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EUROPHYSICS CONFERENCE

European
Group for
Atomic
Systems

ABSTRACTS

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Scientific Program

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Posters from CP 1 to CP 112 will be presented during the first poster session (Wednesday – July 8th, 2009). Posters from CP 113 to CP 211 will be presented during the second poster session (Friday – July 10th, 2009).

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Tuesday, July 7	
18.00 - 21.00	Welcome reception (MB, courtyard)
20.00	EGAS Board Meeting (MB121)

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	Paweł Horodecki						
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Lectures

Quantum information – why is it fascinating?

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Quantum information is a branch of contemporary science which is a highly nontrivial composition of quantum mechanics and information theory that originates from the work of C. Shannon and A. Turing. Historically, first discoveries representing the beginning of modern quantum information field were the idea of quantum money that are impossible to counterfeit (S. Wiesner, 1970) and quantum cryptography with polarized photons (C.H. Bennett and G. Brassard 1984). Elementary analysis of the two phenomena suggests that they are possible because ... quantum sheep, if existed, could never be cloned. In fact, this is true, the no-cloning rule of quantum state (realized by E. Wigner 1969, D. Dieks, W. Wooters and W. Zurek 1982) is one of fundamental rules that govern all information processing. Another phenomenon that plays a fundamental role in quantum information was realized first by Schroedinger and – independently – Einstein, Rosen and Podolsky. This is the so called quantum entanglement. Schroedingers analysis (which he found highly unsatisfactory, though consistent) of that phenomenon, can be easily translated into very surprising conclusion about: "how much disorder you may have in your office if you know the amount of disorder (entropy) in the whole building your office is located in" (provided that the whole building is driven by quantum mechanical rules, of course). Recently (2005) it turned out that the latter issue, which bothered Schoredinger so much, provides even more striking implications in terms of the missing information. What it means if the information we miss is quantum and ... negative? What role is played in this context by quantum teleportation and what the latter is? And finally – what quantum computer is expected to be? These questions will be answered in possible elementary way with some references to quantum-optical setups. In particular, Alice and Bob, the two intelligent "celebrities" in quantum information field, will help us in understanding how quantum computing algorithm can help in fixing the date time quickly. Note that we have already quantum cryptography in the market and one can already buy quantum random generator compatible with PC computer. On the other hand still there are open problems, including some experimental challenges, that make quantum information field very, both dynamical and intellectually fascinating.

Hanbury Brown and Twiss and other atom-atom correlations: Advances in quantum atom optics

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Fifty years ago, two astronomers, R. Hanbury Brown and R.Q. Twiss, invented a new method to measure the angular diameter of stars, below the limit set by the atmospheric fluctuations. Their proposal prompted a hot debate among physicists: how might two particles (photons), emitted independently (at opposite extremities of a star), behave in a correlated way when detected? It was only after the development of R. Glauber's quantum analysis that the effect was fully understood as a two particle quantum interference effect. From a modern perspective, it can be viewed as an early example of the amazing properties of pairs of quantum correlated particles.

The effect has now been observed with boson and fermion atoms, stressing its fully quantum character. After putting these experiments in a historical perspective, I will present recent results, and comment on their significance. I will also show how our individual atom detection scheme has allowed us to demonstrate the creation of atom pairs by non linear mixing of matter waves. This result paves the way to experiments aiming at probing entanglement in atom pairs.

Quantitative experiments on electron-molecule collisions

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The talk will start with a brief overview of areas of application of electron induced chemistry and point out which demands and challenges do these applications place on the fundamental research of electron-molecule collisions. A few examples of how these challenges have been met will be presented:

Combined theoretical and experimental effort has recently improved our understanding and capacity to deliver cross sections for electronic excitation of atoms [1], important for lightning and plasma propulsion.

The emerging Focused Electron Beam Induced Processing (FEBIP) technology inspired the research of electron collisions by directing our attention to new types of compounds – the metalorganic compounds used as precursors there [2]. An example of such a precursor is $Pt(PF_3)_4$ [3] and electron scattering results on this compound will be presented.

Chemical change in polyatomic molecules is very important in the applied systems, but quantitative calculations are nearly always limited to diatomic molecules and absolute measurements are still quite rare. An important recent progress towards improving this situation is the *ab-initio* calculation [4] and absolute measurement [5] of the DEA cross section for the prototype polyatomic molecule acetylene and its di-deutero isotopomer.

The assignment of the resonant bands and our understanding of the dissociative electron attachment mechanism for polyatomic molecules at higher energies – the domain of Feshbach resonances, with two excited electrons – is still very limited. Light has recently been shed into this problem, primarily from experiment, by studying the trends in a large number of compounds [6]. A number of rules and selectivities have been identified and in certain cases qualitatively rationalized by calculations of the potential surfaces of the parent Rydberg states of the Feshbach resonances. These processes still present an unsolved challenge for the theory.

An important conclusion is that electron scattering in the past has often been motivated by the desire to discover new resonances and cross sections were often measured only in relative units, for only one process, and over limited energy and angular ranges to permit the observation of a given resonance. The primary challenge posed by the applications is the need to measure (and calculate) cross sections in absolute units, over wide energy and angular ranges, and for all the accessible processes.

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Observation of ultralong-range Rydberg molecules

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At ultralow temperatures – in so-called frozen Rydberg gases – the scattering of a Rydberg electron and a nearby polarizable ground-state atom can generate an attractive potential. In this case, the scattering-induced attractive interaction binds the ground-state atom to the Rydberg atom at a well-localized position within the Rydberg electron wavefunction (Fig. 1), and thereby yields giant molecules with internulear separations of several thousand Bohr radii.

Here we report the spectroscopic characterization of such exotic molecular states formed by rubidium Rydberg atoms that are in the spherically symmetric s state and have principal quantum numbers, n, between 34 and 40. We find that the spectra of the vibrational ground state and of the first excited state of the Rydberg molecule, the rubidium dimer Rb(5s)-Rb(ns), agree well with simple model predictions. The data allow us to extract the s-wave scattering length for scattering between the Rydberg electron and the ground-state atom, Rb(5s), in the low-energy regime ($E_{kin} < 100$meV), and to determine the lifetimes and the polarizabilities of the Rydberg molecules [1].

Additionally, we report on the observation of trimer states, where even two ground-state atoms are bound by a Rydberg atom.

