcheva are grateful to the colleagues from the Department of Atomic Physics, Faculty of Physics, Madrid for their kind hospitality and support. This work was realized under Academy exchange programme.

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Transition probabilities between Stark states of Helium near the anticrossing field region

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A general method is worked out and presented for theoretical description of nonlinear response of multiplet atomic states to a uniform electric field. Among inert atoms, the atom of Helium is the simplest and the most interesting one, both in theoretical, and in experimental regard. It was just in Helium that the influence of electric field was first discovered experimentally, not only on the spectral line frequencies, but also on their intensities.

We construct Perturbation Theory (PT) for the doublet atomic states in the electric field, which is applicable for triplet Helium levels, as those interacting in pairs. General analysis of a dependence of wave functions of a multiplet state and energy on electric field is carried out on the basis of an iterative procedure for the integral Schrödinger equation written in terms of the Green's function with mean energy $\bar{E}$ of the multiplet levels:

$$\Psi(\mathbf{r}) = \sum_{J'} a_{J'} \left[1 + G'_{\bar{E}}(\mathbf{r}, \mathbf{r}') \left(\hat{V}(\mathbf{r}') - \Delta E \right) \right]^{-1} | \varphi_{nLJ'} \rangle. \quad (1)$$

A uniform algebraic system of equations for the multiplet states $\varphi_{nLJ'}$ superposition coefficients,

$$\sum_{J'} a_{J'} [W_{JJ'} + (\epsilon_{J'} - \Delta E) \delta_{JJ'}] = 0, \quad (2)$$

where $W_{JJ'} = \langle \varphi_{nLJ} | \left[1 + G'_{\bar{E}}(\mathbf{r}, \mathbf{r}') \left(\hat{V}(\mathbf{r}') - \Delta E \right) \right]^{-1} | \varphi_{nLJ'} \rangle$ is the matrix of atom-field interaction operator $\hat{V}(\mathbf{r}')$, allows for writing the solution to the corresponding secular equation for the atomic energy ΔE as a series in powers of field, which is supposed to be on the order of the anticrossing field corresponding to the spin-orbit-coupling breakdown in the atomic multiplet. This procedure makes possible to take into account the interaction of multiplet sublevels with all atomic states, both from the discrete spectrum and from the continuum.

The high-order corrections to energy of Helium triplet states were analyzed in detail in [1]. In this paper we derive general analytical expressions of field dependence for wave function coefficients, radiation dipole matrix elements, and the radiation probabilities in the lowest non-vanishing orders of PT. We input the numerical data for the $n'^3S_1 - n^3P$ transitions in Helium atom. The superposition coefficients in (1), (2) turn out to be expressed in polarizabilities calculated for such states in [1].

Evaluations show that the superposition coefficients change not very significantly, up to the anticrossing region. Nevertheless, it turns out that such field strength corresponds not only to the multiplet splitting minimum, but also to the equivalence of probabilities for two different solutions (in the weak field limit the probabilities differ by the factor 2).

The change of atomic wave functions may be observed experimentally as the change of the corresponding line intensities. Such experiment may provide a good amount of spectroscopic information which can be useful not only for basic studies of the field-matter interactions but also for the development of methods for the dc-field control of atomic structures and for processing quantum information with the use of atomic ensembles in electromagnetic traps.

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Frequency mixing spectroscopy of atoms in electric and magnetic fields

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A dipole-forbidden three-wave resonance frequency mixing process in a gas of free Indium or Thallium atoms becomes dipole-allowed in a dc electric field. In addition, the field induces a coherent forward-scattering amplitude which may be written as:

$$U_{coh}^F = \frac{a}{\varepsilon \varepsilon'} \left[(R_{0\frac{1}{2}} + \frac{4}{5}R_{2\frac{3}{2}})\psi' - (R_{0\frac{1}{2}} + \frac{1}{5}R_{2\frac{3}{2}})\psi_1 + (2R_{0\frac{1}{2}} - \frac{1}{5}R_{2\frac{3}{2}})\psi_2 \right], \quad (1)$$

where $R_{LJ} \equiv \langle nP_{1/2} | r[g_{LJ}^{\omega_1} - g_{LJ}^0] r | nP_{3/2} \rangle$ is the linear combination of two second-order radial matrix elements (g_{LJ}^E is the radial Green's function of the energy E relative the ground state in the subspace of atomic states with orbital and total momenta LJ) for the dc-field-induced two-quantum dipole transition between the sublevels of the ground doublet state, $|nP_{1/2}\rangle$ and $|nP_{3/2}\rangle$; $\varepsilon = E_1 - E_0 - \omega_1 = \Delta - i\Gamma/2$ ($\varepsilon' = E_2 - E_0 - \omega' = \Delta' - i\Gamma'/2$) is a complex frequency detuning of the incident $\{\omega_1, \mathbf{e}_1\}$ and generated $\{\omega' = \omega_1 + \omega_2, \mathbf{e}'\}$ radiation, the factor

$$a = \frac{F_0 F_1 F_2 F'}{648} \langle nP_{1/2} | r | n'S_{1/2} \rangle \langle n'S_{1/2} | r | nP_{3/2} \rangle$$

is the field amplitude dependent factor which includes also the radial matrix elements of the dipole transitions from the upper resonant level $|n'S_{1/2}\rangle$ to the ground-state sublevels $|nP_{1/2}\rangle$ and $|nP_{3/2}\rangle$. The factors

$$\psi_1 = (\mathbf{e}_2 \cdot \mathbf{e}'^*) (\mathbf{e}_0 \cdot \mathbf{e}_1); \quad \psi_2 = (\mathbf{e}_1 \cdot \mathbf{e}'^*) (\mathbf{e}_0 \cdot \mathbf{e}_2); \quad \psi' = (\mathbf{e}_1 \cdot \mathbf{e}_2) (\mathbf{e}_0 \cdot \mathbf{e}'^*) \quad (2)$$

depend on the unit polarization vectors of incident ($\mathbf{e}_1, \mathbf{e}_2$) and generated ($\mathbf{e}'^*$) waves.

A constant magnetic field may also induce the coherent process although its amplitude U_{coh}^B remains dipole-forbidden [1]. Although U_{coh}^B looks similar to (1) and (2), the ratio Q between $E2$ and $M1$ contributions appears here, which is of interest for investigations of the parity nonconservation effects in atomic spectra. Therefore, an additional opportunity appears for determining this quantity from the interference of electrically and magnetically induced amplitudes.

Electrically and magnetically induced effects, both individual and their interference, are studied analytically. The polarization degree and circular dichroism for the coherent cross section are presented in terms of the resonant level widths, resonance detuning and relative orientation of the incident-wave and dc-field vectors. The dependence of the degree on the ratio of $E2$ and $M1$ amplitudes for the dipole-forbidden radiation transition between the first excited and the ground state is also given explicitly.

The analytical data may become useful for the frequency and polarization control of the non-linear process, for determining level position and width and in high-precision measurements of the atomic clock transition frequencies. The relation between $E2$ and $M1$ amplitudes within one and the same transition may be informative for experiments on the parity nonconservation phenomena in atoms.

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Radiative lifetime measurements and oscillator strength determination for transitions in Pr II and Nd II

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Pr II (Z=59) and Nd II (Z=60) accurate transition probabilities are needed in astrophysics for solving problems related to high overabundances of these elements in many types of stars like, e.g., the A and B stars or the ultra-metal-poor giant stars. New radiative lifetimes for 20 levels of Pr II and 24 levels of Nd II have been measured using the time-resolved laser-induced fluorescence (LIF) technique. The combination of these experimental values with theoretical branching fractions (BF) obtained with the pseudo-relativistic Hartree-Fock (HFR) approach [1] has allowed to determine oscillator strengths and transition probabilities for spectral lines of astrophysical interest in these two ions. In Pr II, configuration interaction was explicitly retained among the $4f^36s$, $4f^35d$, $4f^36d$, $4f^25d6p$, $4f^26s6p$, $4f5d^3$, $4f5d^26s$ and $4f5d6s^2$ odd-parity configurations and among the $4f^36p$, $4f^35f$, $4f^4$, $4f^25d^2$, $4f^26s^2$, $4f^26p^2$, $4f^25d6s$, $4f5d^26p$ and $4f5d6s6p$ even-parity configurations while, in Nd II, configuration interaction was explicitly retained among the $4f^35d^2$, $4f^35d6s$, $4f^36s^2$ and $4f^46p$ odd-parity configurations and among the $4f^46s$, $4f^45d$, $4f^35d6p$ and $4f^26s6p$ even-parity configurations. Detailed comparisons between theoretical and experimental lifetimes obtained in the present work and previous measurements will be discussed during the conference.

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Stark-switching technique for fast quantum gates in Rydberg atoms

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Atoms in highly excited Rydberg nL states are very sensitive to the external electric fields. Huge atomic sizes (growing as n^2) and huge dipole moments of Rydberg atoms can give a strong gain in dipole-dipole interaction between neutral atoms. This interaction changes the energies of Rydberg states, and may be viewed as a Stark shift in an atom placed in the dipole electric fields of other atoms. The energy of this atom thus depends on the states of neighboring atoms (whether they are in Rydberg or in low-excited state). This makes the Rydberg atoms attractive for generating the entanglement in experiments on quantum computing [1].

In order to implement such scenarios in practice, fast switching of the atom-light interactions is needed. A natural way would be the use of single-frequency stabilized cw sources with fast external modulators that require, however, a lot of optical elements and electronics. We propose to replace the modulators with much more simple and inexpensive Stark-switching technique.

An important question concerning the applicability of Stark-switching to quantum computers is: would this technique preserve the atomic coherences? The aim of the present work was to explore this problem experimentally for the microwave transitions in sodium Rydberg atoms. We realized a quantum interferometer of Ramsey type using a cw microwave radiation and Stark-switching technique. In the Ramsey interferometer atoms consequently interact with two microwave pulses. In our experiment, an electric field pulse detuned the microwave radiation from exact resonance and provided two interactions. Observation of Ramsey fringes of high contrast would indicate that coherence is really conserved at Stark-switching.

Experiments were made with the $37S_{1/2} \rightarrow 37P_{1/2}$ microwave transition in sodium Rydberg atoms [2]. Interaction with a cw microwave radiation was effectively controlled by a pulse of weak (<1 V/cm) electric field that manipulated the transition frequency near 70050 MHz. The pulse detuned the microwave radiation from exact resonance and induced additional phases to the wave functions of Rydberg states due to the quadratic Stark shifts. As a result, the Ramsey fringes were observable both at scanning the frequency of the microwave field and at scanning the strength of the electric field pulse. The experiment confirmed that this Stark-switching technique provides a fast and effective control of the atom-light interactions and preserves the atomic coherence. Possible applications of this technique to experiments on quantum computers will be discussed.

This work was supported by the Russian Foundation for Basic Research, Grant No. 02-02-16323, and partly by INTAS, Grant No. 2001-155.

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Partial wave analysis of photoionization of Kr into the $4p^45p$ states at the energy of $3d^9np$ resonances.

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Photoionization out of the ground state of the rare gas atoms is described in general by three partial waves: $j = J_1 - 1, J_1, J_1 + 1$ where j and J_1 are the angular momenta of photoelectron and ion, respectively (for $J_1 = 1/2$ only two partial waves are possible). Partial photoionization cross sections (PPICS) determine via the kinematics coefficients (i) the alignment $A_{20}(E_1 J_1)$ and (ii) orientation $O_{10}(E_1 J_1)$ of the residual ion and (iii) the total photoionization cross section $\sigma(E_1 J_1)$ into the respective ion state $E_1 J_1$. Therefore, the measurement of A_{20} and O_{10} together with the normalization condition provides the complete information to determine the *relative* PPICS [1-3]. The knowledge of the PPICS is important for understanding the photoionization dynamics because they are very sensitive to the interference between different photoionization pathways [4].

In the present paper we report measurements of A_{20} and O_{10} for selected $4p^45p(E_1 J_1)$ states of Kr. The experiments were carried out at the beamlines of BESSY II with linearly and circularly polarized radiation. Experimental details are given in [3]. The energy of the exciting photons was scanned with a bandwidth of 10 meV through the lowest $3d^9np$ resonances at 91.200 eV, 92.424 eV, and 92.564 eV. Main emphasis was given to the orientation O_{10} in order to investigate interference effects and deviations from the two-step model as predicted by our calculations for both A_{20} and O_{10} [4]. Preliminary results indicate a good agreement between experiment and theory.

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Radiative decay of doubly excited helium states

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The helium atom in the sense of a three-body-Coulomb-system is still an object of fundamental experimental and theoretical investigations.

Three series of doubly excited singlet states in helium are known. The states labelled (sp,2n+), (sp,2n-) and (pd,2n) were assumed to decay dominantly by autoionization until recently the competing radiative decay of the doubly excited states was observed by detection of the undispersed fluorescence [1,2].

The spectral analysis of the fluorescence was carried out [3] and a theoretical description was published [4] from which the partial fluorescence of the doubly excited helium states for decay into the 1sms and 1smd singlet and triplet states can be extracted.

Our experiments confirm the theoretical predicted broad and complex decay pattern of the (sp,2n-) - states of the singlet system. For n=5 the 1s4s(1S) and 1s4d(1D) - states are favoured in the decay pattern. For n=6 its center moves to the 1s5s(1S) and 1s5d(1D) - states. Furthermore the dominant decay of the (sp,2n+) - states into the 1sns(1S) - states and of the (pd,2n) - states into the 1snd(1D) - states was observed in agreement with the calculations.

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Three-Loop Radiative-Recoil Corrections to Hyperfine Splitting in Muonium

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Recently we initiated a program of calculating of all three-loop radiative-recoil corrections to hyperfine splitting in muonium [1]. Three-loop radiative-recoil corrections are enhanced by the presence of the cube of the large logarithm of the electron-muon mass ratio [2]. All leading logarithm cubed and logarithm squared contributions of this order were calculated a long time ago [2-4]. As the first step of our program we obtained in [1] previously unknown single-logarithmic and nonlogarithmic radiative-recoil corrections of order $\alpha^2(Z\alpha)(m/M)\tilde{E}_F$ generated by graphs with two-loop polarization insertions (irreducible and reducible) in the two-photon exchange diagrams. As the next stage in implementing our program, we present below the results of the calculation of all single-logarithmic and nonlogarithmic three-loop radiative-recoil corrections generated by diagrams with one-loop electron and muon polarization insertions in the exchanged photons. There are four gauge invariant sets of such three-loop diagrams, and we calculate all their contributions. We obtained the three-loop single-logarithmic and nonlogarithmic corrections generated by the one-loop electron and muon polarization insertions in the exchanged photons [5]

$$\delta E_f = \left[\left(6 \zeta(3) - 4\pi^2 \ln 2 + \frac{83}{6} \right) \ln \frac{M}{m} + 29.88049 (6) \right] \frac{\alpha^3}{\pi^3} \frac{m}{M} \tilde{E}_F . \quad (1)$$

Combining this result with the result of our earlier paper [1] we obtain all three-loop single-logarithmic and nonlogarithmic corrections generated by the electron and muon polarization insertions in the exchanged photons

$$\delta E_{tot} = \left[\left(-4\pi^2 \ln 2 + \frac{67}{12} \right) \ln \frac{M}{m} + 9.59318 (6) \right] \frac{\alpha^3}{\pi^3} \frac{m}{M} \tilde{E}_F , \quad (2)$$

or, numerically

$$\delta E = - 0.028 \text{ 8kHz} . \quad (3)$$

This work was supported in part by the NSF grant PHY-0138210. Work of V. A. Shelyuto was also supported in part by the RFBR grant 03-02-16843.

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New Polarization Operator Contributions to Lamb Shift and Hyperfine Splitting

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Nonrecoil corrections of order $\alpha^3(Z\alpha)^5m$ to the Lamb shift and corrections of order $\alpha^3(Z\alpha)E_F$ to hyperfine splitting are generated by three-loop radiative insertions in the skeleton diagrams with two external photons. Respective corrections of lower orders in α generated by one and two-loop radiative insertions are already well known (see, e.g., review [1]). The crucial observation, which facilitates further calculations, is that the scattering approximation is adequate for calculation of all corrections of order $\alpha^n(Z\alpha)^5m$ and $\alpha^n(Z\alpha)E_F$. We calculate radiative corrections to the Lamb shift of order $\alpha^3(Z\alpha)^5m$ and radiative corrections to hyperfine splitting of order $\alpha^3(Z\alpha)E_F$ generated by the diagrams with insertions of radiative photons and electron polarization loops in the graphs with two external photons. We obtained corrections to the Lamb shift, and corrections to hyperfine splitting generated by eight sets of gauge invariant diagrams (for more details see [2]). The sum of all these contributions to the Lamb shift has the form

$$\delta E_L^{tot} = 2.651\,9\,(6) \frac{\alpha^3(Z\alpha)^5}{\pi^2 n^3} \left(\frac{m_r}{m}\right)^3 m, \quad (1)$$

or

$$\delta E_L^{tot} = 0.266\,53\,(6) \text{ kHz} \quad (2)$$

for the $1S$ level in hydrogen.

The sum of all new contributions to hyperfine splitting of order $\alpha^3(Z\alpha)E_F$ has the form

$$\delta E_{HFS}^{tot} = -1.358\,(1) \frac{\alpha^3(Z\alpha)}{\pi^2} E_F, \quad (3)$$

or

$$\delta E_{HFS}^{tot} = -0.001\,74 \text{ kHz} \quad (4)$$

for the ground state in muonium.

We also obtained the radiative-recoil correction to hyperfine splitting in muonium generated by the diagram with the τ polarization loop

$$\delta E_\tau = \left(\frac{6}{5} \ln \frac{m_\tau}{m_\mu} + \frac{51}{25}\right) \frac{\alpha(Z\alpha)}{\pi^2} \frac{m_e m_\mu}{m_\tau^2} E_F, \quad (5)$$

which numerically gives $\delta E_\tau = 0.0022 \text{ kHz}$ for the ground state in muonium.

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This work was supported by the NSF grant PHY-0138210. Work of V. A. Shelyuto was also supported in part by the RFBR grant 03-02-16843.

New Energy Levels of the Neutral Tantalum Atom

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In a continuation of our previous work, we have further investigated spectral lines of the neutral tantalum atom, which appear in high resolution Fourier Transform spectra and which can not be explained as transitions between already known energy levels. The search strategies for finding up to now unknown levels are explained in previous papers [1].

We have set the wavelength of a tunable dye laser to a strong hyperfine component of such an unclassified line, and have searched for laser-induced fluorescence transitions by scanning a monochromator which disperses the light emitted from our source of Ta atoms (a hollow cathode discharge in which Ta atoms are produced by sputtering). The wavelengths of these transitions, together with the information gained from the recorded hyperfine structure of the excited line, allowed us to determine the level energy, the total angular momentum, parity, and the hyperfine constants A and B.