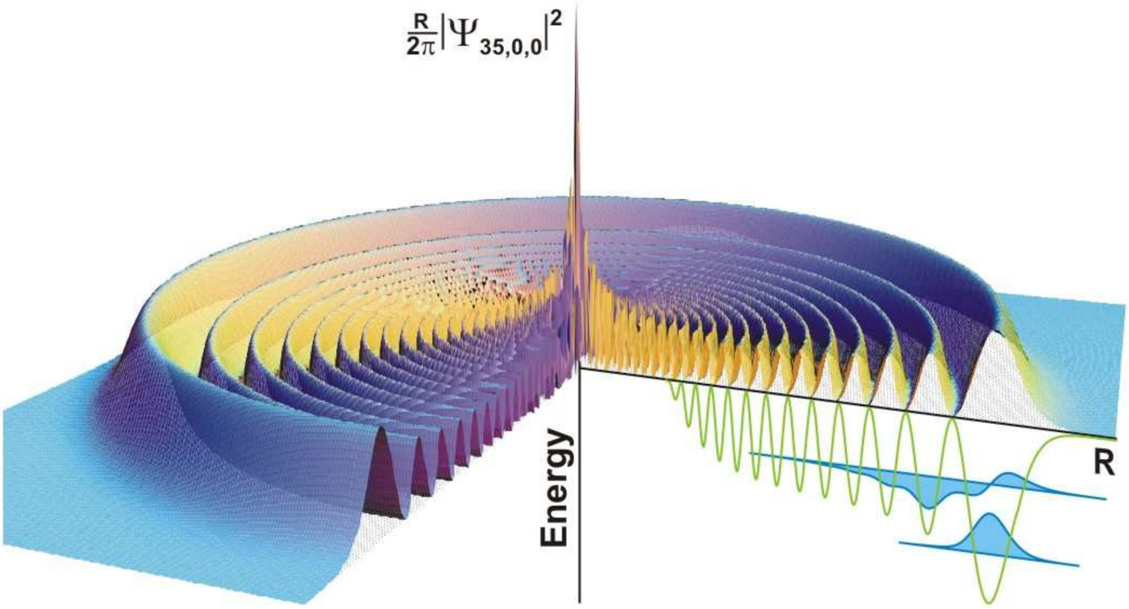

Figure 1: Electron probability density and molecular potential for the state n=35, l=0.

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Dissociative recombination of small molecular ions: The spectroscopic frontier

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Although atomic dielectronic recombination and molecular dissociative recombination share the same mechanism, i.e. resonant electron capture followed by stabilization of the complex, the vibrational degree of freedom offers to the latter a much higher rate, and at the same time lifts the requirement of precise energy matching. The resonant state being generally accessible over a broad Franck-Condon region, structureless cross sections ensue, hiding the spectroscopic details of the molecule. We will demonstrate how high-resolution electron scattering on rovibrationally controlled molecular ions, when coupled to fragment imaging, offers a direct access to the structure and dynamics of the molecule. Anisotropies recorded by three-dimensional fragment imaging point to the symmetries of the autoionizing Rydberg resonances [1]. The detailed evolution of the branching ratios among the various dissociative channels sheds light on the long-range interactions, performing a dynamical spectroscopy similar to what may be obtained by VUV photodissociation experiments.

Such precision measurements are now routinely performed at the TSR facility of the MPI for Nuclear Physics of Heidelberg (MPIK) where an ultracold electron target (500 μeV transverse energy resolution), sophisticated ion sources (e.g. REMPI laser-ion source, multipole trap with buffer gas cooling) and multiparticle time- and position-sensitive detectors have been implemented. This complex arrangement has revealed the uttermost sensitivity of low energy dissociative recombination to the rovibrational state, and the active cooling experienced by molecular ions when merged with cold electrons [2]. The reheating by black-body radiation competes with superelastic electron cooling, and may be circumvented in a cryogenic environment, as offered by the Cryogenic Storage Ring (CSR) under development at MPIK [3]. The inner vaccuum chamber of this electrostatic storage ring will be cooled to liquid helium temperature, allowing for complete rotational relaxation of most infrared active molecular ions. The long storage times (thousands of seconds) will offer the possibility of laser manipulation of the ions, while merged electron and atomic beams will be used to study the reactivity of such ultracold molecular ions, bringing them closer to outer space conditions.

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Photonic entanglement – from fundamentals to applications and back

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Attosecond angular streaking and sub-100-attosecond tunneling ionization dynamics

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It is typically assumed that electrons can escape from atoms through tunneling when exposed to strong laser fields, but the timing of the process has been controversial, and far too rapid to probe in detail. We have used attosecond angular streaking [1] to place an upper limit of 34 attoseconds and an intensity-averaged upper limit of 12 attoseconds on the tunneling delay time in strong field ionization of a helium atom in the non-adiabatic tunneling regime [2]. This is the fastest process that has ever been measured. Our experimental results give a strong indication that there is no real tunneling delay time, which is also confirmed with numerical simulations using the time-dependent Schrödiger equation [3].

In attosecond angular streaking we use close to circular polarized, 5.5-fs long, near-infrared laser pulses with peak intensities ranging from $(2.3 \text{ to } 3.5)\times10^{14}$ W/cm2 (corresponding to a Keldysh parameter variation from 1.45 to 1.17) to tunnel-ionize helium atoms and accelerate the free electrons, whose final momentum is then measured with a COLTRIMS apparatus. This final momentum serves as the hand of a clock, revealing at which time the electron exited the tunnel to first experience the acceleration by the laser field.

To determine the intensity dependence of a possible tunneling delay time $\triangle t_D$ we then fixed the ellipticity to 0.88 and varied the peak intensity from $(2.3 \text{ to } 3.5)\times10^{14}$ W/cm2 (corresponding to a Keldysh parameter variation of 1.45 to 1.17). We define the tunneling delay time $\triangle t_D$ as the difference between the measured streaking angle and the calculated propagation streaking angle taking into account the angular offset due to the Coulomb potential. We measure a weighted intensity-averaged offset of 6.0 as with a standard deviation of 5.6 as: this results in an intensity-averaged upper limit for the tunneling delay time of 12 as.