J	Parity	Energy/cm ⁻¹	A/MHz	B/MHz	$\lambda_{excitation}/\text{\AA}$
9/2	e	33978.883	45(10)	100(100)	6577.695, 6589.95, 6400.11
5/2	e	34514.757	1594(3)	538(30)	6395.804
3/2	e	43781.527	422(10)	-135(50)	4344.872
5/2	e	43826.007	177(10)	-1106(50)	4336.489
3/2	e	47012.63	-477(2)	-1004(15)	4227.226, 4390.668
3/2	e	47124.64	786(4)	-900(50)	4207.298, 4421.992
1/2	e	48535.93	-1076(20)	0	4342.21, 5868.663
7/2	e	49246.359	228(2)	-1490(80)	6347.77, 6395.873, 6557.65
5/2	e	49683.38	742(5)	-380(60)	4260.697, 6374.86
13/2	o	53092.82	256(1)	2920(10)	4237.134
5/2	e	53302.234	388(11)	-280(50)	4461.536, 4495.978, 6730.235
5/2	e	53459.935	475(8)	-243(500)	4371.512, 4537.613
9/2	e	53845.84	945(1)	1145(25)	4479.875, 4494.160
11/2	e	54598.745	700(100)	0(200)	4333.658
11/2	e	54877.28	782(10)	811(50)	4281.958
7/2	o	54304.7	100(50)	3300(500)	4267.734

All given values are preliminary.

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 Part of the work was supported by the Austrian Science Fund, project no. 15625

Magnetically-induced frequency mixing spectroscopy of atoms

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Magnetic field may induce a coherent forward-scattering process of two-colour dipole-forbidden frequency mixing in a gas of free atoms. The amplitude for a double-resonance conversion in In or Tl atoms in their $n^2P_{1/2}$ ground states which includes the $E2$ and $M1$ parts with account for the incident waves and the magnetic field in the lowest (fourth) order, after integration over valence-electron angular variables, may be written as:

$$U_{coh} = \frac{\beta}{\varepsilon^2 \varepsilon'^2} \left[2\varepsilon'(1+Q)\varphi_2 + q \left(\varphi_2 - \varphi_1 - \frac{1-Q}{2}\varphi' \right) \right], \quad (1)$$

where $q = 3\varepsilon + 2\varepsilon'$, $\varepsilon = E_1 - E_0 - \omega_1 = \Delta - i\Gamma/2$ ($\varepsilon' = E_2 - E_0 - \omega' = \Delta' - i\Gamma'/2$) is a complex resonance detuning for the $E1$ -forbidden $|nP_{1/2}\rangle \rightarrow |nP_{3/2}\rangle$ ($E1$ -allowed $|nP_{1/2}\rangle \rightarrow |nS_{1/2}\rangle$) resonance, $\beta = \alpha B F_1 F_2 F' \langle nP_{1/2} | r | n'S_{1/2} \rangle \langle n'S_{1/2} | r | nP_{3/2} \rangle \langle nP_{1/2} | nP_{3/2} \rangle / 1296$ is the field amplitude dependent factor which includes also the radial matrix elements of the dipole transitions from the upper resonant level $|n'S_{1/2}\rangle$ to the ground-state sublevels $|nP_{1/2}\rangle$ and $|nP_{3/2}\rangle$, and $Q = 3\omega_1 \langle nP_{1/2} | r^2 | nP_{3/2} \rangle / (5 \langle nP_{1/2} | nP_{3/2} \rangle)$ is the ratio of the amplitudes $E2$ to $M1$, which is determined by the electric quadrupole radial matrix element of r^2 . The factors

$$\varphi_1 = (\mathbf{e}_2 \cdot \mathbf{e}'^*) ([\mathbf{n} \times \mathbf{e}_0] \cdot \mathbf{e}_1); \quad \varphi_2 = (\mathbf{e}_1 \cdot \mathbf{e}'^*) ([\mathbf{n} \times \mathbf{e}_0] \cdot \mathbf{e}_2); \quad \varphi' = (\mathbf{e}_1 \cdot \mathbf{e}_2) ([\mathbf{n} \times \mathbf{e}_0] \cdot \mathbf{e}'^*)$$

depend on the unit polarization vectors of incident ($\mathbf{e}_1, \mathbf{e}_2$) and generated ($\mathbf{e}'^*$) waves and the unit wave vector $\mathbf{n}$ in the propagation direction. Equation (1) makes possible a detailed analysis of the influence of polarization properties of waves on the cross section and efficiency of the wave-mixing process with generation of radiation with the frequency $\omega' = \omega_1 + \omega_2$. E.g., in the case of *linear polarization of the incident waves*, with the unit polarization vectors

$$\mathbf{e}_{1(2)} = \mathbf{e}_{1(2)}^* = \mathbf{e}_0 \cos \theta_{1(2)} + [\mathbf{n} \times \mathbf{e}_0] \sin \theta_{1(2)},$$

equation (1) may be written as

$$U_{coh} = \frac{\beta}{\varepsilon^2 \varepsilon'^2} \left[a(\mathbf{e}_0 \cdot \mathbf{e}'^*) + b([\mathbf{n} \times \mathbf{e}_0] \cdot \mathbf{e}'^*) \right], \quad (2)$$

where a and b are simple combinations of sine and cosine functions of the angles $\theta_{1(2)}$ with coefficients depending on the complex resonance detuning $\varepsilon, \varepsilon'$ and the $E2/M1$ amplitude ratio Q . As follows from equation (2), the amplitudes for the right and left circular polarization U_{coh}^+ and U_{coh}^- of the generated wave are different, so the degree of the wave's circular polarization

$$D' = \frac{|U_{coh}^+|^2 - |U_{coh}^-|^2}{|U_{coh}^+|^2 + |U_{coh}^-|^2} = \frac{2\text{Im}(a^*b)}{|a|^2 + |b|^2}.$$

may have essentially non-zero values, even far away from exact resonance when the angles θ_1 and θ_2 are thoroughly adjusted.

The circular dichroism may also be observed for one incident wave as the difference of generation efficiency for the right and left circular polarization when another wave is linearly polarized. It also originates from the dissipation processes during the frequency conversion and depends on the resonance level width. The dependence of polarization properties on the $E2/M1$ amplitude ratio Q may be determined from (1), (2) and may be used for measuring experimentally this ratio which is important for testing different calculation methods and for investigating the weak $e - n$ interaction effect on the optical atomic spectrum.

Two-colour frequency mixing spectroscopy of atoms in crossed electric and magnetic fields

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We consider interference of electric-field-induced and magnetic-field-induced amplitudes in a coherent mixing of two laser waves with frequencies ω_1 , ω_2 and the field vectors $\mathbf{F}_1 = F_1 \mathbf{e}_1$, $\mathbf{F}_2 = F_2 \mathbf{e}_2$, on atoms in their nS ground state, with singlet structure of resonant levels.

The dc electric $\mathbf{F}_0 = F_0 \mathbf{e}_0$ or magnetic $\mathbf{B} = B \mathbf{e}_B$ field may induce a coherent forward-scattering process of two laser waves frequency summation or subtraction in an atomic medium. The amplitude of electric field induced generation of a wave with frequency $\omega' = \omega_1 + \omega_2$ and the field vector $\mathbf{F}' = F' \mathbf{e}'$ in the lowest order resonance approximation ($|\varepsilon| \ll \omega'$) with a complex detuning $\varepsilon = E_{n_2D} - E_{nS} - \omega' = \Delta - i\Gamma_{n_2D}/2$ (the width of resonance level n_2D is taken into account), may be written as

$$U_F = A \left[(\mathbf{e}_0 \cdot \mathbf{e}_2)(\mathbf{e}_1 \cdot \mathbf{e}'^*) + (\mathbf{e}_0 \cdot \mathbf{e}_1)(\mathbf{e}_2 \cdot \mathbf{e}'^*) - \frac{2}{3}(\mathbf{e}_1 \cdot \mathbf{e}_2)(\mathbf{e}_0 \cdot \mathbf{e}'^*) \right], \quad (1)$$

where the factor

$$A = \frac{F_0 F_1 F_2 F'}{120\varepsilon} \langle nS | r [g_1^{\omega_1} + g_1^{\omega_2}] r | n_2D \rangle \langle n_2D | r [g_1^{\omega'} + g_1^0] r | nS \rangle$$

includes the field amplitudes, detuning and radial matrix elements of the second-order transition to and from the resonance state with absorption of incident photons and emission of generated one. The notation g_L^E is used for the radial Green's function in the space of states with orbital momentum L and energy E relative the ground state.

A similar equation may be written for the magnetic-field-induced amplitude

$$U_B = -Ab \frac{\alpha \omega' B}{4\varepsilon F_0} \left[([\mathbf{n} \times \mathbf{e}_B] \cdot \mathbf{e}_1)(\mathbf{e}_2 \cdot \mathbf{e}'^*) + ([\mathbf{n} \times \mathbf{e}_B] \cdot \mathbf{e}_2)(\mathbf{e}_1 \cdot \mathbf{e}'^*) \right], \quad (2)$$

where

$$b = \frac{\langle n_2D | r^2 | nS \rangle}{\langle n_2D | r [g_1^{\omega'} + g_1^0] r | nS \rangle} \quad (3)$$

is the ratio of the radial matrix elements for the first-order quadrupole and second-order dipole transition from the resonant excited state $|n_2D\rangle$ to the ground state $|nS\rangle$.

The interference between the amplitudes (1) and (2) in the sum-frequency scattering cross section is strongly dependent on polarization of incident and scattered waves, on the resonance detuning ε and on the ratio (3) of the radial matrix elements. So, for linearly polarized incident waves, $\mathbf{e}_1 = \mathbf{e}_2 \perp \mathbf{e}_0 = \mathbf{e}_B$, the coherent forward scattering cross section is

$$d\sigma \sim |U_F + U_B|^2 = \left| \frac{2A}{3F_0\varepsilon} \right|^2 \left| F_0\varepsilon(\mathbf{e}_0 \cdot \mathbf{e}'^*) + 3B\alpha\omega'b(\mathbf{e}_1 \cdot \mathbf{e}'^*) \right|^2. \quad (4)$$

It becomes evident, that the difference appears between the cross sections for the right and left circular polarization, which may result in the circular polarization degree of the generated wave

$$D' = \frac{d\sigma^+ - d\sigma^-}{d\sigma^+ + d\sigma^-} = \frac{4x}{1 + 4(\Delta/\Gamma_{n_2D})^2 + 4x^2}, \quad (5)$$

where $x = 3B\alpha\omega'b/(F_0\Gamma_{n_2D})$. Maximum absolute value of the degree (5) at exact resonance, $\Delta = 0$, corresponds to $x = \pm 1/2$. The energy dissipation determined by the level width may cause also the circular dichroism $D_{1(2)}$ — the difference of generation efficiency for the right and left circular polarization of the first (second) incident wave when the second (first) one is linearly polarized. The values of D' , D_1 , D_2 at given field strengths provide essential information on the atomic structure quantities, in particular, on the values of b and Γ_{n_2D} .

Transition Probabilities of Ne II Revisited

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A 1997 emission experiment by Griesmann et al. [1] for $3p - 3d$ transitions of Ne II produced some results in strong disagreement with then available calculational results, especially for the intersystem lines. Subsequent calculations narrowed the disagreements substantially, but some significant differences have remained. We have therefore focused a new emission experiment on some of these cases. Specifically, we investigated the branching ratios from three 3d levels. We operated a hollow cathode source in pure neon and measured relative line radiances at a pressure of 200 Pa and at currents from 0.3 to 1.2 A. The experimental setup was similar to that of Ref. [1], and we used again a 2 m monochromator with a photomultiplier for the spectral recording. The lines from each of the three investigated upper levels were measured as a set, and within each experimental run the lines were measured repeatedly to insure that the source conditions remained constant. The line intensities were obtained by measuring the area under each line profile, or, in the cases of partially blended lines, by fitting gaussian curves to the line profiles. The spectral response of the monochromator-photomultiplier system was obtained with a calibrated argon mini-arc, which has a strong signal in the near UV spectral region. Our resulting relative transition probabilities were normalized with available lifetime data. Very good agreement with the most recent calculations has been obtained, and possible reasons for the difference with the earlier experimental results are discussed.

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ATI of H_2^+ with short laser pulses at 228 and 400 nm

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In a recent paper [1] we have proposed a method, of spectral type, to solve the time dependent Schrödinger equation (TDSE) for a molecular ion in a laser field. We showed, in particular, that our approach allows to investigate above threshold ionization (ATI) in molecules. It is based on the expansion of the time dependent solution in terms of B-splines expressed in the prolate spheroidal coordinate system. The first application, in paper [1], concerned two- and three-photon ionization of H_2^+ with a photons energy of 0.6 a.u.. We focus here on the case of longer wavelengths, with (6+S) photon ionization of H_2^+ at the internuclear distances of $R = 2$ a.u. (with $\lambda = 228$ nm) and $R = 10$ a.u. (with $\lambda = 400$ nm). First, one has to solve the Schrödinger equation describing the motion of the electron in the field of the nuclei:

$$(H - E)\Psi = \left(-\frac{1}{2}\Delta - 2\frac{(Z_1 + Z_2)\xi - (Z_1 - Z_2)\eta}{R(\xi^2 - \eta^2)} - E\right)\Psi = 0 \quad (1)$$

We have introduced the prolate spheroidal coordinates $\xi = (r_1 + r_2)/R$, $\eta = (r_1 - r_2)/R$ and ϕ with $1 \leq \xi < \infty$, $-1 \leq \eta \leq 1$ and $0 \leq \phi \leq 2\pi$. The solution of the above equation takes the form $\Psi = Z(\xi, \eta) \frac{e^{im\phi}}{\sqrt{2\pi}}$. In order to solve the equation (1), $Z(\xi, \eta)$ is expanded on a basis of B-spline products:

$$Z(\xi, \eta) = (\xi^2 - 1)^{|m|/2} (1 - \eta^2)^{|m|/2} \sum_{i=1}^{N_\xi} \sum_{j=1}^{N_\eta} c_{ij} B_i^k(\xi) B_j^k(\eta) \quad (2)$$

B_i^k denotes the i th B-spline of order k (see de Boor 1978 [2]). In our case $k = 7$, $N_\eta = 20 - 25$ and $N_\xi = 300 - 400$. The diagonalization of the equation (1) in the basis set of B-spline products directly provides the full spectrum of H_2^+ (bound and continuum states) with a high degree of accuracy. One of the advantage of using the above expansion is that it leads to band-structured symmetric matrices with a matrix band width of $2k * N_\eta$, thus a considerable amount of cpu time and memory is saved. The system is solved within an ellipsoidal box by setting a maximum value ξ_{max} for ξ ($R \xi_{max} = 600 - 800$ a.u. here), with the usual condition $Z(\xi_{max}, \eta) = 0$ at the limit of the box. Once the stationary states and dipole couplings are obtained, the TDSE is solved by expanding the solution on the basis of the field-free stationary states. An explicit Runge-Kutta numerical procedure is used to solve the time dependent equation system.

We have investigated the case of the photoionization of H_2^+ at the equilibrium internuclear distance $R = 2$ a.u., with a laser frequency of 228 nm. The laser pulse has a $\cos^2$ shape with a maximum intensity of 10^{14} W/cm² and its total duration is about 7.5 femtoseconds (fs). The calculations being performed in the approximation of the fixed nuclei, it is only valid for an effective laser-molecule interaction time much shorter than the vibrational period, which is the case here (the period of the lower vibrational state is about 14 fs).

The other case we investigated is the photoionization of H_2^+ at $R = 10$ a.u., with a laser frequency of 400 nm. The other characteristics of the laser pulse are close to the previous ones.

The results, and in particular the ATI spectra, will be presented at the conference.

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Wave packet simulation of the nonadiabatic competitive dissociation of excited bromoacetyl chloride

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The competitive photodissociation of bromoacetyl chloride in the first excited state is now a standard example illustrating the role of nonadiabatic interactions in chemistry. Experimental works by Butler et al. [1] have shown a preferential fission of C-Cl over C-Br following the [n_O , π^*_{CO}] excitation in a photolysis with 248 nm photons. This would not be predicted on the single adiabatic $^1A''$ state because the barrier heights are in favor of the C-Br fission. Very high nonadiabatic interactions with the second $^1A''$ excited state lead to a trapping in the diabatic potential and recrossing of the transition state region. The effect is more efficient for C-Br fission than for C-Cl fission. The ab initio study of this large molecular system is particularly challenging since it concerns excited states. We have adopted a strategy based on a strong interaction between

- Computation of different cuts in the PES with MOLPRO code by a state average CASSCF calculation including the two $^1A''$ excited states
- Quantum dynamics simulation in reduced subspaces with constrained Hamiltonians using the Tnum algorithm [2] which generates the kinetic energy operators automatically in any sets of coordinates.

The different steps in probing the photodissociation are [3]

- Preliminary 2D simulations of the relaxation of C=O and Br-C-C-Cl torsion angle. This shows that the dissociation can be treated in trans geometry.
- 1D test of the nonadiabatic dissociation in trans geometry. Propagations of Gaussian wave packets for each channel give a branching ratio estimated from the asymptotic populations C-Cl:C-Br which reproduces a preferential breaking along the C-Cl bond.
- 2D study in subspaces C=O, C-Br and C=O, C-Cl. A relevant model of diabatic states is fitted to the ab initio PES. Energy resolved cross section are extracted from wave packets.

Perspectives

- 3D study in subspaces C=O, C-Br and C-Cl.
- Modeling of similar polyatomic systems with avoided crossing by the MCTDH method.

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Exciting-photon energy dependence of the N_2 double photoionization cross section into the $N_2^{2+} D \ ^1\Sigma_u^+$ state

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In a recent study [1] the exciting-photon energy dependence of the double photoionization (DPI) cross section for the $N_2^{2+} D \ ^1\Sigma_u^+(v')$ state was estimated by measuring the $N_2^{2+} : D \ ^1\Sigma_u^+(v') \rightarrow X \ ^1\Sigma_g^+(v'' = v') + h\nu_{fl}$ fluorescence. However, due to poor statistics, a complete analysis of the energy dependence of the DPI process has been difficult. Also it was not completely clear why the bands with different vibrational quantum number $v'' \neq v'$ were absent in [1] whereas they have been predicted in [2]. Therefore it appeared worthwhile to investigate the discussed molecular DPI process again, both experimentally and theoretically.

In the present work the photon-induced fluorescence spectroscopy (PIFS) [3] was applied to investigate the discussed molecular DPI process with drastically improved signal-to-noise ratio. The experiments were performed at beamline U 125/1-PGM of the synchrotron radiation source BESSY II, Berlin. Gaseous N_2 in a natural isotope mixture was excited with photons of energies between 50 eV and 66.5 eV using a target cell at a temperature of 300 K. The target gas pressure in the cell was 2.67 Pa. The bandwidth of the exciting-photons was set to 30 meV and the fluorescence resolution to $\Delta\lambda = 0.2$ nm.

To explain the absence of the measured fluorescence corresponding to the $v'' \neq v'$ transitions extensive calculations of the potential curves for the X and D states of N_2^{2+} ion were performed within the Multi-Reference Configuration-Interaction approach. The calculated potential curves of the N_2^{2+} X and D states are obtained very similar around the equilibrium internuclear distance. As a consequence the calculated intensities of the $v'' = v' + 1$ and $v'' = v' - 1$ fluorescence transitions amount to 1/135 and 1/570, respectively, and are very weak with respect to the $v'' = v'$ transition.

The exciting-photon energy dependences of the DPI cross sections, $\sigma_D^{2+ \ ^1\Sigma_u^+}(\omega)$, was calculated within the independent atom approximation taking the monopole rearrangement of electron shells into account. A good agreement between the measured and calculated exciting-photon energy dependences of $\sigma_D^{2+ \ ^1\Sigma_u^+}(\omega)$ was obtained.