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Chemistry at ultracold temperatures: Observation of the smallest droplet of acid

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Acid dissociation and subsequent solvation of its charged fragments, including the hydrated proton, is one of the most fundamental chemical processes. In contrast to ambient bulk water environments, understanding mechanisms that allow for ionization in small networks at ultracold conditions are relevant from atmospheric to interstellar chemistry, but remain largely unexplored.

In Bochum we have set up a He-nanodroplet apparatus in combination with a home-built cw-Optical Parametric Oscillator IR (OPO) with full frequency coverage in the range from 2600 to 3400 cm^{-1}, high output power (up to 2.7 W), and high resolution (0.0001 cm^{-1}) [1]. Briefly (35), helium droplets with an average size of 8500 He were formed in a supersonic expansion of precooled (16 K) gaseous helium through a 5 μm diameter nozzle. These droplets provide a gentle matrix for step-by-step aggregation of molecular clusters, via a controllable pickup process governed by Poisson's statistics [2], allowing for IR high-resolution spectroscopy.

We report the first experimental observation of a microscopic aqueous droplet of acid reported at ultracold (0.37 K) temperatures. Furthermore we will discuss specific reaction mechanism at ultracold temperatures [3]. Here, we report full dissociation of a single HCl molecule with exactly four water molecules in superfluid helium nanodroplets as a result of molecular aggregation at 0.37 K.

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Playing quantum marbles, or how often do atoms interfere with themselves?

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Quantum gases confined by an optical lattices have recently received much attention as simulators for quantum many-particle systems, and they are advertised as important tools for quantum information science. In an alternative "bottom-up" approach small interacting quantum systems can be created with neutral atoms which resembles a bit children playing with microscopic marbles. In this lecture I will present our recent experimental advances where we have taken atomic marbles to the full quantum regime, i.e. to the observation of atomic matter wave interferences at the single atom level. For instance, we have realized the quantum analogue of Brownian motion, the quantum walk, a concept of relevance in quantum information science. New methods to cool single atoms to the motional ground state also open the potential for the creation of degenerate quantum states at the level of few atoms only.

Atomic physics in strong fields: precision experiments with stored and cooled highly charged ions

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The unique combination of the accelerator facilities at GSI makes it possible to accelerate, store, and cool heavy ion beams at their highest charge state. In atomic physics experiments these ion species can be exploited for a stringent tests of Quantum Electrodynamics in the strong and critical field limit and for detailed studies of the correlated many-body dynamics in ultra-short and extremely intense electromagnetic fields. Highly-charged ions also provide a unique access for the determination of fundamental atomic and nuclear properties. In this overview, the present status of the experiments aiming on the precise determination of the 1s Lambshift, the Hyperfine Structure and the g-factor of hydrogenlike ions at high-Z will be given [1]. In addition the novel research opportunities will be reviewed which opens up by the new HITRAP facility [2]. At HITRAP, heavy ions in their highest charges state will be provided even at rest in the laboratory, allowing for a new generation of precision experiments. Further substantial progress can be anticipated by the upcoming international FAIR facility where highest intensities for stable and exotic ion species as well as fast and slow anti-protons will be accessible for experiments [3,4].

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Precision spectroscopy of antiprotonic atoms and antihydrogen

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Experiments with low-energy antiprotons are currently performed at the antiproton Decelerator (AD) of CERN. The main focus of the three experimental collaboration is the study of fundamental symmetries, especially CPT invariance, using antiprotonic atoms and antihydrogen. The ASACUSA collaboration focusses on precision spectroscopy of antiprotonic helium, an exotic three-body system consisting of a helium nucleus, an electron and an antiproton. The antiproton occupies metastable states which allows precision determination of its mass and magnetic moment [1] by comparison to three-body QED calculations. Anthydrogen, the simplest neutral antimatter atom, promises CPT tests of highest precision by comparison to hydrogen, which is one of the best studied atoms. The ATRAP and ALPHA collaborations aim at producing and trapping antihydrogen in a neutral-atom trap and to measure the 1S-2S two-photon transition [2] to a precision similar to the one achieved for hydrogen (relative precision $\sim 10^{-14}$). ASACUSA is preparing an experiment to measure the ground-state hyperfine structure of antihydrogen [3], the corresponding quantity for hydrogen being measured to relative precision of $\sim 10^{-12}$ in the hydrogen maser.

The AD beam energy of 5 MeV is too high for efficient stopping of antiprotons in dilute gases and traps for precision spectroscopy. Furthermore it delivers only pulsed beam which makes experiments of nuclear or particle physics type difficult. This restriction will not apply at the planned FLAIR facility [4] at FAIR, Darmstadt, where the availability of continuous antiproton beams at energies 100 times lower than at the AD will enable measurements not currently possible anywhere in the world. This talk will give an overview on current and planned experiments with low-energy antiprotons.

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Precision parity and time reversal experiments with trapped radioactive isotopes

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At the Kernfysisch Versneller Instituut in Groningen precision experiments are carried out to search for New Physics beyond the Standard Model. Such experiments exploit most modern techniques in atomic, nuclear and particle physics. The research projects at KVI include such which involve optically trapped radioactive atoms, where time reversal symmetry is studied. This scientific question relates to the matter-antimatter asymmetry in the universe. For these measurements new atomic trapping techniques and radioactive beams of highest purity were developed.

The particular focus at KVI is on precision tests of discrete symmetries such as parity and time reversal. To this extent an experiment to measure the weak mixing angle in a single Ra^+ ion stored in a Paul-trap. Parallel to the experimental program our group has performed also calculations of atomic parity violation which show that the Ra^+ experiment has an about 50 times higher sensitivity to atomic parity violation compared to the best experiment so far in atmic Cs.

Further we aim to search for atomic, nuclear and electrom permanent electric dipole moments in optically trapped Ra atoms. As a precursor to this experiment the hurdle of optically trapping heavy alkaline earth atoms was mastered by demonstrating BA atom trapping by using 7 narrowband lasers at the same time.

These experiments at low energies are complementary in their physics potential to accelerator experiments at the highest today possible energies.

Progress Reports

Molecules in intense ultrashort laser pulses

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Recent laser technology allows to generate laser pulses in the infrared with a duration of a few femtoseconds. This paves the route to probe ultrafast processes in, e. g., atoms or molecules. This talk discusses two alternative approaches: one deals with real-time observation of nuclear motion, the other concerns the time-resolved imaging of changes in the electronic structure of molecules.