Acknowledgements

This work was funded by the Deutsche Forschungsgemeinschaft. PhVD gratefully acknowledges the fellowship of the Alexander-von-Humboldt-Stiftung (RUS/1070409).

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The electronic states of isoxazole studied by vuv absorption, electron energy-loss spectroscopies, and He(I) photoelectron spectroscopy

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The VUV absorption spectrum of isoxazole has been recorded for the first time in the energy range 5 to 10.8 eV (250-115 nm). The molecule has also been probed using electron impact with electrons of different incident energies and the He(I) photoelectron spectrum has been re-measured.

Most of the intensity in the VUV absorption spectrum is from excitation of states of $^1\pi\pi^*$ character.

The first two $^1\pi\pi^*$ states are found to lie at about 6 and 7 eV, respectively, and are separated by a state of type $^1\sigma\pi^*$, where σ is nitrogen lone pair. The lowest-lying triplet states, located at about 4.1 eV (290 nm) and 5.3 eV (225 nm), respectively, are $^3\pi\pi^*$.

Short-lived anionic states (electron-molecule resonances) have been detected in both inelastic scattering and dissociative electron attachment channels.

For the first band of the He(I) photoelectron spectrum we find ionisation energies of 9.942 +/- 0.002 eV (adiabatic) and 10.120 +/- 0.002 eV (vertical). Well-defined vibrational structure is apparent in this band. For the second electronic band, two peaks are observed at 11.108 +/- 0.002 eV and 11.258 +/- 0.02 eV, respectively.

Velocity redistribution of excited atoms by radiation trapping studied by field-free imaging of photofragmentation of Na₂

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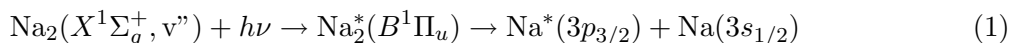
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Photodissociation of state selected sodium molecules,



has been studied theoretically and experimentally using a novel "field-free" ion imaging design. The experiment uses a supersonic Na/Na₂ beam. Prior to the dissociation, the Na₂ molecules are prepared in selected rovibronic levels of the electronic ground state using the STIRAP technique[1]. The Na^{*}(3p_{3/2}) fragments are photoionised (or excited to high Rydberg states) in a permanently field-free reaction zone. The fragments enter the ion optics because of the flow velocity of the beam and are focused onto a position sensitive detector, which provides an energy resolution of about 50 meV.

The measured images show not only the expected relatively fast photodissociation fragments, but also efficient formation of slow Na(3p_{3/2}) atoms. Fast and slow refer to the atomic velocity relative to the centre-of-mass of the dissociating molecule. The ratio of the numbers of slow atoms and fast photofragments is 0.16 and 0.22 for the dissociation of Na₂ from levels v'' = 17 and v'' = 23, respectively.

Table I. Experimental and theoretical data on the ratio of slow to fast Na(3p_{3/2}) atoms for photodissociation from the vibration levels v'' = 17 and v'' = 23.

Na ₂ v''-level	N _{Na_{slow}} /N _{Na_{fast}}		
	Experiment	theory without HFS	theory with HFS
17	0.16	0.26	0.13
23	0.22	0.21	0.19

Several models are analysed to explain the observations. Calculations show that the dramatic velocity redistribution is caused by radiation trapping [2] : the excitation is efficiently radiatively transferred from the fast Na(3p) photofragments to the abundant Na(3s) atoms from the primary beam, whereby the hyperfine splitting of the 3s state must be taken into account. Analytical formulae describing this mechanism show a ratio of slow to fast Na(3p) atoms of 0.13 for v'' = 17 and 0.19 for v'' = 23, which is in very good agreement with the experimental observations (see Table I).

This work was partially supported by INTAS-2001-155.

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Radiative properties, angular momentum and magnetic couplings of ungerade states of Te_2

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The Te_2 molecule is a challenging object for *ab initio* calculations and high-resolution spectroscopy due to the high density and complexity of molecular terms strongly affected by spin-orbit interaction converging to the $^3\text{P}_2 + ^3\text{P}_2$ and $^3\text{P}_2 + ^3\text{P}_{0,1}$ states of separated atoms, i.e. those of particular importance for the laser-induced fluorescence spectroscopy in visible and infrared spectral region. Reliable calculated and measured energetic and radiative properties data concerning these states thus appear to be of interest, especially since tellurium vapor consisting mainly from tellurium dimers is obtainable in quartz glass cells at moderate temperatures, serving as a convenient source of wavelength standards. We present here the study of the system of ungerade electronic states of the tellurium dimer below $20\,000\text{ cm}^{-1}$ by means of the state-selective quasirelativistic version of the multireference many-body perturbation theory [1]. The calculations employed the shape-consistent relativistic pseudopotential of Kr-like atomic cores and extensive bases of density-averaged atomic natural pseudoorbitals. Numerous crossings and avoided crossings of potential functions were located. The predissociation of the $\text{B}1_u$ state can arise from the crossing between the corresponding potential curve and the (quasi) unbound (ii) 2_u one. The $\text{A}0_u^+ - (\text{ii})1_u$ curve crossing can be related to the radiationless decay of the former state. Matrix elements of the electric dipole operator, total electronic angular momentum and magnetic moment between the states under study as functions of the internuclear separation, required to estimate the rates of radiative and predissociative decay as well as lambda doubling of the states under study, were evaluated via perturbative construction of spin-free and spin-dependent one-body transition density matrices [2]. A good agreement of the computed lifetimes and transition dipole moment functions with their experimental counterparts [3] was achieved. The results of the calculations on angular momentum and magnetic transition matrix elements between the $\text{B}0_u^+$ and $\text{B}1_u$ states, as well as $\text{B}1_u$ diagonal magnetic matrix element agree well with there experimentally determined values. As a next step we plan to convert the R -dependences of electronic couplings into rovibronic matrix elements and to re-fit experimental data.

The work has been supported by the NATO SfP 978029 - Optical Field Mapping grant and by the Russian Foundation for Basic Researches (grant No. 03-03-32857), as well as by EC grant G1MA-CT-2002-04063.

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Fourier transform intracavity laser absorption spectroscopy

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We have built an experimental set-up connecting an Ar^+ pumped, home made Sa:Ti laser cavity to a commercial high resolution Fourier transform spectrometer Bruker IFS120HR, to perform ultrasensitive molecular absorption spectroscopy in the near infrared range. We shall report on the experimental technique and results, demonstrating an effective absorption path-length of over 40 km and spectral resolution close to 0.005 cm^{-1} .

Line intensities measurements in $^{14}\text{N}_2^{16}\text{O}$ and their treatment using the effective operator approach. II. The 5200 to 6400 cm^{-1} region

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This work continues a series of publications devoted to the application of the effective operators approach to the analysis and prediction of vibration-rotation spectra of linear triatomic molecules. In that frame, the present work aims at describing line intensities of cold and hot bands of $^{14}\text{N}_2^{16}\text{O}$ in its ground electronic state in the spectral range above 3600 cm^{-1} .

In N_2O , vibrational interacting levels group in polyads, identified by the so-called polyad number $P = 2V_1 + V_2 + 4V_3$, as a result of the relation $2\omega_1 \sim 4\omega_2 \sim \omega_3$ existing between the harmonic frequencies (ω_1 , ω_3 and ω_2 are the harmonic frequencies associated to the symmetric and antisymmetric stretching modes and the bending mode respectively).

The absorption spectra of N_2O , at room temperature, have been recorded in Brussels at high resolution over the whole range between 3600 and 11000 cm^{-1} using a Bruker IFS120HR Fourier transform spectrometer. The measurement and analysis of absolute line intensities in the region between 4300 and 5200 cm^{-1} , involving bands associated with transitions corresponding to $\Delta P = 7, 8$ and 9, was done recently [1]. We are now measuring absolute line intensities for cold and hot bands associated with transitions corresponding to $\Delta P = 10$ and 11, observed in the range from 5200 to 6400 cm^{-1} . Using wavefunctions previously determined from a global fit of an effective hamiltonian to about 18000 line positions [2], parameters of a corresponding effective dipole moment are then fitted to these experimental intensities. Results will be presented and discussed.

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Atomic and molecular spectroscopy with superbright light-emitting diodes

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We shall present our most recent absorption and emission experiments with heavy alkali vapor using superbright light emitting diodes from NICHIA, LUMILED and OSRAM. UV LEDs together with LEDs in the visible spectral region present invaluable narrow band continuum light source for very precise absorption measurements. We used all-sapphire cells in a usual absorption arrangement high resolution scanning monochromators. Beside self-broadened alkali resonance lines we investigated molecular bands and diffuse bands of alkali dimers similar to experiment in ref. [1].

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Nonradiative processes in the molecular systems with squeezed vibrational states in intensive laser field

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The multiphonon transitions in the eximer molecules in the field of the intensive electromagnetic wave are theoretically studied. The calculations are executed in the adiabatic approximation. The adiabatic potential of the excited electron-vibrational state is described by the parabolic dependence on the normal coordinates and the adiabatic potential of the ground electron-vibrational state of eximer molecule is presented as the repulsive term. It is shown, that the nonradiative decay processes of the eximer molecules in the intensive laser field are significantly activated and as result the luminescence processes are considerably suppressed. The probability of the nonradiative transition is calculated in the model of the line-coordinate perturbation [1]. If the creation of the eximer molecules is carried out by the supershort laser pulse, then in the excited electronic state the packet of the stationary states of the harmonic oscillator is formed (the squeezed vibrational states [2]). The existence of the squeezed vibrational states intensifies the processes of the multiphonon decay of the eximer molecules and modifies the kinetic processes. The conditions at which the time of the nonradiative decay can be commensurable with the radiation life time of the excited state of the eximer molecules were formulated

The theory of nonradiative transfer of the electronic excitation energy in the electron-vibrational systems in the field of an intensive electromagnetic wave is constructed too. The influence of the intensive electromagnetic radiation on the nonradiative transfer of energy in molecular (including excimer's) systems with nonzero electrical dipole moment is explicitly investigated. It's shown, that the squeezed vibrational states, which ones are derivated in the excited electronic state by means of a ultrashort laser radiation pulse, significantly increase probability of the energy transfer in molecular systems. In this case, the noticeable increase and nonmonotonous dependence of the transfer rate of energy on the electromagnetic field intensity are predicted.

The physical interpretation of the obtained results and the conditions of their experimental observation are also discussed.

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POSTER SESSION P2

The Effect of the Halogen Depletion Instability on Deposited Power in High Pressure Discharge Sustained XeCl Laser

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Theoretical studies of a phototriggered XeCl excimer laser have been performed through the development of a zero-dimensional model and used for conditions close to experiment for about 50 to 100ns laser pulse duration with electron power deposition in the MW/cm³ range and inside a 300 cm³ chamber. Time variation of the electron density is obtained by integrating the transport equation coupled to the heavy kinetic and the external circuit. This study provides the time variation of the discharge characteristics as well as the influence of the gas composition on these characteristics. The results have been discussed and analyzed. Calculated discharge current and voltage are also compared with experimental results. Finally, the use of the present model allows a good comprehension of the halogen depletion phenomena, which is the principal cause of laser ending and allows a simple study of the evolution of a large-scale non uniformity in preionization density and its effect on electrical and chemical plasma properties.

Modeling of argon glow discharges

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The basis of this work is one-dimensional fluid model of electrical properties of a argon glow discharge with planar electrodes. The results from this model are the spatial profiles of electric field, the charged particle densities, and ionization source term. The range of current densities considered is between 0.1 and 0.6 mA/cm². To calculate the gas temperature, we solve the one dimensional heat transport equation. The gas temperature profile is reintroduced into the electrical model. In the fluid model, the electrons and ions are described by their continuity and momentum transfer equations in the drift diffusion approximation, and these equations are solved together with Poissons equation for the electric field.

Teaching optical spatial filtering : a simple method to calculate the image filtered intensity

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Spatial filtering is a rather common topic in Modern Optics [1] as a method of image processing. The dark ground and phase contrast methods (the latter one has recently been used for probing Bose-Einstein condensates) are typical applications of the technique [2].

The principle of the spatial filtering method is the following: the image of a partially transmitting plane object (Ω) characterised by its transmission function t is formed using a lens. The Fraunhofer diffraction pattern displays the spatial frequency spectrum of the object. Modifying the amplitude and/or the phase of this spectrum by means of a filter results in a alteration of the image. The filter is characterised by its transmission function T . The problem is to compute precisely the intensity distribution of the altered image. A natural procedure consists (i) in calculating the diffracted complex amplitude A of the object and (ii) considering A as a new input, determining the complex amplitude diffracted in the image plane.

The application of this brute force method depends strongly on the particular set-up used and leads to lengthy and cumbersome calculations. The difficulties arise from the fact that the mentioned calculations yield both the phase and the amplitude of the wave in the image plane: if one is only interested in the intensity, the knowledge of the phase is useless.

The method we propose consists in two steps:

(i): determine the intensity in the image plane as a function of the intensity on the back side of the object (Ω), assuming that the optical imaging system can be properly treated in the limit of geometrical optics (no limitation of the light beams by the lenses). No spatial filter is used at this step.

(ii): consider the imaginary object (Im) which would give a diffracted amplitude exactly equal to the filtered one. One easily finds that the transmission function of (Im) is equal to the convolution product of t by the Fourier transform of T .

Applying step one to the transmission function of the imaginary object leads to the intensity of the filtered image at any point of the image of (Ω).

Applications of the method will be given.

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Tracking Ground-State Selected Ba^+ Ions in an Expanding Laser Plasma Plume Using Time-Resolved Vacuum-UV Photoabsorption Imaging

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Photoabsorption imaging using tuneable optical lasers is a well established technique for tracking the expansion of dilute dynamic samples (e.g., time of flight measurements on expanding atomic Bose-Einstein condensates [1]). However, for more dense samples (e.g., laser plasma plumes) the analysis is complicated by the need to invoke radiation transfer. Moving to the VUV spectral range, where one can excite inner shell and multiply-excited resonances, which decay predominantly by electron emission, can eliminate this restriction thereby permitting a description of the beam attenuation by the simple Beer-Lambert law. Probing plasma plumes with VUV light has a number of other advantages over optical probing, including the ability to access the resonance lines of ions most of which lie in the VUV and also reduced refraction of the VUV probe beam by the plasma (electron) density gradient. The data presented, representing as they do the non-emitting species in the plume, complement the usual optically filtered ICCD emission images which provide insight into spatial distribution excited state plasma species only [2].

We report initial results from a study of the ion column density and expansion dynamics of ground state-selected Ba^+ ions in a laser-plasma plume with a new experimental facility at the NCPST, DCU called VPIF (Vacuum-ultraviolet Photoabsorption Imaging Facility). Details of the setup are in the press [3]. Briefly, a laser produced gold plasma constitutes the continuum source which provides VUV pulses of ca. 25 ns duration at a repetition rate of 10 Hz. The barium 'sample' plasma is produced by a second electronically synchronized laser. The VUV beam is monochromatised and collimated before being directed through the expanding Ba plasma plume. The Ba^+ ions are tracked by recording the time resolved attenuation of the pulsed VUV beam as the expanding (Ba) plasma plume moves through it. The Ba^+ ions are selected by tuning the VUV pulse to the 5p-6d inner-shell resonance. The attenuated beam is allowed to fall on a CCD array where the spatial distribution of the transmission $I(x,y,t)/I_0(x,y,t)$ is recorded. Maps of equivalent width (W_E) are constructed from the raw $I(x,y,t)$ and $I_0(x,y,t)$ images [4]. From a knowledge of the Ba^+ (absolute) photoionization cross section [5], corresponding maps of ion column density are constructed. In addition, Ba^+ ion expansion velocities are extracted and compared with an adiabatic model of plasma expansion.

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Digital box-car system implemented in a single CPLD device.

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Many physical phenomena observed as nonstationary random processes are characterized by highly localized events, relatively to the time of observation [1]. The analysis of such processes is applied in time-of-flight mass spectrometry or time resolved spectroscopy when the decay time of the population of the excited atoms is observed. Digital box-car systems or real time multichannel scaler – RTMS [2] are usually applied as measuring systems to the case of processes consisting of a sequence of ions randomly distributed in time.

The optimal measuring system should be characterized by a high time-resolution and very small dead-times. Counting systems, such as the box-car or the RTMS, based on ECL devices, usually have a resolution of the order of several nanoseconds. On the other hand such systems are characterized by a very small dead-time. In many applications a resolution of the order of several nanoseconds is absolute sufficient. In such cases the measuring system can be simply design using VHDL method and implemented in a single FPGA device. The box-car system implemented in the Lattice ispLSI2128 165LJ programmable device consists of three synchronous counters. One of the counters has a function of the programmable delay line, while the second one has a function of programmable gate. The third counter, clocked by the input pulses is counting the number of input pulses while the gate is open. Each measuring cycle is initialized by the trigger pulse and can be repeated when the data (number of counts) are transferred to the computer memory.

The most important advantage of such a system is simplicity. However, in that case the resolution is strongly limited to 10 ns. The box-car system, working with a 100 MHz clock can accept the pulses of minimal width equal to 3 ns separated by a minimal time interval of 7 ns.

The box-car system configured as an ISA card was used for instance in time-resolved mass spectroscopy for detection of Ca ions produced by multiphoton ionization as well as for ion detection during the laser ablation experiment.

Acknowledgments

This work was supported by Polish State Committee for Scientific Research KBN Grant No. 8 T10C 035 20

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Combining laser spectroscopy with the VUV undulator radiation of beamline i411 at MAX-lab

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Soft X-ray photoelectron spectroscopy (XPS) is a well established technique for studying the electronic structure of atoms, molecules, clusters, and surfaces. At beamline I411 of the MAX II storage ring in Lund (Sweden) high resolution electron spectra can be obtained with an Scienta SES200 electron analyzer in a energy range from 60 to 1500 eV. The experimental chamber allows for studying both gas phase and solid targets.

While XPS is mostly applied to the target's ground state the possibility to study excited and polarized probes opens up new fields of interest. To address these types of experiments a continuous wave (cw) laser system has been installed at the beamline. The laser system delivers 1 W continuous radiation in a wavelength range from 690 to 1000 nm using a Titanium doped sapphire (Ti:Sa) crystal as gain medium. The option to use a liquid dye jet instead of the Ti:Sa crystal allows for expansion of the wavelength range into the visible light. The Ti:Sa laser is pumped by a commercial 10 W cw 532 nm Vanadate laser.

The cw laser system can be used to optically pump the probes into well defined states. This method has been used for pumping free atomic transition metals into magnetically oriented states in order to measure their magnetic dichroism in the photoemission in comparison with the solid state[1,2]. Additionally it will be possible to perform photoionization out of excited states of atoms, molecules and surfaces. The narrow band width of less than 500 kHz allows for selecting single transitions and is a good basis for investigating coherent effects. On the other hand the laser system can be used to ionize atoms after excitation with synchrotron radiation [3] or to detect specific photoionization products by using laser induced fluorescence techniques.

In this presentation the setup of the laser system will be introduced and the status of the experiments will be presented.