First, it is demonstrated how an ionizing ultrashort laser pulse can induce a vibrational wavepacket not only in the formed ion, but also in the non-ionized neutral molecule. This phenomenon, dabbed *Lochfraß*, is of purely quantum-mechanical origin and lead after its theoretical prediction [1] to the so far fastest nuclear motion that could be experimentally observed in real time [2]. In fact, the wavepacket induced in the case of a homonuclear molecule like H_2 is shown to be extremely stable and behaves like a quantum pendulum or molecular clock. Interestingly, it was recently claimed that starting from a more incoherent initial state can lead to even more coherence induced by *Lochfraß* [3]!

In the second part of the presentation the possibility to image orbital structures in a time-resolved fashion is discussed. For this purpose, the relation between the orientational dependence of strong-field ionization and the shape of the highest-occupied molecular orbital is demonstrated, but also possible problems are indicated. The consequences for the possibility of watching chemical reactions in real time will be addressed.

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Nonlinear resonances and dynamics of atomic Bose-Einstein condensates

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We investigate nonlinear dynamics of atomic Bose-Einstein condensates which provide an ideal system to study the effect of atomic interactions on delta-kicked atoms. The signatures of nonlinear dynamics appear in abrupt cutoff on leading resonances which is due to an excitation path combining both Beliaev and Landau processes. Other manifestations of dynamical instabilities in nonlinear condensate evolution, such as phase separation, soliton formation and the effect of critical flow velocities, may be studied in static optical lattices.

Few-electron dynamics in intense short XUV pulses studied with coincident momentum spectroscopy

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The emission of few electrons from atoms, molecules, clusters or solids constitutes one of the most fundamental processes occurring when intense VUV or X-ray radiation interacts with matter. Recent development of the **F**ree electron **LAS**er in **H**amburg (FLASH), delivering femtosecond VUV light pulses at unprecedented intensities along with the progress in high-harmonics generation made multi-photon multi-electron transitions in this energy range experimentally accessible, triggering enormous theoretical interest and opening the way for a variety of time-resolved imaging schemes.

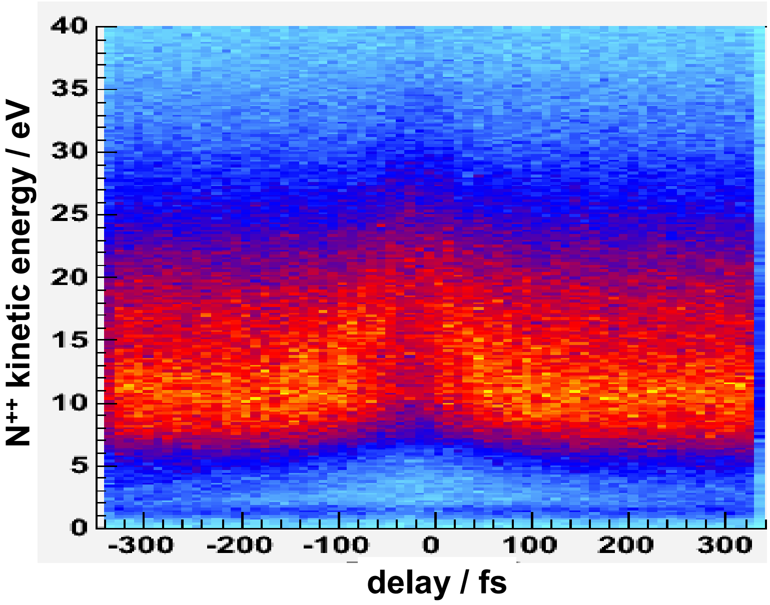

Figure 1: Kinetic energy of N^{2+} ions as a function of the delay between two 38 eV pump- and probe pulses delivered by FLASH

Here an overview of recent experimental studies on few-photon-induced fragmentation of rare gas atoms and simple diatomic molecules performed at FLASH employing coincident cold-target recoil ion and electron momentum spectroscopy will be presented. Particular examples include a disentanglement of sequential and direct ('non-sequential') pathways for few-photon double ionization of Ne and He [1], identification of dissociation and Coulomb explosion channels in FEL-induced fragmentation of simple diatomic molecules (N2, O2, D2) [2], and the results of the first VUV-VUV pump-probe experiments. As illustrated in Fig. 1, the latter measurements not only allow for a time-resolved mapping of fragmenting molecular states, but also yield valuable information on the properties of the FEL pulse via channel-selective analyses of autocorrelation-like patterns.

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Rydberg dark states

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We will describe our experiments on Rydberg dark states [1] and show how the extreme polarizability of the Rydberg energy level leads to a giant Kerr effect [2]. We will also discuss rf dressing of dark states and potential applications in electrometry. Finally, we will show the strong interactions between Rydberg atoms leads to a modification of the dark state [3], and discuss potential applications in single photon non-linear optics.

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Interferences in the Autler-Townes effect

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The Autler-Townes effect is manifested when two levels are coupled by a strong coherent radiation field. When one of those levels is coupled by a weak probe field to a third level, the typical doublet can be observed in the probe excitation spectrum [1]. A number of detailed studies in atoms [2] and molecules [3] exist. The present report is focused on the possible applications of the Autler-Townes effect to population switching, and the effects of resolved and unresolved hyperfine structure on the formation of laser-dressed (adiabatic) states.

We consider a three-level system as in Fig. 1 coupled by two laser fields. If the strong field P is coupled between levels g and e, then the excitation spectrum of level f obtained by scanning the S field does not exhibit the expected doublet; instead, peculiar broad lineshapes are observed [4]. These lineshapes can be explained by Ramsey-type interference of the laser-dressed states. Moreover, such interference can be used in order to achieve switching of the population of level f via variation of the S-field frequency from a maximum to a minimum of the Remsey fringes.

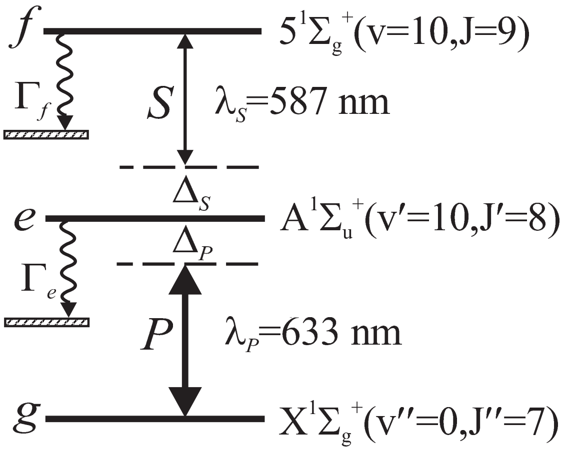

Figure 1: Three-level linkage scheme in Na_2.