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Particle-in-cell Code Library for Numerical Simulation of the ECR Source Plasma

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A summary of recent development of physical and mathematical basements and the first version of computer code library based on the particle-in-cell method are presented. The code library is aimed for the 3D simulation of the ECR plasma and ion production in an ECR ion source. The particle-in-cell method is one of the most powerful methods for the numerical simulation of multicomponent ECR plasma and electron-ion beams. This method allows studying the detailed characteristics of plasma, taking into account distribution functions of particles real self and external fields, particle-particle interactions and others. This technique promises to provide very precise numerical simulations and optimizations of ECR ion sources. The first results of simulations of ECR source plasma are presented.

A versatile X-ray source for highly charged ions

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X-ray emission from highly charged ions is of substantial interest for a wide range of investigations, such as atomic physics, plasma physics, astrophysics, metrology and other fields of basic research. Further on, X-rays from highly charged ions can also be used in applied research as for instance in X-ray projection microscopy and material analysis.

With the Dresden EBIT (Electron Beam Ion Trap) a compact table-top ion source for the production of very highly charged ions has been developed [1,2]. In this ion source highly charged ions are derived by successive electron impact ionization in a high-dense electron beam with energies up to 15 keV in the typical pressure range of 10^{-8} mbar to 10^{-10} mbar. In order to reach sufficient high ionization factors the ions are trapped inside the source by electrostatic fields for any choosen time. During the ionization time in the trap X-rays from direct excitation (DE), radiative recombination (RR) and dielectronic recombination (DR) processes are emitted. The intensity of the produced X-rays is high enough for energy as well as for high-resolution wavelength dispersive X-ray spectroscopy. Typical radiation powers of electric dipole lines from highly charged ions are in the order of nW. Up to now in the Dresden EBIT bare nuclei of elements up to nickel ($Z=28$) [3], helium-like ions such as Ge^{30+} and Kr^{34+} [4] and neon-like ions such as Xe^{44+} , Ce^{48+} and Ir^{67+} [5] have been produced.

The Dresden EBIT is equipped with spectroscopic Be-windows that provide spectroscopic measurements in a simple experimental arrangement. If neccessary as in the case of low-energy spectroscopy the ion source also can operate in a windowless regime. In order to demonstrate the ability of the source to investigate different basis processes such as DE, RR and DR a choice of energy and wavelength dispersive measured X-ray spectra from the trap, as for instance spectra from Ar^{17+} , Ti^{20+} , Xe^{44+} and Ir^{q+} ($q \leq 67+$) ions, are shown.

Ions produced in the Dresden EBIT also can be extracted from the ion trap with ion currents of nA per pulse. This is the prerequisite for experiments to measure X-ray emission from the interaction of slow highly charged ions with solid state surfaces. Beside ion extraction spectra examples of X-ray spectra from the process $\text{Ar}^{q+} \rightarrow \text{Cu}$ ($q \leq 17$) are shown.

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Reduction of Dicke narrowing of cadmium line perturbed by Xe

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In this work we have verified the possibility of observation of the Dicke narrowing of atomic spectral lines in optical domain. Experimental results obtained by means of a laser-induced fluorescence method for the ^{114}Cd 326.1 nm line perturbed by xenon[1] were carefully reanalyzed using a line shape model which takes into account the speed dependence of collisional broadening and shifting, the velocity-changing collisions and the collision-time asymmetry[2]. Our analysis clearly shows that in case of the 326.1 nm ^{114}Cd line perturbed by Xe Dicke narrowing is not observed.

It was shown that the possible small contribution of Dicke narrowing which can not be excluded owing to the accuracy of our experiment is significantly smaller than that calculated on the basis of the mass diffusion coefficient. We believe that the correlation between the velocity-changing and dephasing collisions is responsible for this almost complete elimination of the Dicke narrowing in the case of the line under investigation.

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QED theory of discharge of the meta-stable nuclei during negative muon capture and a search of the possible high power source of monochromatic γ radiation

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A negative μ meson captures by a metastable nucleus may accelerate the discharge of the latter by many orders of magnitude (c.f.[1,2]). For a certain relation between the energy range of the nuclear and mesonic levels the discharge may be followed by the ejection of a meson, which may then participate in the discharge of the other nuclei. In this paper we present a consistent QED theory for phenomenon of discharge of a nucleus with emission of γ quantum and further meson conversion, which initiates this discharge. Traditional process of the μ meson capture are in details studied earlier and here is not considered. Within an energy QED approach (c.f.[1,2]) with QED scattering matrix, a decay probability is presented as an imaginary part of the energy shift. The intensities of satellites are linked with imaginary part of the "nucleolus core+ proton +meson" system. For radiative decays it is manifested as effect of the retarding in interaction and self-action. Three channels should be taken into account: 1). Radiative purely nuclear 2^j -poled transition (probability P1; this value can be calculated on the basis of known traditional formula); 2). Non-radiative decay, when a proton transits into the ground state and a meson leaves the nuclei with energy $E=N-M$, where N is an energy of nuclear transition, M - is an energy of bond for meson in the 1s state (probability P2); 3). A transition of proton into the ground state with excitement of meson and emission of the γ quantum (probability P3). Within the QED perturbation theory [1-3], a full probability is divided into the sum of the partial contributions, connected with decay into definite final states of system. These contributions are equal to the corresponding transitions probabilities (P_i). For example, under condition $N \ll M$ the probability definition reduces to the QED calculation of probability of the autoionization decay of the two-particle system. The corresponding QED expression is derived. There are also discussed the key moments of calculational procedure on the basis of our atomic numerical code [3-5]. For a sample with a sufficiently high density of metastable nuclei and a sufficiently intense meson beam above considered process can result in a sharp increase of γ radioactivity of the sample and may be used as the basis of operation of a high power source of monochromatic γ radiation [2,5].

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Energy transfer and account of influence of the rotational and V-T relaxation on multi-photon excitement and dissociation for CF_3Br within stochastic kinetic model

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Phenomenological approach to description uncollisional excitement of number of molecules (CF_3I , SF_6 , OsO_4 etc.) has been realized in papers of Letokhov, Stown etal [1]. At the same time a problem of correct influence of collisions on dynamics of multi-photon processes, selectivity of dissociation, absorption and energy transfer etc. requires a further studying. In this paper within new stochastic, quantum kinetics model it is studied a link between the integral characteristics of the multi-photon excitement and dissociation with parameters of relaxation in a medium of the buffer gas (N_2). It is calculated the output of multi-photon dissociation and absorbed energy for molecules of $^{12}\text{CF}_3\text{Br}$, $^{13}\text{CF}_3\text{Br}$. We describe a process of excitement into continuum within generalized kinetical equations model [1,2]. A key moment is connected with account of the stochastic diffusion mechanism in quasi-continuum. To describe an excitement on the lowest discrete levels it is used a modified model of Letokhov etal. Within it, the lowest levels system is described by two velocities: radiative velocity of excitement of some separated levels, which is proportional to pressure, and the rotational relaxation velocity. We calculate a dependence of the absorbed energy ^{13}E and dissociation output $^{12}\beta$, $^{13}\beta$ upon a summarized pressure $p_\Sigma = p(\text{N}_2) + p(\text{CF}_3\text{Br})$ [$p(\text{CF}_3\text{Br})=0,5$ Torr] for a number of laser lines of the CO_2 laser (1048,66; 1043,16; 1035,47 cm^{-1}). It is carried out an analysis of absorption by molecules in the quasi continuum, molecules on the lowest levels, contribution of the V-T relaxation. It is shown that in the pressure interval p;50-100Torr a dissociation output is mainly determined by influence of the rotational relaxation and the V-T relaxation is not significant. Above 200Torr the dissociation output is mainly determined by concurrence of two processes: the V-T relaxation and involving the molecules from the lowest levels Stochastic model block is manifested in more correct description of the excitement dynamics in the quasi continuum.

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A new type of weak localization of the electrons in disordered media

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The mechanism of weak localization of relatively fast electrons scattered with a fixed energy loss from disordered media is examined. The main focus of this paper is to put forward an explanation for why coherent enhancement of electron scattering in the inelastic-scattering channel takes place at angles which differ from π . A simplified kinematic model is proposed to determine basic properties of the weak localization of electrons in the inelastic scattering channel. The model easily reproduces the range of scattering angles typical for the weak localization of electrons with the fixed energy loss. The procedure does not require calculation of contribution from the crossed diagrams. The results agree with those based on the dynamical theory associated with the calculation of the crossed and ladder diagrams. It is possible to follow the transition from the weak localization of the new type to the ordinary weak localization with decreasing energy loss is about the energy of an optical phonon.

The weak localization of conduction electrons and backscattering enhancement of classical waves in disordered media have been the subjects of intensive study. Both phenomena are intimately related. They are connected with the constructive interference of random wave fields. A coherent phenomena are also interesting in the scattering of external particles (such as electrons) with a fixed energy incident on disordered samples. Weak localization of external electrons (with energies from tens to thousands of eV) has been studied in the works of R.Berkovits and M. Kaveh and also in the work of E. Gorodnichev, S. Dudarev, D.Rogoskin.

It is commonly belief that inelastic scattering destroys the phase memory and forbids the quantum interference effect. However, in some cases, the inelastic processes do not lead to phase memory loss. Moreover, quantum interference can occur even if an electron suffers single inelastic scattering while interacting with an incoherent electromagnetic field. There are two ways to realize this process, since it can either start or end with an inelastic collision. The interference of electron waves associated with these complementary processes has been proved to be constructive [1]. It manifests itself in the enhancement of electron scattering through an angle which differs from π very impressive. The new coherent phenomenon was called "new" type of weak localization. The angular distribution of particles and radiation undergoing weak localization in disordered medium can be found by calculating the contribution of the crossed (or so-called "fan") diagrams into an electron (radiation) cross section or density matrix. However, it is also useful to have a simple physical model explaining why coherent phenomena are particularly pronounced in particle scattering at certain angles. In the case of ordinary weak localization, there is a particularly simple graphic method [2] which provides insight into phenomenon and explains why the angle π is specific for the weak localization of regular kind. The main goal of this work, which has been done, was to find physical interpretation and to build the same graphic method for the fact that constructive interference of the new weak localization is pronounced at scattering angles different from π .

Finally, we have shown that there is no wall between new and ordinary weak localizations. These phenomena are two different manifestations of constructive quantum interference of electron waves.

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Coincidence measurements of electron impact excitation of the 5^1P_1 state of Cd.

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The coherence analysis technique has been used to determine a state of a polarization of 228.8 nm radiation emitted by cadmium atoms excited to 5^1P_1 state by electron impact. The experimental set-up and first results for incident electron energy of 100 eV were described elsewhere [1].

Photons of a wavelength 228.8 nm resulting from the decay of the 5^1P_1 state were detected in a direction perpendicular to the scattering plane and analysed for either linear or circular polarization. The scattered electrons were selected for the scattering angle θ and for the energy loss of 5.4 eV using electrostatic electron energy analyser. The electron pulses started the time – to – amplitude converter and the photon pulses, suitably delayed, were used to stop it. The output of the converter was monitored continuously with a multichannel analyser operated in a pulse – height – analysis mode to form electron – photon coincidence spectra.

The main procedure involved for each electron scattering angle accumulating electron – photon coincidence spectra at appropriate positions of the polarization analyser. Signals required to determine a single polarization data point, were accumulated by repeating a cycles of two 600 second long measurements at different polarizer positions.

The atomic beam used in the experiment was obtained by evaporation of a natural mixture of Cd isotopes. As such it contained 75% of atoms with zero nuclear spin I and 25% fraction of ^{111}Cd and ^{113}Cd characterised by $I = 1/2$. The fluorescence of the latter was partially depolarised due to the hyperfine interaction. However, the experimentally determined Stokes parameters could be easily corrected for the effect, using the well - known formalism of the perturbation coefficients [2,3].

In this report we present new data obtained for incident electron energy of 80 eV and 100 eV for extended range of the scattering angles of 10° to 50° . Reduced Stokes parameters and electron impact coherence parameters (EICP), characterizing the state of the excited atoms immediately after the collision, have been extracted from the measurements and compared with results of relativistic distorted – wave approximation calculations [4]. Theoretical predictions are in a good qualitative agreement with experimental values.

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Collisional ionization of Rydberg atoms of Sodium

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Electron transfer in weakly bound quasi-molecular systems plays an important role in many physical processes, e.g., laser excited vapours and low temperature plasmas. Temporary quasi-molecular systems are formed in collisions of excited atoms. Such collision complexes may, at certain internuclear distances, couple to ionization continua and emit an electron. Depending on the excitation energy and relative positioning of the covalent and ionic molecular potential curves, collisions may lead to atomic and molecular ionization through Penning and associative processes. Conventional theory treats such processes deterministically, as interaction of a few bound states with the continuum. However, exact quantum mechanical description of such systems often fails due to the complexity of calculations. This drawback of deterministic description of ionization dynamics could be overcome by complementing it by a newly developed approach, the stochastic ionization model in a single collisional event [1,2]. This alternative approach treats the process as an escape of weakly bound electron during the collision due to its stochastic migration along overlapping multiple ionization channels.

The aim of the present work was to test the theoretical predictions of [1,2] experimentally. The process of electron detachment in the collisions of ground-state and Rydberg sodium atoms has been studied. Experiments were performed in a vacuum chamber with effusive thermal atomic beam at the 10^8 - 10^{10} cm $^{-3}$ density. Temperature of the atomic beam was varied in the 550-650 K range. Rydberg nS and nD states of sodium were excited by two pulsed tunable lasers (Rhodamine 6G dye-laser and the second harmonic of Ti:sapphire laser) running at a 5 kHz repetition rate. Electrons appearing in the associative and Penning ionization processes were detected by channeltron multipliers. 50 V/cm electric field was applied to guide electrons to the channeltrons. Ionization signals were observed at the moment of laser excitation (multistep photoionization by intense laser pulses), and during 2-10 μ s after the excitation. The latter corresponded to ionization of Rydberg atoms.

We have measured the ionization signals for the states with $n=10$ -30. The signals were analyzed to take into account various processes that can contribute to the ionization of Rydberg atoms: associative and Penning ionization, collisions with background gases, photoionization by the black-body radiation (BBR), spontaneous decay and BBR induced transitions. An influence of BBR was investigated by varying the temperature of the detection system from 77 to 300 K. Dependence of the collisional ionization rates on n and its comparison with theory and other experiments will be presented and discussed.

This work was supported by INTAS, Grant No. 2001-155, and partly by the Russian Foundation for Basic Research, Grant No. 02-02-16323.

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Coherent resonances obtained by multi-frequency excitation of Cs atoms

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Coherent resonances in alkali atoms have been observed by utilizing mainly two approaches: coupling of (i) two ground-state levels of different energies by means of two-frequency laser field, and (ii) two ground-state levels of equal energy by two polarization components of the laser field. In both cases resonances in the fluorescence or in the transmitted light are observed, whose FWHM is orders of magnitude less than the natural width of the optical transition. It has been shown [1] that when Cs atoms are placed in a constant magnetic field that is small enough to cause only linear splitting of the two ground-state Zeeman sublevels, the coherent superposition of the sublevels caused by bichromatic field leads to observation of a narrow resonance. This occurs when the frequency difference between the laser field components equals the frequency difference between the split sublevels. This kind of resonances are applied for precise measurement of magnetic fields. For such applications, the width of the resonances should be as small as possible in order to increase the sensitivity of measurements.

In this communication we present the results on the comparison of the resonance parameters for three different cells: evacuated cell with pure Cs vapour, a cell with coated walls and a cell with buffer gas added. Due to the strong decrease in the spin-exchange collisions, the FWHM of the resonances in the coated and buffer gas cell is an order of magnitude less than in the vacuum cell. However, the amplitude of the resonances in the first case is also lower due to the increased optical pumping to the ground-state non-interacting with the laser field. The signal-to-noise ratio decrease is compensated for by using of lock-in detection technique.

As has been shown in [2], for the fluorescence line starting from the ground state $F_g = 4$, bright resonances have been observed in a vacuum cell. In a buffer gas cell, when the population of the Zeeman sublevels of the Cs excited state is mixed due to collisions with the buffer gas atoms, the bright state is transformed into a dark one. Here we present a more detailed investigation of this transformation. An interesting phenomenon is observed: the transformation of the bright into a dark state with buffer gas pressure increase starts earlier for atoms in the wings of the Doppler profile than for atoms at the maximum of the fluorescence line.

The accuracy of the magnetic field measurement with this experimental set-up makes possible the experimental registration of the light shift of the Zeeman sublevels due to the laser power and its dependence on the laser frequency detuning within the spectral profile of the fluorescence line. In conclusion, it should be pointed out that with a proper choice of the laser power and type of Cs cell, magnetic field change of the order of $10 \mu G$ is measured. Further investigations are in progress for improving the sensitivity of measurement and clarification of the mechanism of transformation of the bright state into a dark one.

Acknowledgements: The authors thank the EC for the financial support (Contract G6RD-CT-2001-00642) and the BNS Council (Grant F-1005/00) for the partial support.

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The cold atom micromaser in a vertical configuration

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The properties of the cold atom micromaser in a vertical configuration will be presented. The cold atom micromaser (also referred to as maser for microwave amplification via z-motion-induced emission of radiation) consists in the interaction of a cold atomic flux in an excited state through a high- Q microwave cavity. This system was first described by Scully *et al.* [1] where it was shown that the use of cold atoms in the system requires a quantum-mechanical treatment of the center-of-mass motion and results in a new kind of induced emission inside the cavity. This strongly modifies the properties of the field generated inside the cavity by the incident excited atoms. In Scully's paper and all following ones related to this subject (see e.g. Ref. [2] for a review of these papers), the atoms were supposed to move along an horizontal axis without consideration of the gravitational effects. In the present study, these effects are taken into account and a complete quantum description of the atomic motion in the gravitational field when the atoms interact with the maser cavity is given. The motion is supposed in the vertical direction to keep the one-dimensionality of the problem.

Interesting new effects will be discussed. Particularly, we have analyzed how gravity affects the induced emission probability of a photon inside the cavity by an atom initially in the excited state. We will show that the free fall introduces quasi-bound states inside the cavity that enhances significantly this probability. More generally, we have shown that the maser behavior in the vertical and horizontal configurations differs significantly.

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Localization of three-level atoms in standing wave via quantum interference

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The problem of subwavelength localization of cooled atoms in standing waves is of great interest for atom optics and nanolithography. The special interest in this area is the localization scheme by laser-induced phenomena in multilevel atoms. Several models have been proposed using the measurement of the phase shift due to an off-resonant standing-wave field [1], the entanglement between the atom's position to internal state [2]. Recently the localization of three-level atoms that interacts with two fields, a probe laser field and a strong classical standing wave has been considered in [3]. The main advantage of this scheme is that the localization of atoms occurs immediately in the subwavelength domain of strong standing wave field as spontaneous emission is recorded during the atom motion in the standing wave. At the same time the theoretical model of atom localization used in [3] for non-stationary Schroedinger equation was not strong enough to obtain this effect by using the real parameters of experimental setup.

Here we consider the same scheme of laser-atom interaction by matrix density technique, which allows us to obtain the new results about both the degree of localization and the parameters of laser field (intensities and detunings). Moreover, we show also that such localization is not stable and we find the life-time of this structure. Thus, we demonstrate the possibility to apply this technique to atom nano-litography.

This work was financially supported by the grants of the Program "Universities of Russia" YP.01.01.040, Education Ministry of Russian Federation E02-3.2-287, and Russian Foundation of Basic Research 02-02-17686.