New effects of hyperfine structure on the formation of laser-dressed states have also been identified. We consider a scheme as in Fig. 1 but with strong coupling in the second step and a weak probe in the first step, while each level has hyperfine sublevels. Hyperfine magnetic sublevels are fully resolved in the Autler-Townes spectra if the number of hyperfine levels in the two laser-coupled states is equal. If the number of hyperfine levels is different, then the dark states are formed, which limits the hyperfine resolution.

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Chemical applications of laser- and sympathetically cooled ions in ion traps

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The recent progress in the generation of translationally "cold" atoms and molecules has enabled to study physical and chemical processes in a new regime. A particular intriguing perspective is the investigation of reactive molecular scattering processes at ultralow collision energies to characterise quantum-mechanical effects which dominate the chemical reactivity at very low temperatures. However, such studies have thus far been prevented by the difficulties to detect and analyse the small number of scattering events per experimental cycle limited by the low number densities of cold molecules that can be produced with present-day sources.

We have recently developed a novel experimental setup to study reactive collisions between translationally cold ions and neutral molecules which overcomes these difficulties [1,2]. Our new experiment consists of a linear Paul trap for the laser- and sympathetic cooling of atomic and molecular ions combined with a quadrupole-guide velocity selector for the generation of translationally cold neutrals [3]. The high detection sensitivity which can be achieved using Coulomb-crystallised ions allows us to study cold ion-molecule reactive collisions on the single-particle level. In the presentation we review recent results on selected cold ion-molecule reactions, discuss the experimental parameters influencing the collision energy and chemical reactivity and explore further developments towards fully quantum-state selected experiments at even lower energies.

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Towards scaling quantum simulations in an ion trap(array)

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We can not translate quantum behavior arising with superposition states or entanglement efficiently into the classical language of conventional computers. A shortcut was proposed by Richard Feynman, via simulating the quantum behavior of interest in another quantum system, where all relevant parameters and interactions can be controlled and observables of interest detected sufficiently well. We realized two proof of principle demonstrations of an analog quantum simulator based on trapped ions. The complete mode of operation of a quantum simulator will be described on the basis of a simple model case on two spins [1]. We reveal the difficulties in describing a quantum system classically for the case of a quantum magnet, where we introduce and explain the role of superposition states, entanglement and tunneling (quantum fluctuations) by means of our experimental data.

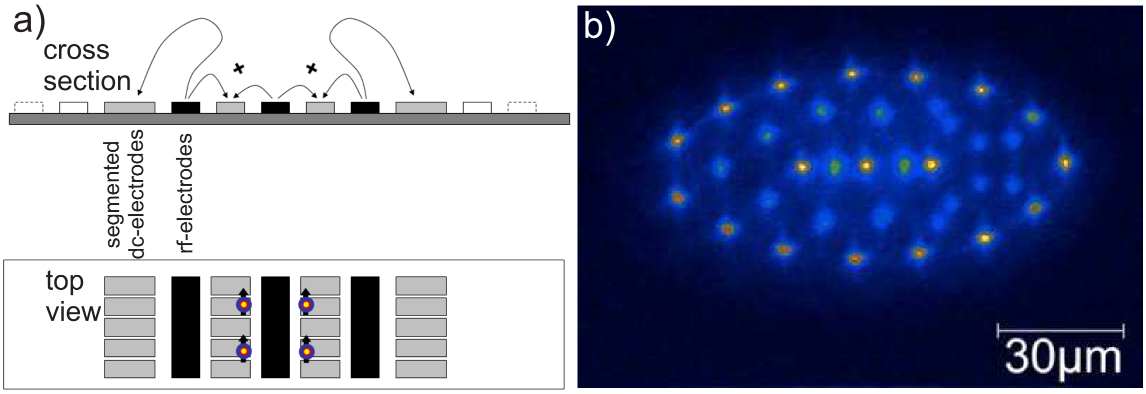

Figure 1: a) Schematic view of an ion trap with the RF- (black bars) and segmented DC-electrodes projected on a surface. We plan to position segmented linear ion traps at a distance that allows for stiff single ion confinement and a Coulomb interaction between ions being similar in two dimensions. b) Fluorescence light of a 3D Coulomb crystal – 35 laser cooled $^{25}\mathrm{Mg}^{+}$ ions in the experimental zone of our segmented linear Paul-trap. In our current experiments we are dealing with linear chains of 5 ions only.

We summarize our recent results on the implementation of a radial phase gate operation at a fidelity exceeding 97%, radial motional side band cooling of up to 5 ions and the implementation of a quantum walk of a single ion[2].
Finally, I will try to describe our vision (see Fig. 1), how we plan to bridge the gap between proof of principle experiments and quantum simulations providing deeper insight into complex quantum dynamics intractable on classical computers.

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Realistic quantum-enhanced interferometry

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It is widely recognized that the use of nonclassical states of light allows one to overcome the shot-noise limit in precision measurements. The enhancement comes from exploiting inherently quantum features, such as entanglement, that are sensitive to decoherence. The outstanding challenge is to design quantum-enhanced measurement schemes that remain robust in realistic environments. We review recent work in this direction for optical interferometry.

Contributed Papers

Dielectronic recombination of H-like highly charged ions

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We present theoretical investigation of the process of dielectronic recombination (DR) of H-like highly charged ions. Dielectronic recombination together with radiative recombination plays the main role in the process of capture of an electron by ion. For calculation of the cross section of the electronic recombination in the framework of QED, we employ the Line Profile Approach (LPA) [1,2]. The LPA was first developed for QED calculation of the energy levels (particular, quasidegenerate levels) of the highly charged ions [1], recently, it was applied for QED calculation of the transition probabilities [1,2]. The advantage of the LPA is the possibility to calculate the interelectron interaction with high level of accuracy. Within the LPA the interelectron interaction is partly included to all orders in the QED perturbation theory. For the present calculation the LPA was generalized for the systems containing an electron from the continuum.