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Role of symmetry principles in the electromagnetically induced transparency

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The electromagnetically induced transparency (EIT) [1,2] has aroused considerable interest in recent years. It has led to many interesting applications such as lasing without inversion [3,4] and light speed reduction [5,6]. In the EIT phenomena, the absorption rate of a weak probe field which is resonant with an atomic transition is substantially suppressed by the application of a strong coupling field. In this paper, we show that basic symmetry principles underlie the EIT.

We may choose the Λ -type EIT as a typical example to illustrate the mechanism of the EIT. The probe field is resonant with the transition $|1\rangle \rightarrow |3\rangle$, where $|1\rangle$ is the ground state and $|3\rangle$ is an excited state. The coupling field is resonant with the transition $|2\rangle \rightarrow |3\rangle$, where $|2\rangle$ is an excited state lower than $|3\rangle$. There are two paths between $|1\rangle$ and $|3\rangle$. In the first path, the atom jumps from $|1\rangle$ to $|3\rangle$ by absorbing one probe laser photon. Its transition amplitude is designated by $T_{31}^{(1)}$. The second path involves a three-photon process. First, the atom jumps from $|1\rangle$ to $|3\rangle$ by absorbing one probe laser photon. Then it drops to $|2\rangle$ by emitting one photon with the same frequency of the coupling laser photon. Finally it jumps from $|2\rangle$ to $|3\rangle$ by absorbing one coupling laser photon. Its transition amplitude is designated by $T_{31}^{(3)}$. It is surprising that $T_{31}^{(1)}$ and $T_{31}^{(3)}$ are always of opposite signs in diverse atoms! Therefore there is always a destructive interference between these paths, which suppresses the absorption rate of the probe laser. The aim of this paper is to gain deeper insight into the long-standing subtle question "why on earth do the competing paths in the EIT system evolve so robustly to produce destructive interference in diverse circumstances?". We show that the destructive interference arises naturally as a consequence of both the time-reversal symmetry and the gauge symmetry.

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Dynamical stability in nonlinear traps

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We extend the classical and quantum pseudopotential approach given in [1] and [2] to the motion of charged particles in nonlinear traps with rapidly oscillating electromagnetic fields. The stability properties of a single trapped ion and the collective motion of ion clouds can be described in terms of pseudopotentials for suitable nonlinear parametric oscillators. We assume that the electric potential can be decomposed into a time independent static part and a time dependent part given by

$$\Phi(\mathbf{r}, t) = a(t)G(\mathbf{r}) , \quad (1)$$

where a is a time periodic function of period $T = 2\pi/\Omega$ with $\langle a \rangle = 0$ and $a_{max} = 1$. Here $\langle \rangle$ denotes the time average over a period. Consider the time dependent functions v and s such that $dv/dt = a$, $ds/dt = v$, and $\langle v \rangle = 0$. For an ideal Paul trap $a(t) = \cos \Omega t$ and $\langle v^2 \rangle = 1/2$.

The classical motion can be described by separation into a slow part and a high frequency part. In the case of slow dynamics for a trapped particle of mass m and charge q , with a small displacement s , the electric potential Φ is approximated by the pseudopotential

$$\Phi_{eff} = \frac{\langle v^2 \rangle}{2m\Omega^2} (\nabla G)^2 . \quad (2)$$

A rigorous control of the pseudopotential approximation may be given in terms of normal forms [1]. We obtained perturbatively high order terms in $1/\Omega$ for the pseudopotential.

The laser cooled ion dynamics must be treated quantum mechanically. The solution of the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = (H_0 + q\Phi)\Psi , \quad (3)$$

can be approximated by

$$\Psi_{eff} = \varphi \exp(-ivG/\hbar) , \quad (4)$$

where H_0 is a time independent Hamiltonian and φ is the solution of the effective Schrödinger equation

$$i\hbar \frac{\partial \varphi}{\partial t} = (H_0 + q\Phi_{eff})\varphi . \quad (5)$$

We characterize the trapping stability and the validity of pseudopotential approximations by a frequency independent stability functions $\xi = |\nabla[(\nabla G)^2]|^2/|\nabla G|^2$. The stability function η defined in [3] can be written as $\eta = 2 \langle v^2 \rangle \sqrt{\xi}/m$.

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A dark state magnetometer in Hanle configuration

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Destructive quantum interference of two resonantly excited transitions within a Λ -type level scheme enables a medium to get coherently prepared in a superpositional dark state via optical pumping. As a condition the transitions must satisfy two photon resonance. Correspondingly a distinct enhancement of radiation transmission is observed around zero Raman detuning, which is well known as Electromagnetically Induced Transparency (EIT). Due to the quantum interference nature of this effect a very narrow linewidth down to the Hz region can be observed [1]. Consequently, if a lambda system is constructed within the Zeeman sublevel manifold of a hyperfine state, the medium transmission is very sensitive to magnetic field deviations.

We present first results of sub-kHz EIT resonances, observed in a Hanle configuration by single laser frequency excitation on the Rb^{87} D_1 line: We use an extended cavity diode laser system, which is externally stabilized to the excited transition $5S_{1/2}, F=2 - 5P_{1/2}, F=1$ using the DAVLL setup. The linear polarized beam excites σ^+ and σ^- transitions while the magnetic field is scanned around zero value in the direction of the laser beam propagation, thus forming Λ -systems within the Zeeman manifold of the excited transition. Hence additional to the Hanle signal a significant EIT peak is observed.

There is a high potential for magnetometers based on optical methods: Such devices have already reached very high resolution which allows to resolve the magnetic fields produced by the beating human heart [2]. Recently even the SQUID sensitivity of typically a few $\text{fT Hz}^{-1/2}$ has been outperformed by an optical magnetometer showing sub-fT resolution [3]. Our groups' efforts are concentrated on the aim to build a portable EIT based magnetometer with high accuracy and high spatial resolution, which works at room temperature. It could be used in human health care as well as in the monitoring and standardisation of working conditions.

This work is supported by the European Union as a collaboration with groups in Italy and Bulgaria (Contract G6RD-CT-2001-00642).

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Coherent evolution of a mixed state

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We analyze coherent evolution of a mixed state under the action of a Hermitean Hamiltonian. We determine the limitations on the evolutions of the populations that derive from the Liouville equation. Such limitations are imposed, for example, by the constants of motion $\text{Tr } \hat{\rho}^n = \text{const}$ ($n = 1, 2, \dots, N$), where $\hat{\rho}$ is the density matrix operator and N is the number of states.

In the case when the system is initially in a *completely incoherent* superposition of states, the maximal value for each population cannot exceed the largest initial population. Moreover, the population dynamics in this case is separable in the sense that each initial population evolves independently of the others. Then each population can be represented in the classically intuitive manner as a (incoherent) sum over the initial populations weighted by the respective transition probabilities.

When the system is initially in a *partially incoherent* superposition of states, the population dynamics is considerably more complex. In this case, each population can exceed the largest initial population for an appropriately chosen Hamiltonian. The maximal value of each population depends on the degree of coherence. We quantify the size of the Hilbert space by using the constants of motion and, in particular, the Bloch vector length [1].

We apply the general formalism in some detail to two cases of particular interest: population transfer in two-state systems [2] and STIRAP in three-state systems [3].

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Influence of additional magnetic field on the Electromagnetically-Induced Transparency resonances in Hanle-configuration

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Electromagnetically-Induced transparency (EIT) resonances in Hanle configuration have been investigated for several alkali atoms (Na, Rb, Cs). What makes such resonances interesting is their linewidth, which is orders of magnitude less than the natural width of the optical transitions. This makes possible their use in high resolution spectroscopy and for precise measurements [1-4].

In this communication we present results on experimental and theoretical examination of the influence of additional magnetic field B on the resonance profile. In the experiment, Rb vapour contained in a glass cell is irradiated by a linearly polarized single-frequency diode laser light tuned to the different fluorescence components of the D_1 line. The Rb fluorescence is registered in dependence on magnetic field applied along the direction of the light propagation axis and scanned around zero value. For hyperfine transitions with quantum number of the ground state F_g higher than that of the excited state F_e , EIT resonance is observed in the fluorescence dependence on the magnetic field, centered at $B = 0$. Additional constant magnetic field B_{ort} is applied parallel or orthogonal to the polarization vector of the light E . In the case of $B_{ort} \perp E$, fast broadening and destruction of the EIT resonance is observed, while the application of $B_{ort} \parallel E$ leads to an increase in the resonance amplitude and broadening of its profile. Similar behaviour is observed experimentally also for a complex-shape EIT resonance in Rb [3].

A theoretical consideration about the additional magnetic field B_{ort} influence on the CPT resonance has been performed for the $F_g = 1 \rightarrow F_e = 0$ transition. Exact solution was found for the system of equations for the density matrix components in an irreducible representation, describing an atomic system at rest in the driven and additional magnetic fields arbitrarily mutually oriented. The theoretical calculations show that a small $B_{ort} \perp E$ destroys the resonance. For the influence of $B_{ort} \parallel E$, the theoretical results are also in qualitative agreement with the experiment. These calculations are in qualitative accordance with the results obtained in [5], where the influence of a parasitic magnetic field on the Hanle signal is discussed.

The results from this investigation are of great importance for the application of the EIT resonances for precise magnetic field measurements.

Acknowledgements: The authors wish to thank the EC for the financial support (Contract G6RD-CT-2001-00642) and the BCSR for the partial support of the investigation (Grants F-1005/00 and F-1006/00).

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Coherent evolution of laser-driven four-state systems

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We present an analytic treatment of the laser-driven population dynamics of four-state systems in several configurations: chain, diamond and tripod. Such linking patterns can be created, for example, when a degenerate two-level system is driven by an elliptically polarized laser pulse.

The theoretical description of the method is based upon the Morris-Shore transformation [1-3], which decomposes the four-state system into a set involving independent two-state subsystems and possibly also decoupled dark states. In each of these decoupled two-state systems, one state is a coherent superposition of ground sublevels only and the other state is a coherent superposition of excited sublevels. The decoupled dark states are superpositions of ground sublevels.

This approach allows to find analytic solutions for four-state systems using known two-state analytic solutions, such as the Landau-Zener model and the Rosen-Zener model, applied to each of the decoupled two-state systems. It also allows to derive various general properties for four-state systems using the limitations imposed by the Morris-Shore decomposition.

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Addressing single atoms in a dipole trap: towards a quantum shift register

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We report the addressing of single neutral atoms in a standing wave optical dipole trap. Using adiabatic passage techniques atoms initially prepared in one hyperfine state are transferred into another hyperfine state with high efficiency. By applying a magnetic field gradient we can select single atoms at a desired position along the standing wave. An intensified CCD-camera monitors and spatially resolves the atoms within the dipole trap. A state-selective atom removal from the trap allows us to read out the state of each individual atom. These results form the basis for preparation and read-out of an elementary quantum register. To enable controlled interaction between neighboring atoms of the register we have set up a high finesse optical cavity. A small mode volume and low mirror losses enable us to reach the strong coupling regime. Using an off-resonant lock laser the mirror spacing of this cavity is reliably stabilized to a precision of 100fm. It will soon allow us to entangle atoms by the exchange of virtual cavity photons.

Cooperative Raman-type scattering of entangled photons as a mechanism of squeezing or entanglement in the spin subsystems of macroscopic atomic ensembles

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Squeezing or entanglement is an important property, which matter can get due to quantum nature of interaction existing between different micro or even macroscopic objects. Spin subsystems of macroscopic ensembles are just the confirming examples where macroscopic entanglement can appear. Atomic ensembles consisting of ultracold atoms, which are isolated from environment, can store the induced quantum correlations inside their long-lived spin subsystem. The unique property of squeezing or entanglement is a potentially important as far as it can be further utilized in different quantum information protocols or can form a basis for the quantum computing algorithms.

We describe here an optical mechanism of how the squeezed or entangled states can be created in the ground state spin subsystems of macroscopic atomic ensembles. In the proposed mechanism as well as in other schemes of spin squeezing or entanglement the quantum state is mapped into the macroscopic spin fluctuations of originally coherent spin state with 100% spin orientation. Our proposal is based on cooperative Raman-type scattering of the correlated photon pairs generated by optical parametric oscillator operating in far subthreshold regime. In this presentation we consider an example of the Lambda-type excitation channel organized between the lower $F = 1$ and upper $f = 1$ atomic states, where F and f are the corresponding total angular momenta of atom in its ground and excited state. The proper example of optical transition can be found in the hyperfine manifolds of alkali atoms. For such a transition we consider the Raman scattering channel initiated in orthogonal circular polarizations for the right-hand circular polarized quantum mode and for the left-hand circular polarized classical mode. It is shown that due to quantum correlations existing between the photons of the quantum mode the final spin states of atoms becomes also correlated. Accumulating this type of correlations during the interaction cycle the final macroscopic spin state becomes squeezed or entangled.

The work was supported in part by RFBR under grant 01-02-17059 and by INTAS under grant INFO 00-479.

Coherent excitation of a two-state system by a Gaussian pulse

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We present an analytic description of coherent excitation of a two-state system by an external driving pulse of Gaussian temporal profile. We consider the two most important types of detunings: constant (transform-limited pulse) and linear (chirped pulse). The theoretical method is based upon the Dykhne-Davis-Pechukas approximation [1] and the adiabatic condition. We derive very accurate estimates for the final transition probability as a function of the Rabi frequency, the detuning and the pulse width. These analytic results allow us to determine the specific features of excitation by Gaussian pulses, in comparison with various exactly soluble analytic models with different pulse shapes (constant and hyperbolic-secant). We derive the frequency of the Rabi oscillations for a constant detuning, and the linewidth of the excitation profile, which shows a very weak (logarithmic) power broadening. For a linear detuning, we derive the conditions for complete population inversion and discuss the consequences of nonlinearities.

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Controlled light storage in a medium of four-level atoms

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It has been shown both theoretically and experimentally [1],[2] that a light pulse propagating in a medium composed of three-level atoms in a Λ configuration, suitably driven by another pulse, can be stopped and later released in a controlled way. Extending such a configuration by adding a coherently coupled fourth level opens new possibilities of an external control of such a process. Light storing in the form of atomic coherences joins the advantages of the efficiency of light as an information carrier and of an atomic medium as an information store. Thus, it might be a question of a practical importance how to modify in a controlled way the properties of the released light by processing the atomic medium during the storage stage.

In a Λ system with fourth level or in a double Λ system it is possible to change the light frequency of the stored light or even release two pulses of different frequencies by applying two control fields, properly chosen and delayed in time. At the beginning of the process the control field ϵ_2 is on, so the medium is electromagnetically induced to be transparent. When the signal field ϵ_1 has entered the medium the control field is switched off. The velocity of the signal is reduced to zero and atoms remain in a coherent superposition of the two lower states b and c . When the control field is switched on again the pulse is released in a process which is time reflection of the stopping stage. Switching on any interactions involving any of the two lower states modifies the coherence σ_{bc} , which later influences the released pulse or pulses [3].

We present two possibilities of controlling the released pulse or pulses by modifying the atomic coherence due to the stopped light: both consist in an additional coupling of the Λ system with fourth level. We show that the Rabi oscillations due to the new interactions modify in a coherent way the properties of the released light. One can in particular release two pulses of different frequencies or polarizations, with their envelopes being regulated in a continuous way.

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Speed-gradient control of cooled atoms in potential standing waves

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One of the main problem of nano-lithography with cooled atoms: How to choose appropriate parameters of the optical radiation to achieve the most efficient focusing of the cooled atoms in periodical potential wells of standing wave? It means that we can obtain the very narrow width of cooled atoms (much less than wavelength λ of optical radiation) by focusing in standing wave. As it known [1], the dynamic of cooled atoms in standing wave in neglecting of diffusion term can be represented as dynamics of pendulum with friction term. It is not possible to obtain the width of the localization of atoms much less than wavelength since the light force does not cool atoms near of the minimum of the potential wells. In this paper we consider the possibility to increase the efficiency which means obtaining the very narrow width of atoms by controlling of an atom dynamics in periodic potential of standing wave. Such control achieves by using the additional laser field that leads to additional terms in dynamic equation for an atom movement

$$\frac{d^2x}{dt^2} + \beta \left[1 + u \left(x, \frac{dx}{dt} \right) \right] \frac{dx}{dt} + \omega^2 \left[1 + u \left(x, \frac{dx}{dt} \right) \right] \sin(2kx) = 0, \quad (1)$$

where $\beta = (4\hbar k^2 g^2 / M \gamma^2) (\sin kx)^2$ is the coefficient friction for atoms, $\omega^2 = 8\hbar k^2 g^2 \sin^2 kx / M |\Omega|^2$ is determined an oscillation frequency of atoms into single potential well (g is Rabi frequency, γ is the half of the natural width of an atom transition, Ω is the detuning, M is an atom mass), and $u(x, dx/dt)$ is the function of the control, which is different for each atom and depends on its initial position and velocity.

To calculate the width of atoms after the focusing with additional control function, we obtain the solution of Eq.(1) by the speed-gradient method [2] for each point of the phase space. We consider two additional possibilities of atom focusing to comparing with usual focusing without control function. The first, the control function was chosen so that all atoms fall into potential wells of standing wave. In this case we obtain the increasing of atom number in five times (compare with ordinary focusing). At the same time, the width of atom distribution function dw inside wells is about $dw \sim \lambda/20$. In the second case, the control function was chosen so that all atoms prepare on the hills of the periodical potential. For such unusual focusing we demonstrate that the width of atoms dw can be done extraordinary narrow $dw \sim \lambda/100=6 \text{ nm}$ and an atom number increases in one hundred times.

This work was financially supported by the grants of the Program "Universities of Russia" YP.01.01.040, Education Ministry of Russian Federation E02-3.2-287.

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Equivalency of Kadanoff–Beym and Keldysh approaches in theory of Bose-Einstein condensate

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We are discussing here the adequate "language" to formulate the valid theory of Bose–Einstein condensation in alkali gases and, in particular, the dynamics of vortices in trapped dilute Bose–Einstein condensates (BECs) as the subject of great interest, stimulated by the experimental achievement of BECs. Vortex-like excitation exists in atomic Bose–Einstein condensates as example of topological defects. The vortices obtained from the Gross–Pitaevskii (GP) equation are analogous to vortices in classical hydrodynamics.

The formulation of the quantum kinetic theory of dilute Bose–Einstein condensed gases is possible in terms of nonequilibrium Green's function and their Kadanoff–Baym (KB) equations. As it was recently shown in [1], GP and KB approaches are equivalent. Nevertheless, the vortex structure of BECs is investigated mostly with the GP technique.

Our basement is the general fact that Kadanoff–Baym approach and Schwinger–Keldysh formulation are equivalent in *every* nonequilibrium model (and this fact seems to be not well-known). Both of them, KB [2] and Keldysh [3] approaches are applied to the theory of BECs. Our unified KB–Keldysh formulation allows us to describe easier properties of BECs and their vortex structure.

This work was financially supported by the grants of the Program "Universities of Russia" YP.01.01.040, Education Ministry of Russian Federation E02-3.2-287, and Russian Foundation of Basic Research 02-02-17686.