We performed QED calculation of the total cross section of the electronic recombination of H-like uranium. The cross section is presented as a function of the energy of incident electron. Due to the DR process the cross section shows resonances corresponding to the doubly excited $(2s, 2s), (2s, 2p), (2p, 2p)$ two-electron configurations. These resonances are investigated in details. The interelectron interaction for the ns, np, nd-electrons (the principal quantum number $n \leq 3$) is taken in all orders of QED perturbation theory (PT). The interelectron interaction for the other electrons (including the negative part of the Dirac spectrum) is considered in the first order of PT. The dominant part of the radiative corrections (self-energy and vacuum polarization) is also taken into account; the self-energy vertex corrections which are not resonant are missing.

Results of the present calculation are compared with previous calculations [3,4]. The interelectron interaction is taken into account in the present work more precisely compared to the previous works. Since the LPA is *ab initio* QED approach, the QED effects are considered systematically. The major discrepancy between the calculations reveals itself in the lineshapes of the resonances.

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Progress in the analysis of the odd parity configurations of tantalum atom

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Classification of electronic levels belonging to odd parity configurations system in tantalum atom, based on semiempirical calculations (described in [1]) was extended to further newly discovered levels. Calculations of A and B hyperfine structure constants, performed also for new levels, did not yield satisfactory agreement with experimental values obtained with laser spectroscopic methods by experimental group in Graz. Calculations performed with additional inclusion of some interactions in second order of perturbation theory did not result in a substantial decrease of these discrepancies.

Within the frame of a new theoretical approach to the description of hyperfine structure, recently developed in Poznań, new calculations concerning parametrization of configurations interaction were undertaken. These include the following kinds of excitations: open shell - empty shell and closed shell - open shell. Results of calculations obtained, as well as hyperfine structure analysis and classification of the levels belonging to odd parity configurations in tantalum atom, are discussed in detail within this work.

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Population transfer in four-level atomic or molecular systems with far-optical transitions

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The possibilities to control quantum systems, e.g., to obtain desired coherent superposition states using external electromagnetic fields, have been studied intensively during the many decades since the period of development of the Nonlinear Optics and are considered nowadays because of their significance for implementation of contemporary problems in Quantum Informatics. The techniques which allow robust transfer of population between the specified states in quantum systems are of interest. From this point of view, adiabatic passage in atomic and molecular systems is a well established tool to achieve this goal. The main advantage of processes based on adiabatic passage is their relative robustness against the fluctuations of the characteristic parameters in experiments (such as the pulse area). However, the control of population transfer is problematic in quantum systems where the main transitions are at least in the UV domain. In these cases, the problem requires multiphoton excitation. The latter is effective if the energies of the excited states of a three-level atomic configuration are close to each other with a nonzero transition dipole moment [1], otherwise the states of the system should possess mean dipole moments [2].

In the present work, we propose the multiphoton adiabatic population transfer mechanism in four-level systems with far-optical transitions via the two dipole coupled quantum states close to each other, or with a mean dipole moment in the excited states (for a three state system with this configuration, the multiphoton population transfer mechanism resembles "multiphoton STIRAP", see [3, 4]). In the considered model systems, the two coupling laser fields induce multiphoton transitions between the initial and target states, which we call IMAP - induced multiphoton adiabatic passage. The time evolution of such systems is found analytically by the developed nonperturbative multiphoton resonant theory for atom-two strong waves interaction. Performing also numerical simulations, we show that by using two time-delayed-overlapping laser pulses it is possible to produce the complete population transfer in quantum systems with high energy transitions. The proposed IMAP schemes for four-level quantum systems of high energy transitions may have diverse applications for molecules or molecular ions, as well as for hydrogen-like atoms/ions with the required structure due to the Coulomb random degeneration.

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Line strength measurements for selected Ne I spectral lines and comparison with strengths of analogous transitions in Ar I

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Applying the emission spectroscopy method line strengths for several selected 3s - 3p and 3s - 4p transitions have been measured. A wall-stabilized high-current arc operated in neon with some admixture of argon was applied for excitation of neon atoms. The electron density of the arc plasma ($N_\mathrm{e} = 8 \cdot 10^{15}\mathrm{cm}^{-3}$) and temperature ($T$ = 13 000 K) assured partial local thermal equilibrium conditions among energy levels with principal quantum number n $\geq$ 3. Details of the experimental setup, the data acquisition, and determination of line strengths are described in a paper recently published by one of us [1].

The studied Ne I transitions occur between energy levels belonging to two groups of terms with different atomic core configurations: $2\mathrm{s}^2 2\mathrm{p}^5(^2\mathrm{P}^\mathrm{o}_{3/2})$ and $2\mathrm{s}^2 2\mathrm{p}^5(^2\mathrm{P}^\mathrm{o}_{1/2})$. Each set of measured line strengths: (i) 3s-3p; 3s-3p'; 3s'-3p; 3s'-3p', and (ii) 3s-4p; 3s-4p'; 3s'-4p; 3s'-4p', has been individually normalized to the strongest transition within each set - $3\mathrm{s}[3/2]^\mathrm{o}_2$ - $3\mathrm{p}[5/2]_3$, and $3\mathrm{s}[3/2]^\mathrm{o}_2$ - $4\mathrm{p}[5/2]_3$, respectively.

These measured relative line strengths are compared with (relative) line strengths of analogous transitions in Ar I. The corresponding line strengths have been taken from NIST data base [2].

Regular behavior along the homologous sequence (Ne I - Ar I) is encountered in the case of transitions involving levels belonging to the same parent term, i.e. without changing the atomic core configuration. This regularity is observed for transitions originating from upper levels with the principal quantum number n = 3 as well n = 4. Very large discrepancies (between relative line strengths of neon and argon) are found in the case of transitions occurring between levels belonging to different parent terms, i.e. for transitions 3s - 3p', 3s - 4p', 3s' - 3p, and 3s' - 4p.

This observation seems to be in accordance with line strength data reported for the 3p - 3d transition array (3p - 3d; 3p' - 3d; 3p - 3d'; 3p' - 3d') in Ne I [1], where significant departures from the J-file sum rule are found.