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Atomic collisions in a ring trap: the atomotron

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During the last decade the development of techniques to cool and to trap neutral atoms has promoted a great deal of possibilities in the investigation of cold atomic collisions. Elastic and inelastic process occurring at the mK regime have allowed a profound understanding of long range interatomic potentials as well as precise determination of scattering length. Those investigations have been crucial for the achievement of Bose-Einstein Condensation and related topics. One of the problems in studies of atomic collisions in a symmetric trap is the lack of orientation. Atoms interact in all direction and the measured quantities correspond to an average involving all contributions. Experiments involving excited states with polarization dependence, like photoassociation and others, cannot be investigated in traps. To overcome such a problem, we have used a ring-shaped distribution of trapped atoms to investigate polarization effects in cold collisions. This system we have called Atomotron. The Atomotron is a type of storage ring for neutral atoms where they behave like in an atomic beam.

The Atomotron is obtained in a magneto-optical trap when Gaussian laser beams are adequately placed forming a race-track geometry [1]. In such a geometry, we create a coordinate-dependent macroscopic vortex force which combined with the conventional trapping forces promotes the stabilization of the atomic orbits. The formed storage ring can combine up to 10^9 atoms in a temperature that ranges from 100 to $250\mu K$ for Rb atoms. Those atoms are like an atomic beam in circular motion. Using the Atomotron we have investigated polarization dependence for photoassociation of Rb and the production of ground state molecules. The obtained results show evidences of different states participation as well as their involved selection rules.

During this presentation we shall discuss the principles involved in the formation of the Atomotron as well as the obtained results concerning cold collisions. This work has received financial support from Fapesp and CNPq - Brazilian Agencies.

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Laser Cooling in the Case of Exact Resonance

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As is well known laser cooling in the fields with nonuniform polarization appear additional forces leading to sub-Doppler laser cooling of atoms. In the majority of works have been used the fields, formed by circular polarized counterpropagating light waves $\sigma_+ - \sigma_-$ configuration, or formed by linearly polarized light waves with a mutual angle between their polarization vector [1,2]. In all these cases the direction of a kinetic process (heating or cooling of atoms) is governed by the sign of laser detuning from atomic resonance. In particular, for atoms with $J \rightarrow J + 1$ optical transition cooling takes a place under red detuning $\delta < 0$. The use of elliptical polarization gives additional features in atom-light interaction that leads to new forces on atoms. In the present work we consider 1D laser cooling in a field of more general polarization configuration. This field formed by counterpropagating waves with opposite elliptical polarization ($\varepsilon - \theta - \bar{\varepsilon}$ field configuration). With ε is the parameter of ellipticity and θ is the angle between major axes of waves polarization ellipses. As was predicted in our earlier paper [3] in such field appears a new fore that acts on atom even in the case of exact resonance, where the usual sub-Doppler force vanish.

We consider the laser cooling of atom with optical transition $Jg = 1 \rightarrow Je = 2$ (Jg and Je are the total angular moments for ground and excited states correspondently) and show that in the case under consideration atomic kinetics depends not only on field detuning δ , but also on waves ellipticities ε and angle θ . Moreover, for the case of close resonance $|\delta| < \gamma$, where γ is natural linewidth, there exists area of parameters $\varepsilon - \theta$ in which the direction of kinetics process (cooling or heating) is opposed to well known field configuration $\sigma_+ - \sigma_-$ and $lin \perp lin$. The laser cooling temperature is analyzed in this area as function of light waves ellipticities.

This work is partially supported by RFBR (grants N01-02-17036 and N01-02-17744, and N03-02-06047) and by grant E00-3.2-153 of Ministry of Education of Russian Federation.

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Laser Cooling in a Standing Light Wave with Uniform Elliptical Polarization

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Initially (before 1988) the mechanical action of resonant light on atom and, in particular, the atom motion in a light field was entirely considered in the frame of simple two-level atom model [1,2]. This description has allowed to understand the physical mechanisms and nature of the force on atom in light field, to estimate the limit of laser cooling (so-called Doppler limit) $k_B T_D \simeq \hbar \gamma$, where γ is the natural linewidth of excited state. In the present work we consider quasiclassical laser cooling of atom with degenerated energy levels in standing light wave with uniform elliptical polarization. For atoms with a simple optical transition $Jg = 1/2 \rightarrow Je = 1/2$ (Jg and Je are the total angular moments for ground and excited states correspondingly) we obtain analytical expressions for the force on atom, friction and diffusion coefficient. For linear field polarization these expressions coincide with well-known results for two-level atom. However for elliptical polarization they contain additional terms. These terms leads to qualitatively new result in comparison with two-level atom. In the case of low field intensity and large detuning ($\delta \gg \gamma$) the new term in friction coefficient exceed the usual friction coefficient for two-level atom as δ^2/γ^2 that leads to significant increasing the rate of laser cooling. In intense laser field these terms in friction and diffusion coefficient give peculiarities in temperature of laser cooling:

- In a field with ellipticity $\sin^2(2\varepsilon) < 1/3$, where ellipticity parameter ε ($|\tan(\varepsilon)|$ is equal to the ratio of the semiaxes of polarization ellipse) the result qualitatively corresponds to two-level atom, i.e. there exists two region in detuning for laser cooling: the small region in red detuning and the major one in blue detuning.

- Apart from previous case of intense laser field with ellipticity $\sin^2(2\varepsilon) \geq 1/3$, the result qualitatively differ: the laser cooling takes place only for red detuning.

Additionally we perform numerical calculation for atom with optical transition $Jg = 1 \rightarrow Je = 2$. The laser cooling for these atoms corresponds to two-level model only for laser field with circular polarization. Predicted new terms in friction and diffusion coefficient appears even in the case of liner polarization and they became more significant in elliptically polarized light field.

This work is partially supported by RFBR (grants N01-02-17036 and N01-02-17744, and N03-02-06047) and by grant E00-3.2-153 of Ministry of Education of Russian Federation.

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Prospects of VNIIFTRI Cesium Fountain

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Russian State Time and Frequency Service relies on a group of H-masers and classical Cs-beam primary frequency standard. H-masers are used as time keeper with a long term stability near $\sim 10^{-15}$, while Cs standard is used for H-maser calibration and it has $\sim 2 \times 10^{-14}$ uncertainty.

We started our Cs fountain project in the spring 1999, minding to get uncertainty at list one order less. The present paper is a brief review of the latest research data obtained at IMVP GP VNIIFTRI in this topic area. The VNIIFTRI Cs Fountain (optical system, physical package, control system, etc) was previously described in details [1,2]. We recall here only preliminary results.

They are in following:

The investigation of a prototype fountain system have been carried out. First the operation in a MOT regime was investigated. Two 80 mm in diameter anti-Helmholtz coils were installed on a MOT section. The distance between them was 60 mm. The magnetic flux density gradient value could exceed 10 Gauss/cm. Unbalanced horizontal beams were used. The beams with linear polarization in X and Y directions were retroreflected by mirrors in -X and -Y directions using $\lambda/4$ plates, respectively (in future it is planned to get balanced horizontal beams.

After the MOT magnetic fields were switched off, the atoms were further cooled in a 1-3S phase when the lasers changed their frequency from 6MHz to 60 MHz bellow $F = 4 - F' = 5$ resonance frequency. The intensity of the beams did not change at the time. In 0.2 s after atoms release a TOF signal was obtained in the detection zone. Its width is 7 ms and evaluated cooled atoms temperature is 20 μ K.

To check operation in molasses phase, we surrounded the MOT and detection zones by a single layer of the magnetic field. We obtain a molasses operation, and the cold atom temperature is determined by measuring the optical thickness of the ballistically travelling sample cold atoms as a function of the time. The evaluated molasses temperature was found about 2–3 μ K. These values are in the reasonable agreement with an important predictions of the theory [3].

In the near future , the installed experimental devices will be used in order to obtain cold fountain Ramsey fringes for the hyperfine structure components of Cs atoms in the ground state.

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Production of cold ground state heteronuclear molecules

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Over the past years, many experiments have been devoted to the study of excited-ground state collisions using a sample of trapped cold atoms [1]. Recently, several theoretical studies have been published, proposing new experiments involving two different species of atoms trapped together: two BEC species and heteronuclear cold photoassociation [2]. The natural extension of those investigations is the experimental study of the heteronuclear photoassociation by laser spectroscopy techniques, already well developed for the homonuclear cold samples [3]. In this work we present the first production of cold ground state heteronuclear KRb molecules.

According to Wang and Stwalley [2] the K-Rb sample is one of the most suitable for photoassociation due to its high relative heteronuclear Franck-Condon factor; nevertheless high atomic density are required. Therefore, the heteronuclear loss rate must be small in order not to compromise the performance of the binary sample. In order to characterize the K-Rb sample we had performed trap loss experiments to evaluate the heteronuclear losses imposed by the samples to each other. Our results show that the heteronuclear collisions do not compromise the MOT densities and number of trapped atoms. To detect the ground state molecule we ionized with a pulsed dye laser and detect the ions [3]. Briefly, in the experiment there are a trapping and probe phases. During the probe phase the heteronuclear pairs, which were photoassociated during the trapping phase are photoionized by a pulsed laser (100 mJ/pulse, 4 ns, $\lambda \sim 603$ nm). The ions are collected by a channeltron and analyzed by a boxcar integrator gate. By time-of-flight the atomic ions can be discriminated from the molecular ions. We observe K_2 , Rb_2 and KRb ions in our laboratory. Important features like molecules temperature as well as the involved molecular states are investigated. By scanning the frequency of a photoassociation probe laser, we shall be able to obtain the bound states of the K-Rb molecule, and extract important information like the scattering length, etc. The production of heteronuclear cold molecules opens up new possibilities in the electrostatic traps of molecules. This work has received financial support from Fapesp and CNPq - Brazilian Agencies

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The variable phase method used to calculate and correct scattering lengths

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We demonstrate a numerical method to show how the s-wave scattering length for a pair of colliding atoms can be obtained as the limit, at infinite atomic separation, of the accumulated scattering length that satisfies the first order ordinary differential equation derived from variable phase theory [1]. The accumulated scattering length $a(R)$, at separation R , is equal to the scattering length calculated for an interaction that is truncated at R and when the interaction supports bound vibrational molecular states, as it certainly does for alkali metals, the accumulated scattering length has poles corresponding to the turning points of the zero energy molecular vibrational wave-function and the usual numerical algorithms for solving ordinary differential equations cannot be used. We show how the differential equation satisfied by the accumulated scattering length can be rewritten as a Riccati equation satisfied by the log-derivative [2] so that a suitable integrator for the log-derivative, a *symplectic* integrator [3,4], may be used. We provide a numerical tabulation of $a(R)$ for Cs-Cs scattering *via* a model potential interaction [5]. From the differential equation satisfied by $a(R)$ we derive simple expressions for the correction to the scattering length, evaluated as $a(R_c)$ at some cut-off separation R_c , that arises from the first order effect of the interaction over the range $[R_c, \infty]$. We show that one of our expressions overestimates (algebraically) the scattering length while the other underestimates it, and we show, for typical inverse power dispersion interactions, how the two expressions may be combined to yield a better estimate. We relate our expressions to those obtained elsewhere [6,7,8,9,10] and demonstrate that one of them can be obtained from secular perturbation theory [11,12]. Finally we discuss higher order corrections obtainable from the differential equation and relate them to the higher order corrections predicted by secular perturbation theory.

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Rydberg States of Barium in Crossed Fields

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We report recent experimental results obtained by laser spectroscopy of Barium Rydberg atoms in crossed external electric and magnetic fields. The geometry of the experiment was chosen such that the laser beam propagates in a direction parallel to the magnetic field direction, and an effusive atom beam propagates in a direction perpendicular to this magnetic field. By the selection of left or right circular polarisation of the laser radiation it is possible to distinguish the σ^+ and σ^- states of the Barium atoms in the magnetic field [1]. By applying an electric field across the atom beam perpendicularly to the magnetic field it is possible to correct for the motional Stark effect induced by the motion of the atoms in the magnetic field [2]. At suitable magnetic field strengths, spectral regions where the influence of the quantum numbers is reduced can be accessed through the application of various electric fields relative to this compensation field.

The beam of atoms is excited to high-lying Rydberg states ($n = 40$ to 60) by a pulsed, tuneable, single-mode, Nd:YAG pumped OPO laser system (20mJ, 4ns, 10Hz), giving a bandwidth of 400MHz. This represents more than a five-fold increase in spectral resolution to that reported in the most recently published experimental data [1,3]. The excited atoms are field ionised and the detached electrons detected on multi-channel plates.

With this experimental set-up we have compiled Stark-Maps for Barium in several wavelength regions and at various magnetic field strengths. We have carried out preliminary statistical analysis on the experimentally determined level spacings at selected areas in the Stark Maps. The aim of this analysis was to understand the transition in the semi-classical limit from an ordered quantum system to a classically chaotic one. The crossed-field spectrum presents some specific properties as compared with the pure magnetic field problem, in that the presence of the electric field breaks all the known quantum numbers of the atom except z-parity.

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Coherent Population Trapping in an Open Λ -System of Samarium Atom

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Coherent population trapping (CPT) resonances were the subject of interest in the variety of experiments during the last years [1, 2, 3]. CPT resonances were mostly studied in nearly closed Λ - systems of alkali atoms. Nevertheless the coherent population trapping in an open Λ - system has some interesting features, untypical to the closed one. The contrast of the CPT resonance in the open Λ - system strongly depends on the depolarization rate of its lower levels, while the width of the resonance is practically insensitive to it [4]. Such dependence is unusual for closed systems [2].

It is well known that in a closed Λ - system collisions with buffer gas lead to the narrowing of CPT resonance in a wide range of buffer gas pressures. The velocity selective optical pumping (VSOP) practically does not affect the observed CPT resonances even for relatively high buffer gas pressures [1, 3]. On the contrary, in the case of an open system the VSOP strongly affects the observed resonances.

We represent the results of experimental study of an open Λ -system of Samarium atom in bichromatic electromagnetic field. The dependence of the contrast and the width of observed CPT resonance on buffer gas pressure was investigated. The results were interpreted considering the competition between CPT and VSOP processes at relatively low buffer gas pressures (up to 100 Pa).

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New schemes for laser selective detecting the single atoms and products of nuclear reactions

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Laser photoionization detecting the atoms in a beam and the buffer gas attracts a great interest for systematic studying the short-lived isotopes and nuclear isomers in experiments in the real time of accelerator work which is used for their generation [1]. We propose a new approach to construction of the optimal schemes of the laser photoionization method for further applying to problem of the nuclear reactions products detecting. It's studied the reaction of spontaneous Cf(252) isotope fission on non-symmetric fragments, one of that is the caesium nucleus. The corresponding experiment on detecting the reactions products is in details described in [1]. Usually the foil with implanted Cf ions is disposed before exit of the surface barrier detector that is sensitive to the nuclear decay fragments. Intensity of the fission reaction is of order of one event per second. Laser beam crossed the axe of collector of the nuclear fragments. The braking is realized in the gas mixture 990The heavy fragment of the Cf nucleus fission created in the ionized track 106 electrons which are collected on the collector during 2 ms. The collector is charged negatively 40ms later after nuclear decay and 10ms before the laser pulse action. The photo electrons, arisen due to the selective two-stepped photoionization are drafted into the proportional counter for their detecting. Usually a resonant excitement of Cs is realized by the dye laser pulse, the spectrum of which includes the wavelengths of two transitions 6S(1/2)-7P(3/2) (4555Å) and 6S(1/2)-7P(1/2) (4593Å). This pulse also realizes non-resonant photoionization of the Cs excited atoms. The disadvantages of the standard scheme are connected with non-optimality of laser atomic photoionization one, effects of impact lines broadening due to the using the buffer gas, the isotope shift and hyperfine structure masking etc. We proposed and carried out a modelling new laser photoionization scheme, which is based on a selective resonance excitation of the Cs atoms by laser radiation into states near ionization boundary and further autoionization decay of excited states under action of external electric field [2]. Detailed calculation data regarding the dependence of ionization velocity of excited atom upon the electric field strength for states with quantum numbers $n=8, 9, 16$ and $m=0, n2=n-1$ for Cs and also other alkali atoms are presented. It is found a set of parameters when velocity of ionization in a field is more than the radiation decay velocity. The corresponding parameters of laser and electric fields, atomic transitions, states, decay parameters, scheme realization conditions etc are calculated within the density matrix formalism to atomic dynamics, the optimal governing theory and quantum-mechanical methods [1,2].

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Experimental Hyperfine Structure Investigation in Scandium I

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As a continuation of our hyperfine structure studies of 3d-shell elements [1] hyperfine structure investigation in the spectrum of atomic Scandium has been performed by laser opto-galvanic detection in a discharge of a hollow cathode lamp. The element Scandium possesses just one stable isotope of odd mass number 45, whose nuclear spin is $I = 7/2$.

Using a Titan-Sapphire-ring laser as a light source we were able to investigate transitions of Scandium I in wavelength region between 750-780 nm for the levels of the configurations $3d^24s$, $3d^24p$ and $3d4s4p$. In the spectral region from 625 nm to 650 nm we have investigated transitions of the levels of the configurations $3d4s4p$, $3d4s^2$ and $3d4s5s$ by using a cw-ring dye laser.

The magnetic dipole hyperfine constants A of the three odd levels and the five even levels have been evaluated for the first time. The results of our measurements are presented together with a list of all hyperfine constants of Scandium I known up to now. These data serves as basis for a parametric study of the hyperfine structure shown in our another poster.

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Plasma plume oscillations during welding of thin metal sheets with a CW CO_2 laser

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The automobile industry has recently incorporated a new technology in order to improve the quality of its products: the laser welding process. The faults we are interested in are those defects that can be produced during the laser welding process. These are holes, porosity, surface appearance and partial penetration. In the car manufacturing process, the stage that follows the laser welding one is stamping, where the different car body parts take shape. If the weld has defects, it probably will break. This will introduce delays in the whole manufacturing process. During high speed CO_2 laser welding, faults may occur due to the state of the cross section of the specimen, gap, flow rate of the assist gas, travel speed and laser power. The defects are monitored in real time, in order to prevent continuous occurrence of defects, reduce the loss of material and guarantee good quality. Also, the shape of the weld bead is the main factor in deciding the strength of the workpiece. Therefore, development of a monitoring system in laser welding which detects weld defects and bead shape is required. During the laser welding process, an intense beam ($I > 1MW\ cm^{-2}$) focused on the surface of a workpiece, creates a thin capillary in a moving material called the keyhole.

Any distortion of the pressure balance generates pressure fluctuations inside the keyhole [1,2]. Irregular oscillations are observed in the radiation of plasma expanding from the keyhole [3]. It is obvious that by suppressing the plume oscillations or making them more regular (periodic) better welding results [4] can be obtained without faults. There are several reasons for investigating the problem. Firstly, the models of laser welding that describe the observed pressure oscillations are scarce [1,2] and need experimental validation. The cause of the oscillations is not clear. It has been concluded that unstable laser power leads to the oscillations [1]. Because at any given value of the absorbed laser power only one stable keyhole radius exists [1,2], it has been suggested that it is the interaction of laser beam with the plasma plume which results in a change of beam power density which is the cause of keyhole oscillations. So far, the physics of keyhole dynamics is not fully understood and experimental data are needed to establish a reliable theoretical model of the oscillations. Second, the optical signals emitted during laser welding can be used for real time quality monitoring system. The dependence between observed signals and the depth of penetration as well as seam quality must be known. In this paper, a study of the electromagnetic spectrum of the plasma laser-induced in the laser welding is shown. This emission spectral analysis allowed us to determine most significant wavelength intervals to detect the plasma oscillations. Secondly, the plasma oscillations are correlated with defects in the seam and the weld quality.

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Laser monitoring of atmospheric and aerosol medium parameters

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Paper is devoted to development of new methods for monitoring and diagnostics the parameters of aerosol, atmospheric and plasma mediums with using non-linear spectroscopic effects [1,2]. It is considered a non-linear multi-photon process of resonance interaction between laser radiation and medium. Within energy approach it is calculated the probability of two-photon absorption on vibration-rotational transitions in molecules on the example of two-photon absorption of the CO₂ laser radiation in the 010 water vapour band. In process of the IR laser radiation (LR) resonance absorption in atmosphere it occurs the redistribution of molecules on energy levels of internal freedom degrees. Creation of the excited nitrogen molecules due the resonance excitation transmission from carbon dioxide molecules leads to the medium polarizability changing. We consider the role of the resonant spectroscopic effects in the forming of the non-linear behaviour of the gas atmosphere for propagation of the powerful LR pulses in it under different conditions and atmosphere models and apply these phenomenon for determination of the whole number of the atmosphere parameters. As a basic model for the absorbed energy relaxation description it's used 3-mode kinetic processes model. It is numerically shown the change in the time dependence of the resonance radiation absorption coefficient for carbon dioxide under different conditions. In paper within the operator perturbation theory form and QED moment technique [3] it is also developed the effective approach for description of the LR atmosphere multi-photon absorption and Stark dynamic shift (these effects can be used as the physical basis for new distance methods of environment laser diagnostics). Under consideration of the two-quantum transitions in ground vibration band $v=0 - v=1$ for diatomic molecules with zeroth projection of electron impulse moment on inter-nuclear axe, it is necessary to account for contribution of electron intermediate transitions. This contribution dw into the frequency Stark shift value dw_{st} of the vibration-rotational transition 1-2 can be simplified according to Letokhov et al approach [1]. For example, using the resonance condition and sum rule for oscillator strengths one can obtain for dw the estimate: $dw \approx 8\pi^2 w_v I / \nu^3$, where I is the resonance radiation power density, w_v is a frequency of vibration transition, $w \approx w_v/2$ and other notations are standard. In a case of multi-atomic molecules under calculation of the vibration-rotational transition frequency Stark shift in resonance field, every vibration mode can be approximated by an "effective" diatomic molecules [1]. We have estimated an effect of the two-photon absorption of laser radiation on vibration-rotational transitions of molecules, in particular, of the CO₂-laser radiation (radiation intensity $I=10^7 \text{ Wt/cm}^2$ in the band 010 of water vapour. Our estimates for the electron transition shift is $dv=dw/2\pi$ is $3 \cdot 10^{-2} \text{ G/(Wt/cm}^2)$; probability for two-photon absorption is $G=(3-4) \cdot 10^9 \text{ s}^{-1}$. This value is correlated with estimate, obtained by Letokhov et al [1]: $G=(1-1,5) \cdot 10^9 \text{ s}^{-1}$.

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Precision Differential Optical Measurement of the 2S Hyperfine Interval in Atomic Hydrogen

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Precision measurements of the frequency of the 2S hyperfine interval $f_{\text{HFS}}(2S)$ in hydrogen-like atoms open the possibility to test the quantum-electrodynamics theory (QED) to the level up to α^4 and $\alpha^3 m_e/m_p$. In spite of the fact, that the accuracy of a direct theoretical prediction of $f_{\text{HFS}}(2S)$ is restricted by an insufficient knowledge of the proton structure, the specific combination of the 1S and 2S hyperfine intervals $D_{21} = 8f_{\text{HFS}}(2S) - f_{\text{HFS}}(1S)$ can be calculated precisely due to significant cancellations of nuclear structure effects [1]. The precision of theoretical calculations of D_{21} in atomic hydrogen far exceeds the experimental accuracy, thus demanding further experimental improvements.

During the last decades the frequency $f_{\text{HFS}}(2S)$ in atomic hydrogen has been measured twice using radio-frequency spectroscopy on a hydrogen thermal beam with a relative accuracy of 150 – 300 ppb [2,3]. We have applied a completely independent method based on precision two-photon UV spectroscopy on a cold hydrogen beam [4]. We have used the second harmonic of a 486 nm dye laser locked to an extremely stable reference cavity to excite 1S – 2S transitions in atomic hydrogen. The laser frequency, shifted by a double-pass AOM, is tuned separately to excite the $(1S, F = 0) \rightarrow (2S, F = 0)$ and $(1S, F = 1) \rightarrow (2S, F = 1)$ transitions between the hyperfine levels. The Hydrogen beam is shielded from external magnetic and electric fields. Using the cavity as a frequency flywheel with a very high short-time stability and a predictable drift and the well-known value for $f_{\text{HFS}}(1S)$, we deduce $f_{\text{HFS}}(2S)$ as a frequency difference between two laser excitation fields.

The differential measurement cancels a number of important systematic effects intrinsic to two-photon spectroscopy on atomic beams (e.g. the AC-Stark shift and the 2nd order Doppler effect). The frequency of the 2S hyperfine interval has been measured during 16 days at different background gas pressures. For the averaged data, we find a preliminary value of 177 556 859(15) Hz which is up to now the most accurate experimental value for $f_{\text{HFS}}(2S)$. This experimental result along with the previous ones [2,3] are in moderately good agreement ($< 2\sigma$) with the value deduced from theoretical D_{21} calculations.

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Energy spectra of elementary excitations and their dispersion in tetragonal crystals ZnP_2 and CdP_2

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Dispersion of elementary excitations in several directions of wave vector was investigated in isostructural tetragonal crystals ZnP_2 and CdP_2 . Photoluminescence spectra, one- and two-phonon Raman scattering and spectra of edge absorption were recorded experimentally. Both of these crystals are indirect semiconductors. Vibration spectra are similar for both compounds, but spectra of exciton-phonon transitions are quite different. Each of mentioned crystals could exist in two enantiomorphous modifications, which transform one into another by means of inversion operation. Symmetry of the right modifications lattices is characterised by space group $P4_12_12$, left ? $P4_32_12$ and belong to crystal class which is described by point group 422. Since both of enantiomorphous modifications are related to one crystal class, energy spectra don't depend on of modification type.

For analysis of dispersion of energy states in the crystals method of projective representations of wave vector groups was applied. The following points of Brillouin zone were taken into consideration: Γ , Λ , Z , S , A , V , M , Σ . At each of these points one- and two-valued irreducible projective representations of wave vector groups were constructed for two enantiomorphous modifications. For Λ , S , V and Σ points these projective representations were defined as functions of wave vector.

Influence of time inversion on energy spectra of elementary excitation at these points also was taken into consideration by means of Herring criterion, which gives the possibility to define the degeneracy of energy states in certain point of Brillouin zone in the absence thereof external electric or magnetic fields. Compatibility correlations between projective representations in following directions: $\Gamma \rightarrow \Lambda \rightarrow Z$, $Z \rightarrow S \rightarrow A$, $\Gamma \rightarrow \Sigma \rightarrow M$, $M \rightarrow V \rightarrow A$ were built using projective representations of mentioned points. These compatibility correlations describe behaviour of corresponding wave functions of energy states with integer and half-integer spin. It was determined, which of examined points of Brillouin zone are points of zero slope and points where dispersion curves of energy states have extremum by $\vec{k}\vec{p}$ -method. This analysis and data obtained from energy spectra allow determining the minimum of conduction band.

Bare state ladder system for X-ray lasing without inversion

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A scheme for obtaining laser without inversion in the deep x-ray regime is proposed based on the principle of gain without inversion. A ladder scheme is proposed in Ar^{+8} system. In this system conventional lasing with population inversion in a neon-like fashion. This lasing field is proposed for the drive field on the higher transition of the ladder. A coherent field obtained in the high harmonics ultrashort laser provides the probe field to be amplified. The ground level is incoherently pumped into the highest level, while the latter is incoherently depumped into the ground level, at a different adjustable rate. A detailed density matrix calculation of the ladder configuration is performed [1]. The system is extensively investigated in the steady state regime and the influence of various system parameters on lasing is explained. We derive conditions on that the incoherent pump rate must fulfill in order to achieve lasing without inversion. Numerical calculations in the bare state picture exhibits gain at resonance and at the Rabi side bands, for appropriate choice of system parameters, i.e., the strength of the driving field, the strength of the incoherent pump that provides the required energy needed for the inversionless amplification and the deexcitation rate. The latter rate is detrimental to lasing as it increases. Numerical calculation of the density matrix elements is obtained both for resonance and off resonance cases. Populations and coherences are shown to oscillate at the Rabi and double Rabi frequencies, with the highest gain peak for the probe laser is observed to occur at the first Rabi cycle. Also the spectrum and line shape are explored both for resonance and off resonance situations. Probe line shape is seen to be constructed of two symmetrical dispersion-like features each centered at the generalized Rabi side bands. This is testimony of the quantum interference occurring at these locations. At line center we observe very narrow gain peak. The real part of probe coherence, responsible for index of refraction consists of two somewhat asymmetrical Lorentzian lineshapes joined together at line center. Again this is interpreted as arising from quantum coherence and interference. An interesting observed feature is the effect of refractive index enhancement occurring at the Rabi sidebands, where vanishing absorption is accompanied by large refractive index.

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Frequency stability comparison of diode lasers locked to Doppler- and sub-Doppler resonances

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This presentation concerns what constitutes - to our knowledge - the first quantitative and systematic comparison of two Extended Cavity Diode Lasers (ECDL) stabilization schemes based on, respectively, Doppler and Sub-Doppler spectroscopy in Rb atomic vapour cells.

The sub-Doppler laser stabilisation based on saturated absorption is widely applied in the field of precision instrumentation, e.g., atomic frequency standards, or magnetometers. It is the object of this study to investigate whether or not the significantly simpler method of Doppler stabilization can be used instead without compromising the required instrument performance.

Our experimental studies realised in Observatoire de Neuchâtel use two identical and completely independent laser systems based on ECDLs that can be stabilised to either Doppler-(absorption) or sub-Doppler (saturated absorption) reference lines. The relative stability of these two stabilized lasers was measured by a heterodyne method. We are therefore able to characterise and compare the frequency stability of both schemes.

In addition to the relative Allan variation plot we describe and explore the qualitative behaviour of some resonance lines in various experimental conditions and the results of our systematic study aiming to quantify the frequency shifts caused by parameters like, e.g., magnetic field, laser intensity, pointing stability of the laser beam, and cell temperature.

The impact of the resulting stability on the applications of the two schemes in atomic clocks and magnetometers will be discussed.

Acknowledgment

This work was supported by the Swiss National Science Foundation (SCOPES 7BUPJ062412). GM, CA thank the European Space Agency (ESA contract 15280/01/NL/US). DS, SC, CA thank the Bulgarian National Scientific Council (F-1005/00).

The sensitivity of the coherent population trapping resonances to stray magnetic fields

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The CPT resonances obtained in 2-level system in ^{87}Rb were investigated. The experiment was performed in a vacuum cell containing natural mix of Rb isotopes on D_1 line. The resonances were obtained in level-crossing type experiment - sweeping the magnetic field around zero point and using a single laser beam. So the two-photon resonance which appears as fluorescence cancelling around the zero point, when the Rb levels are degenerated. Its width is determined mainly by the relaxation processes in the cell and time of interaction of the atom with the laser beam. CPT signals with complex shape (a narrow resonance $\sim 2\text{kHz}$ superimposed on a wide one $\sim 120\text{kHz}$) were observed [2]. The influence of weak transverse magnetic fields on the amplitude and width of the two components was measured. Due to its narrow width and sensitivities to the magnetic fields these resonances are very promising for small magnetic field measurement.

The CPT resonances were observed with linear, circular and elliptical polarized laser light. Transverse magnetic field widens the resonances obtained by linear and circular polarization but splits the resonance created by slightly elliptical polarized laser light. This splitting shows high sensitivity to magnetic fields- $0,13\text{ kHz/ mG}$. The dependence of this splitting on the elliptical ratio and experimental geometry were investigated. An possible reason for this splitting could be two axes alignment caused by the elliptical polarized excitation beam [3].

The authors would like to acknowledge the EC for the financial support of the project (G6RD-CT-2001-00642) and the Bulgarian NSFB for the partial support of the work (grant F-1005/00).

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Resonance enhanced multiphoton ionization in combination with mass spectrometry as an ultrasensitive tool for the investigation of self-assembled monolayers

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Many nanotechnological applications presently under development rely on functionalized surfaces with (sub)monolayer coverages of complex organic molecules such as self-assembled monolayers (SAMs) [1]. This involves that standard surface characterization techniques such as SIMS, XPS, and AES, must become increasingly sophisticated and sensitive to keep up with the constant reduction of the amount of material available for analysis. In this contribution, we demonstrate that photoionization in combination with particle induced desorption and mass spectrometry could be the basis for analytical techniques suitable for characterizing nanosystems.

The irradiation of a surface with energetic particles, induces the emission of secondary particles such as atoms, molecules and clusters. Although the desorbed particles are distributed over different charge and excited states most of them are neutrals. To probe these neutral particles, we apply photoionization employing a nanosecond lasersystem. A widely used technique to ionize free molecules is non-resonant multiphoton ionization. By using ns-lasers, this technique needs high photon fluences to have a reasonable ionization efficiency, which increases the probability of the photofragmentation process. If one uses resonance enhanced photoionization, the ionization efficiency increases drastically, and as such lower photon fluences are needed to ionize the molecules.

Resonance enhanced multiphoton ionization is used to detect neutral molecular fragments emitted from the surface during cation and electron irradiation of SAMs. As model systems we selected different phenyl- and biphenyl-alkanethiols that covalently bind to an Au/mica substrate [2]. To enhance the ionization efficiency of the molecular fragments, the laserwavelength is turned to a resonance of the phenyl chromophore. To differentiate between molecular fragments emitted from the surface and molecular fragments originating from photodissociation, the mass distribution of photoionized molecules obtained during the irradiation process are compared with the mass distribution of the photoionized parent molecules in the gasphase. Additional information about the photofragmentation of the emitted molecules is obtained by using different photon fluences in the photoionization process. Another advantage of using photoionization of secondary neutrals is that it is possible to determine the kinetic energy of the desorbed particles. We show that the energy and the mass distribution of the emitted particles contains valuable information to characterize the desorption process on SAMs [3].

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This work is financially supported by the Belgian Fund for Scientific Research - Flanders (F.W.O.), the Flemish Concerted Action Research Program (G.O.A.) and the Interuniversity Poles of Attraction Program (I.A.P.) - Belgian State, Prime Minister's Office - Federal Office for Scientific, Technical and Cultural Affairs. The financial support of the National Science Foundation, the National Institutes of Health, the Office of Naval Research, and the Polish Committee for Scientific Research Fund and Maria Sklodowska Fund MEN/NSF-97-304 are gratefully acknowledged. E.V. is a Postdoctoral Fellow of the F.W.O.

Laser spectroscopy of neutron deficient titanium isotopes in bunched ion beam

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Optical isotope shifts of the unstable ^{44,45}Ti isotopes, as well as of the stable ^{46–50}Ti, have been investigated by collinear laser spectroscopy in fast ion beam using an ion guide isotope separator with cooler-buncher. Changes in mean square charge radii across the $\nu 1f_{7/2}$ shell are deduced. A significant difference with the symmetric parabolic behaviour of the nuclear charge radii of the neighbouring element Ca on the neutron number is observed. The evolution of the Ti nuclear radii as the isotopes become more neutrons deficient shows a generally increasing tendency and suggests that a proton skin may be developed. Obtained Ti mean square charge radii changes were compared with theory predictions for this region of nuclei. The self-consistent relativistic mean-field (RMF) theory [1] predicts in the case of Ti a continual increase in the charge radius going from $N = 28$ to the $N = 20$ shell closure. The general trend of nuclear charge radii in the whole titanium isotopic chain is described qualitatively very well. The RMF theory predicts also a typical shell closure effect, i.e. a sudden increase of Ca, as well as of Ti, charge radius at the $N = 28$ shell closure but fails to reproduce the parabolic shape in $1f_{7/2}$ shell in the case of Ca. The experimental value of ⁴⁴Ti ms charge radius is in a good agreement with the recent predictions of the strictly restricted dynamic model (SRDM) for ν -cluster type nuclei [2]. A continuation of the optical investigation of Ti isotopes to the lighter ⁴³Ti and especially to ⁴²Ti at the $N = 20$ shell closure will provide a definitive answer as to whether titanium has started to form a proton skin still several neutrons away from the proton drip line in the neutron deficient $1f_{7/2}$ shell.

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The satellite structure of palladium L_{α} and L_{β} X-ray transitions excited by fast oxygen and neon ions

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The high-resolution x-ray spectra of $L_{\alpha_{1,2}}(L_3M_{4,5})$ and $L_{\beta}(L_2M_4)$ transitions in palladium excited by fast oxygen and neon ions were measured in order to investigate the process of multiple ionization and the structure and relaxation of excited multi-vacancy states. The measurements were performed at the Philips cyclotron in the Paul Scherrer Institute (PSI) in Villigen, Switzerland using the beams of highly charged O^{7+} and Ne^{6+} ions accelerated to energies 178-376 MeV. The x-rays were detected by a von Hamos type crystal spectrometer[1] having an energy resolution of about 1 eV for 3 keV. Consequently, the absolute energies of x-rays studied were determined within 0.3-0.5 eV.

The measured spectra of Pd L-x-rays clearly show the pronounced satellite and weaker hyperatellite structures due to the additional (spectator) vacancies in the M- and N-shell. The relative intensities of these satellites reflect the vacancy configuration during x-ray emission, and thus give an access to extract the information on the multiple ionization in the moment of collision as well as the vacancy rearrangement processes. In this way, the ionization probabilities for the M- and N-shells were extracted from the data and compared with the predictions of the semiclassical approximation (SCA)[2] and the so-called "geometrical model" (GM)[3].

The measured satellite structure of $L_{\alpha_{1,2}}(L_3M_{4,5})$ and $L_{\beta}(L_2M_4)$ x-ray transitions in multiply ionized palladium are interpreted in terms of the multi-configuration Dirac-Fock (MCDF) calculations treating, at the present stage, up to three additional vacancies in the M- and N-shell. This calculations reproduce reasonable well the experimental results for oxygen ions, being dominated by configurations with two spectator vacancies in the M-shell. For neon ions much more complex multi-vacancy configurations are needed to explain the data. For this reason, in order to interpret the data we use presently a simplified approach, which based on the binomial model of multiple ionization combined with average MCDF energy shift per vacancy for the M-, N- and O-shells. The final understanding of the present results asks for more extended MCDF calculations, which are in progress.

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Temperature and spatial distribution of the highly charged ions in an electron beam ion trap

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In this work, we present the results of an experimental study of the temperature and spatial distribution of the highly charged ions in the plasma of an electron beam ion trap. Using magnetic dipole (M1) transitions of highly charged argon ions in the visible range (Ar^{9+} , Ar^{10+} , Ar^{13+} and Ar^{14+}), the distribution of trapped ions under different conditions (intensity of electron beam, depth of axial potential trap, atomic beam density, etc) was observed. The information provided by these direct image measurements can be used in the research of the dynamics of trapped highly charged ions, as a test for the plasma models, and also contributes to the improvement of atomic data measurements. We have also measured the temperature of ions of different charge states (Ar^{9+} and Ar^{13+}) at varying plasma conditions. The experimental techniques and the line broadening (Doppler, Zeeman effect, etc) are discussed in detail, and the results are compared with theoretical predictions. For the first time, the temperature differences for different ion charge states are presented. Our measurements and results can help to understand the production, confinement, heating and cooling processes in modern highly charged ion plasma devices.