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Enhancement of radiative recombination of U^{92+} ions with cooling electrons for the lowest n=1 and n=2 states

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The enhancement observed in experiments on radiative recombination (RR) of bare ions with cooling electrons in ion storage/cooler rings [1,2,3] have attracted a wide interest in last years to interpret this effect theoretically [4,5]. More precisely, these experiments have shown that the radiative recombination rates, measured by detecting the recombined ions, agree with the theoretical predictions for relative electron energies higher than the transverse electron beam temperature $T_{\perp}$, while for the lower electron energies an increase, called the enhancement, of the measured rates with respect to the RR prediction is observed, which saturates below the longitudinal electron beam temperature $T_{\parallel}$. It was found [1] that the excess of the recombination rate depends on the magnetic guiding field in the electron cooler, however, the existing interpretations [4,5] of the enhancement effect do not fully explain these observations.

In order to investigate the enhancement effect in more details, the state-selective x-ray radiative recombination experiment has been performed in the electron cooler of the ESR storage ring with decelerated bare U^{92+} ions of energy 23 MeV/amu recombining with electrons having relative energies in the range 0-1000 meV [6]. In this experiment the x-ray K-RR and L-RR photons emitted from direct radiative recombination into the K- and L-shells were measured in coincidence with recombined U^{91+}ions both for on- and and off-cooling electron energies. In this way, by comparing the measured K-RR and L-RR rates with fully relativistic RR calculations [7] reproducing the data for off-cooling electron energies quite well, the enhancement of RR for the n=1 and n=2 states was derived for the cooling condition. The importance of the present results for interpretation of the enhancement effect will be discussed in details.

Acknowledgment

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Experimental Stark broadening studies of the O I multiplet 3p ^{5}P–3d ^{5}D^o at 9264 Å.

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A high current wall-stabilized arc with flat carbon electrodes, operated at atmospheric pressure in helium and argon, with small admixture of oxygen and hydrogen was applied as excitation source of the studied spectra. The radiation of the plasma emitted from nearly homogeneous plasma layers in end-on direction was detected by applying a grating spectrometer equipped with a CCD detector. This instrumentation provides spectra with a reciprocal dispersion of 0.043 Å/pixel. The apparatus profile was determined by applying low-pressure krypton- and neon-discharge lamps of a Plücker type, which were also used as standard sources for wavelength calibration. At the entrance slit – 26 μm of the spectrometer, the apparatus profile is of Gaussian type with a FWHM of 0.08 Å. The radiance calibration was carried out against light outputs originating form a tungsten strip radiation standard.

The arc current was varied from 31 to 54 A in order to obtain different plasma conditions: electron densities from the range $2.5{\cdot}10^{21} - 1.4{\cdot}10^{22} m^{-3}$, corresponding to electron temperatures between 10000 and 13700 K. The electron density N_e was determined from measured FWHM of the hydrogen H_β line and using theoretical broadening data of Gigosos and Cardeñoso [1]. The plasma temperature T_e was determined by measuring total line intensities of three infrared OI multiplets (at 7773 Å, 8820 Å, 9264 Å) and applying the standard Boltzmann plot method. The transition probability data have been taken from NIST Atomic Spectra Database [2].

The multiplet 3p ^{5}P–3d ^{5}D^o consists of nine fine structure components. Because of the small differences in wavelengths between spectral lines involving the same lower level, this multiplet appears – at our plasma conditions and spectral resolution – in form of three spectral features, each consisting of three fine structure components.

Spectral lines of neutral atoms emitted from plasmas are usually affected by a few broadening mechanisms. In the case of non-hydrogenic transitions the main contribution arises from collisions between emitters and fast moving electrons, producing shifted Lorentzian-like line shapes. Collisions with ions lead to some additional broadening and cause an asymmetry of the profile. Such profiles can be described by an asymmetric so-called $j(x)$ function introduced by Griem [3, 4]. These $j(x)$ profiles convoluted with the corresponding Doppler and apparatus profiles were fitted to our experimental data. In this way the electron impact widths of fine structure components of the investigated multiplet were determined. The evaluated Stark broadening parameters are compared with theoretical data of H.R. Griem [4].

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Ne I excitation rate coefficients for C-R models applied to electric propulsion

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Because of the possible use of Ne as a fuel gas in electric propulsion devices, we are developing a Collisional-Radiative (C-R) model valid for low temperature Ne plasma, encompassing the neutral Ne atom and its first ion, with Ne III as a continuum [1]. This "zero dimension" model is meant for non-intrusive emission spectroscopy diagnostics giving the local electronic temperature T_e and density n_e inside a plasma thruster; it can also be used as a basis for development of a detailed full dimensional model [2]. Validation of the C-R model is underway, mainly by use of a Ne-filled hollow cathode lamp experimental facility in which the positions and intensities of the principal Ne I and Ne II spectral lines have been measured. The theoretical spectra obtained by the C-R model rely on transition probability (A_{ij}) and electron impact collision excitation (σ_e) data. In the present contribution we focus on evaluation of the σ_e and of the corresponding excitation rates for the lower levels of Ne I. In addition to the available experimental and theoretical results [3], we have used the following theoretical methods [4] for the σ_e evaluations: i) The Born approximation (high energy region) in which the structure parameters are of paramount importance. ii) Distorted Wave (DW) approximation and First Order Many Body Theory (FOMBT) at electron impact energies approaching the threshold, using the online interface to the Los Alamos National Laboratory atomic physics codes [5]. iii) Quasi-classical evaluations based on the Hamiltonian formulation of the few body problem, following numerical CTMC studies.

Acknowledgment

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Complete active space multiconfiguration Dirac-Hartree-Fock calculations of hyperfine structure constants

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Ab initio calculations of atomic properties can now be performed routinely, both in the framework of the MCDHF theory, as well as many-body perturbation (MBPT) theory. Both these methods are designed to evaluate in a systematic manner the electron-electron correlation effects, which constitute the dominant correction to all *ab initio* calculations based on the central-field approach. However, the complexity for neutral atoms increases rapidly with the atomic number, and fully correlated calculations, in which all electrons are explicitly correlated, are still possible only for very light elements. For heavy atoms both theories can only be applied in a limited model (one- and two-body correlation effects) or only to certain atoms (closed-shell systems or alkali-like systems). We will present an attempt to carry out a fully correlated calculation of hyperfine structure constants of a heavy atom within the framework of the MCDHF theory. Calculated expectation values for the hyperfine splittings of two levels of atomic gold, together with experimental values of the electric quadrupole hyperfine structure constants, allowed us to extract a nuclear electric quadrupole moment $Q(^{197}\mathrm{Au})=521.5\,(5.0)$ mb (see figure).