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Diagnostics of elementary processes in a collisionally pumped plasma and search of the optimal plasma parameters for x-ray lasing

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The X-ray laser problem has stimulated a great number of papers devoting to development of theoretical methods for the modelling the elementary processes in a collisionally pumped plasma. Very 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 which was carried out in the Lawrence Livermore National Laboratory (University 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-m laser driver of intensity 10^{17} W/cm². Significant improvement in efficiency is indicated for shorter laser pulse lengths. At the same time, low temperature plasma sources are more efficient and less expensive devices. They show promise for producing lasing in the vacuum ultraviolet and soft X-ray region. Preliminary investigations of capillary spark discharge were made (c.f.[1-4]), which show the possibility of their use as effective plasma sources for the generation of a soft-X-ray or extreme ultraviolet amplified spontaneous emission. Two key theoretical problems must be solved in order to develop a special code and to predict necessary plasma parameters needed for generation of a soft-X-ray or extreme ultraviolet amplified spontaneous emission. First one is a highly accurate definition of the rate coefficients for elementary processes in the plasma that are responsible for the forming emission lines spectra. The second problem is connected with necessity of development new adequate kinetics calculation schemes for defining the level populations, inversions, line intensities and gain coefficients at definite plasma parameters. Despite of great number papers, devoting to solving cited problems (c.f. [1-5] and references in them), they are at present time quite far from final adequate solution. The most consistent approach to considered problems solving must base on the quantum electrodynamics (QED). In our paper the generalized energy approach in consistent gauge invariant formulation has been at first used for consistent QED description of elementary electron processes in collisionally pumped laser plasma [6,7]. It is developed an optimal scheme for gauge invariant calculation of the electron-collision strength and rate coefficients for the de-excitation (excitation) processes in the Ne-like multicharged ions plasma with further estimate of the optimal plasma parameters for X-ray lasing.

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Spectroscopy of non-LTE laser plasmas. Application to a Xenon spectrum.

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In hot plasmas, for each ion species, the numbers of populated levels, whence, of dipolar-electric lines emitted are so large that, due to the various line-broadening phenomenons, the lines coalesce into broad bands. In the simplest cases, these broad bands can be identified as *Unresolved Transition Arrays* (UTAs), each of them being the totality of the transitions between the quantum states of two electronic configurations. If the Local Thermodynamical Equilibrium (LTE) is obeyed, the intensities of the UTAs can be calculated by applying the Boltzmann statistical law, for the relevant electronic temperature T_e .

In the non-LTE cases, one must take into account the numerous atomic processes for calculating the level populations. This is usually done by means of the Collisional-Radiative Model (MCR), which consists in solving a system of coupled linear balance equations (one equation per level). When the number of levels is huge, one must resort to global MCR methods. Initially, it was proposed to group the levels by configurations, as it has been observed, in results of the standard MCR, that the level populations of a given configuration C nearly obey a Boltzmann-like law, for a temperature T_C specific of that configuration [1].

However, dozens of thousands of relevant configurations must generally be introduced. More recently, we have proposed to build an MCR model with one linear equation per *superconfiguration* (SC) [2]. The temperatures T_{SC} of the SCs are defined like those of the configurations. We have chosen to use SCs defined by the occupation numbers of the atomic *shells* (Layzer complexes). The system of linear equations can be split into two systems. The first one yields the populations of the SC average state. The second one yields the SC temperatures.

We will give details of the method, with its application to the interpretation of an Xe spectrum recorded at LULI (École Polytechnique, Palaiseau, France) in a plasma with $T_e = 450$ eV and density $n_e = 1.2 \cdot 10^{20} \text{ cm}^{-3}$, for 6 ions, 8 processes, and 109 SCs containing about 66 millions of levels. The calculated emission spectrum agrees very well with experiment [3].

This work was performed under the auspices of the US Department of Energy by the University of California Lawrence Livermore National Laboratory under contract no W-7405-Eng-48.

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Free-free and free-bound radiative transitions in electron collisions with heavy ions

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Polarization channel of free-free and free-bound radiative transitions of electrons in fields of multicharge ions in hot plasmas is under investigation. The polarization radiative channel is connected with a dynamical polarization of heavy ions cores in an electric field produced a colliding electron on the ion. The contribution of the polarization radiation channel can be comparable with a standard channel connected with Bremsstrahlung and radiative recombination. The contribution of the polarization channel is taken into account in the frame of statistical (Tomas-Fermi) model of complex ions. The specific cases of *Mo*, *W*, *U* ions in a hot plasma with the temperature $T_e = 0.5$ keV are considered.

The contribution of the polarization channel is characterized by the factor $R(\omega, T_e, Z)$ being a ratio of spectral (or total) radiative losses in polarization ($k_{pol}(\omega, T_e, Z)$) and ordinary static ($k_{stat}(\omega, T_e, Z)$) channels:

$$R(\omega, T_e, Z) = k_{pol}(\omega, T_e, Z)/k_{stat}(\omega, T_e, Z) \quad (1)$$

and

$$R^{total}(T_e, Z) = k_{pol}^{total}(T_e, Z)/k_{stat}^{total}(T_e, Z) \quad (2)$$

The result of calculation of $R(\omega, T_e, Z)$ as a function of Z for $T_e = 0.5$ keV is presented for *W*, *Mo*, *Fe*. It follows that contribution of polarization channel increases with the nuclear charge being 10% for *Fe* and 60% for *W*. The total radiative-recombination rates as functions of temperature T_e for polarization and static radiative channels are under calculations as well for Unarium ions under coronal ionization equilibrium.

It is shown that the contribution of polarization channel is comparable with standard static radiative channel. It follows from consideration above that contribution of polarization channel must be taken to account in considerations of continuum plasma spectra by multiplying the standard static results by the factor $(1 + R)$ where R is the enhanced factor for spectral or total radiative losses. Such procedure can result in a change of the effective quantum charge Z_{eff} , it being less than it follows from standard static radiation model.

This work was supported in part by a grant from the Russian Ministry of Industry, Science and Technology and in part by the grant 01-02-16305 from the RFBR.

4d-4f narrow-band emission from plasmas containing tin as a highly efficient euV/soft x-ray source

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The wavelength of choice for the next extreme UV lithography (EUVL) step, 13.5nm, is based on the availability of MoSi multilayer mirrors with excellent reflectivity (Approx. 75%) at this wavelength with a reflectance bandwidth of approximately 0.5nm. It is envisaged that a suitable exposure tool will be ready for insertion in the 70nm node alongside excimer laser sources by 2005 and will be sole choice for the 65nm node which will be reached by 2007. A wide variety of pulsed discharge sources using xenon or xenon/helium mixtures are being actively investigated and developed by a number of companies and laboratories. However all of the conversion efficiencies reported to date for these devices are close to 0.5%. Considerable work has also been expended on exploring the feasibility of using laser produced plasmas of xenon clusters produced by supersonic jets or gas puffs from nozzles or solid xenon targets. The highest conversion efficiencies (1.2% into 2% bandwidth) have been achieved using solid xenon. In xenon, the transitions responsible are $4p^6 4d^8 - 4p^6 4d^7 5p$ in Xe XI. Since this is an open shell species, plasma modeling puts the maximum population attainable at 45% and the strongest emission will arise from $4p^6 4d^8 - 4p^5 4d^9 + 4d^7 4f$ lines that are almost a factor of 100 stronger than the 4d-5p. The required conversion efficiency figure has now been revised upwards to better than 3% conversion into a 2% bandwidth. This is necessary as the exposure tool needs to be capable of a throughput of at least eighty wafers per hour. We have identified tin as potentially the brightest emitter at this wavelength. However solid tin targets emit a large amount of debris and experimental results on the distribution of particles will be presented. The transitions responsible in tin arise from $4p^6 4d^n - 4p^5 4d^{n+1} + 4d^{n-1} 4f$ lines from stages VIII through XIII that merge to form an unresolved transition array (UTA) [1-3]. If the tin concentration is reduced to <10%, the peak brightness increases due to enhanced radiation transport at lower density. Furthermore, if the remaining >90% of the constituents are low Z materials the radiation emitted is concentrated in a band 1-2nm wide centred near 13.5nm. The profile width is determined to a large extent by final state $4p^5 4d^{n+1} + 4d^{n-1} 4f$ configuration interaction [4] that causes the features to overlap in successive ion stages. The overlap, like the intensity, is strongly related to the localisation of the 4f wavefunction and its overlap with the 4d. Indeed, the extreme brightness of these features is a direct result of the transfer of oscillator strength from the continuum 4d-ef resonance known to dominate the EUV absorption of the neutral and low ion stages to discrete 4d-4f transitions. This type of UTA emission is brightest and narrowest in the lanthanides, where all ion stages containing open 4d subshells possess highly localised 4f wavefunctions. It is in fact optimum in cerium where we have measured a conversion efficiency of $4.2 \pm 1.5\%$ at 8.6nm using cerium doped glass targets [5].

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Super intense laser field on surface with forming the femto-second laser plasma and new laser spectroscopy of nuclear isomers

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It well known that using the super short light pulses changes principally a character of interaction of the laser radiation with substance (surface) [1]. Under laser radiation intensities more than 10^{15} Wt/cm^2 During the laser pulse electrons get energy of 100-1000eV and it is realized a process of forming the femto-second laser plasma.(FLP) In this paper we consider possibilities of governing by processes, which are taken a place in the FLP in nano-structured porous materials (Si). Nano-structured porous materials consists of the separated clusters set, that forms the fractal structure or regular net. The main 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. For porous materials one may wait for the sharp increasing the hot electrons generation and X-ray radiation. Under large intensity of laser field it is observed a new type of the hydrodynamic ablation, which has the explosion character. Experimental estimates show that a velocity of the plasma flying of the strongly porous samples Si ($1 \times 10^{16} \text{ W/cm}^2$) is 10^8 cms^{-1} , that is corresponding to energy 21 MeV [2]. We carried out the modelling of FLP forming in the porous materials on the basis of the energy balance equations and Green's function formalism for non-ordered materials. Special attention is devoted to the modelling the system: nano-structured porous material with clusters, on surface of which there is a great number of bonds with H and OH groups. In a case of the D-and OD group's one can wait for realization of the cluster explosion process and reaction $\text{D} + \text{Da} + \text{n}$ (3,8MeV). In the high density plasma there is possible an excitement of the low lying isomers (level energy less 20 keV) by means of the following channels: photo excitement by own X-ray plasma radiation, the electron impact excitement, electron conversion etc. Atomic-nuclear numerical code [3-9] is then used for calculating the stable and long lived nuclei low lying isomers characteristics (time of life, spin, energy, decay channels etc.).

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Spectroscopic studies of a sputtering copper ion laser excited in a longitudinal hollow cathode discharge

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The plasma in the longitudinal hollow cathode discharge (HCD) exhibits significant axial non-uniformity [1,2], which affects strongly the excitation efficiency of the discharge. The longitudinal inhomogeneity is even more pronounced in the case of sputtering metal vapour lasers working at a higher current density (above 0.5 A/cm^2). Usually, to increase the sputtering efficiency of the HCD, i.e. the metal atom density and, hence, the laser power, a small portion of Ar (or Ne) is added to the main pump gas He. As it is reported recently [3] the few percents Ar admixture plays a significant role not only for the production of metal atoms, but also for the production and excitation of the other plasma species responsible for laser line excitation.

To study the influence of Ar concentration on the discharge excitation efficiency we have measured the axial emission intensity of He, Cu and Ar atom and ion lines in an experimental set-up consisting of several alternating hollow cathodes and anodes at different Ar concentration. The measurements are performed at discharge conditions typical for laser oscillation in He-Cu HCD. The discharge tube design allows measurements in hollow cathodes with a variable length - from 1 cm to 7 cm each. The axial emission profiles of all lines are characterized with a maximum near the anode ends of the cathode and a minimum at the cathode center. For the He and Ar lines the intensity decrease is not so pronounced, while the intensity of Cu atom and especially of Cu ion lines drops rapidly and is almost zero at 1.5-2 cm. When increasing the Ar concentration, the He lines intensity decreases, the Ar lines intensity grows, and there is no change in their axial emission profiles. The emission intensity of the Cu atom and ion lines changes in a different manner. As it is expected, their intensity is higher at higher Ar addition. The axial emission profile of all Cu lines also changes with increasing the Ar concentration in the discharge. The narrow maximum observed near the cathode end in the He discharge becomes wider at higher Ar percentage, increasing the part of the cathode volume efficient for laser excitation. For the same experimental conditions numerical modelling is performed using the lately developed modelling network for a He-Cu HCD laser [4]. Reasonable agreement between the measured data and the results from calculations is achieved.

Acknowledgements: This research is sponsored by the NATO Science for Peace Programme SfP 971989. It is also supported by the Flemish Fund for Scientific Research (FWO) and Bulgarian Academy of Sciences (BAS) in the framework of agreement for scientific cooperation.

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Ion broadening of sodium nS-3P transitions

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Recent measurements of the shift and shape of sodium nS-3P (n=5-7) atomic lines emitted from high pressure sodium discharges [1, 2, 3] have revealed the existence of a small but significant red asymmetry of all investigated atomic lines. The spectral line profiles of sodium nS-3P transitions radiated by excited sodium atoms in a high pressure arc discharge are influenced by three main broadening mechanisms: the Stark broadening (by electrons), the van der Waals broadening (by dissimilar atoms) and the resonance broadening (by similar atoms). However, the dominant shift and broadening mechanism in this experiment is the Stark broadening by electrons. To find out the reason for the observed asymmetry we compared the measured and the calculated, synthetic line shapes. According to Stormberg [4], the synthetic emission line shape can be successfully simulated by convoluting the impact line profiles and the quasistatic line profile to obtain a resultant profile describing simultaneously the line core and the line wings. In our analysis the synthetic line profiles were obtained by numerical convolution [5] of the line shapes caused by abovementioned broadening mechanisms: (1) reduced Stark profile accounting quasistatic approximation for ions and the impact approximation for electrons, Eq. 4-88 [6], (2) profile caused by broadening by neutral sodium atoms, and (3) profile caused by van der Waals broadening by cadmium (or mercury) atoms. Finally, the synthetic line shape was used in Bartels' method [7] to simulate the true line shape emitted by the discharge. The comparison of the simulated synthetic line shape and the measured line shape shows that the noticed red asymmetry of sodium atomic lines can be only partially explained by foreign gas broadening (by dissimilar, cadmium or mercury atoms). However, if ion broadening is correctly accounted for one can obtain excellent agreement between measured and calculated line shapes. The comparison reveals also the new experimental data for the Stark broadening parameters (d_e , w_e and A) of the sodium nS-3P (n=5-7) transitions.

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Energies of circular transitions in sigmonic atoms

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An exotic atom is formed when a particle, with a negative charge and long-enough lifetimes, slows down and stops in matter. It can then displace an atomic electron, and become bound in a high principal quantum number atomic orbital around the nucleus. Exotic atoms are named after the particle captured in this way. If the particle is a negative sigma Σ^- , a baryon with spin 1/2 and a lifetime of 1.48×10^{-8} s, a sigmonic atom is thus created.

Due to the particle mass, transition energies are much higher than the corresponding electronic ones (a sigma is ≈ 2343.4 times heavier than an electron). The de-excitation of the exotic atom will start via Auger processes, in a manner equivalent to internal conversion for γ -rays, while the level spacing is small and electrons remain to be ejected, and subsequently via radiative (E1) transitions, producing characteristic X-rays while cascading down its own sequence of atomic levels until some state of low principal quantum number. One thus can end with a completely stripped atom, provided the mass of the exotic particle is large and the atomic number of the atom not too high.

Since sigma particles are fermions we obtain their energy and wave function by solving numerically the Dirac equation. The effects of the vacuum polarization in the Uehling approximation, which dominates radiative corrections, is included to all orders by adding the Uehling potential to the nuclear Coulomb potential. Other vacuum polarization terms included in this work, namely the Källén-Sabry term and the Wichmann and Kroll term, were calculated by perturbation theory. The theoretically orbital binding energy is obtained as follows. The energy obtained from the Dirac equation is corrected for the reduced mass as well as for the relativistic recoil. The theoretical energy is the sum of all these terms. We account for remaining electrons by writing the atom wave function as the product of a Slater determinant representing the electronic part and of a sigma particle wave function.

Energies of the circular $(n, \ell = n-1)$, $1 \leq n \leq 20$ levels have been calculated for several (hydrogenlike) sigmonic atoms throughout the periodic table, using the current world average sigma mass. We also computed the electronic shift in systems like $(\Sigma^- + N_e e^- + \text{nucleus})$, where N_e stands for the number of electrons. Hyperfine structure will be also investigated.

Quantum Confinement Effect on ZnP₂ Clusters and Molecules in Zeolite

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ZnP₂ nano-clusters and molecules incorporated into cages of zeolite (with the radius of about 7.5 Å) have been studied for the first time. The photoluminescence (PL) spectra of the clusters have been measured at the temperatures 2 K and 77 K. Samples in quartz tubes were dipped into superfluid helium (2 K) or liquid nitrogen (77 K) during the optical measurements.

Three bands B₁, B₂ and B₃ with the energy in maximum 2.2848 eV, 2.0832 eV and 1.9158 eV have been observed at both the temperatures. The relative intensities of the bands depend on the loading density of ZnP₂ into zeolite. In the spectra of samples with low loading densities the highest-energy B₁ band has the intensity sufficiently exceeding the intensities of B₂ and B₃ bands. In the spectra of the samples with higher loading densities the intensities of B₂ and B₃ bands are almost the same as comparing to one of B₁ band. Proceeding from these data we have made a conclusion that B₁, B₂ and B₃ bands originate from one molecule, two and three molecule clusters incorporated into cages of zeolite. These bands are characterized by the blue shift from the exciton energy in bulk β-ZnP₂ crystal (1.5591 eV) of 0.7254 eV, 0.5238 eV and 0.3564 eV respectively. The origin of the blue shift is the quantum confinement of ZnP₂ clusters in zeolite cages. As the exciton Bohr radius a in bulk β-ZnP₂ crystal is 15 Å that is higher than radius R of zeolite cage (about 7.5 Å), the strong confinement case takes place in our samples. The theoretical estimation of the value of blue shift of the ground state energy of cluster with respective relative size $R/a = 0.5$ gives $32Ry$, where Ry is the exciton rydberg in the bulk crystal. The experimental values of the blue shift obtained from the spectral positions of B₁, B₂ and B₃ bands are $16.8Ry$, $12.1Ry$ and $8.2Ry$ respectively, where $Ry=43$ meV for the dipole allowed C-exciton in bulk β-ZnP₂. Considering the fact that one, two and three molecule clusters have very small quantity of atoms, experimental and theoretical values of the blue shift are in quite good agreement. Differences of the ground state energies of one and two, and two and three molecule clusters can be obtained from the spectral positions of B₁-B₃ bands as following: $E_{12} = E_{B1} - E_{B2} = 0.2016$ eV and $E_{23} = 0.1674$ eV. So, the dependence of the cluster ground state energy on the quantity of molecules in cluster $E(n)$ does not demonstrate the saturation even to one-molecule limit.

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