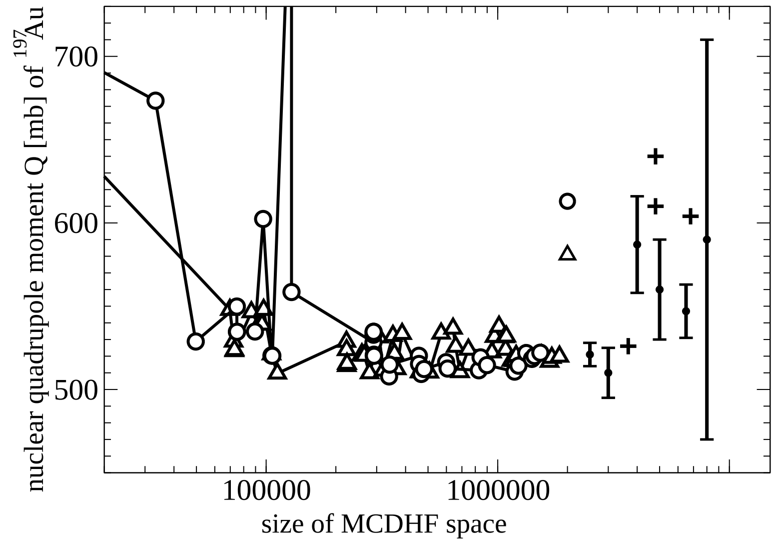

Figure 1: Nuclear quadrupole moment Q [mb] of the ^{197}Au isotope obtained from the calculated electric field gradients, as a function of the size of multiconfiguration expansions for the states $5d^96s^2\ ^2D_{3/2}$ (triangles) and $5d^96s^2\ ^2D_{5/2}$ (circles), compared with other theoretical and experimental results.

Is two-photon resonance optimal for STIRAP?

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The technique of stimulated Raman adiabatic passage is a highly efficient tool for coherent population transfer in a chainwise-connected three-state system, 1-2-3. It is widely accepted that two-photon resonance between the two end states of the chain, 1 and 3, is crucial for the success of the process. This assumption, which is almost never questioned, is perfectly justified when the two driving pulses-pump and Stokes-produce nearly equal couplings for the two transitions, 1-2 and 2-3. We show, numerically and analytically, that when the pump and Stokes couplings differ significantly, the two-photon excitation profile is distorted and asymmetric with respect to two-photon resonance. We present examples when the line profile is shifted from the two-photon resonance so much that the optimal operation of STIRAP demands significant two-photon detuning. The results are of potential importance for a number of applications of STIRAP, particularly in situations when the pump and Stokes fields are of different nature.

IR luminescence of Xe_2 excimers produced in dense Xe gas by electron impact

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We discovered the emission of an infrared (IR) continuum centred at 1.3 μm ($\tilde{\nu} \approx 7800$ cm^{-1}) due to the decay of Xe_2 excimers produced in dense Xe gas excited by 70-keV electrons [1].

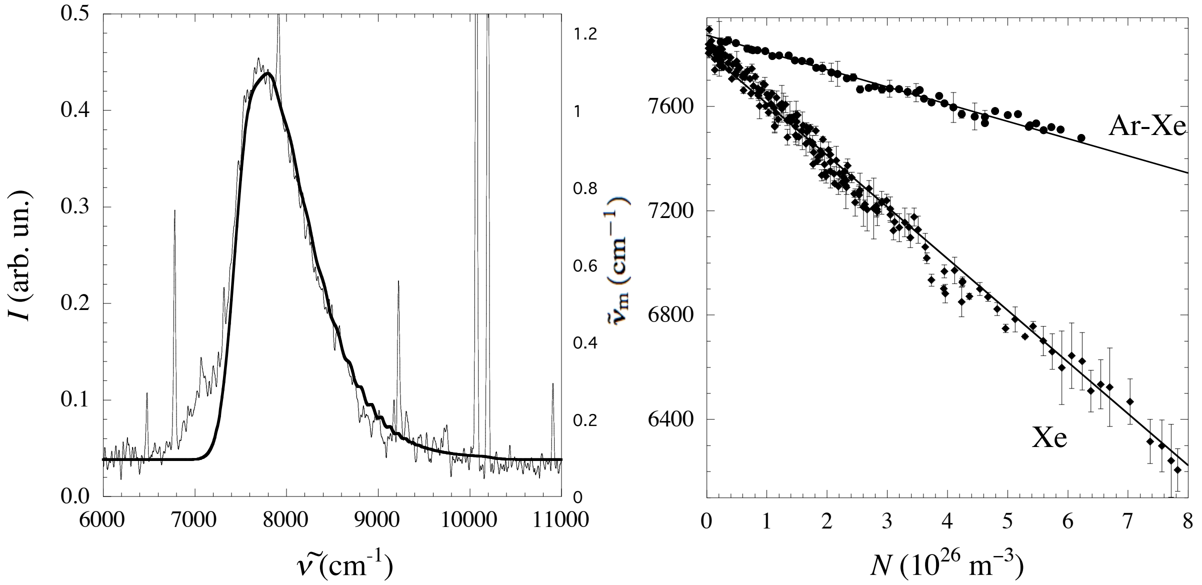

Figure 1: Left: Xe_2 IR emission spectrum. Thick line: FC calculations. Right: Density dependence of the peak wavenumber in pure Xe gas and in an Xe–Ar mixture.

In the left panel of Fig. 1 we show the spectrum for $P = 0.1\,\mathrm{MPa}$. The continuum is due to a bound–free transition between the 0_u^+ state related to the $6p(^1D_2)$ atomic limit and the 0_g^+ dissociative one related to the $6s(^3P_1)$ limit. This assignment reproduces the spectrum shape by means of Franck–Condon calculations [2]. A unique feature of the spectrum is that the wavenumber of its peak ν_m is red-shifted as the gas density N increases. In the right panel of Fig. 1 ν_m is plotted vs N for $P \leq 3.3$ MPa in pure Xe gas and in an Ar-Xe mixture. The shift is explained by accounting for the dielectric properties of the gas and the quantum multiple scattering of the optically active electron whose wavefunction extends over many atoms [1].

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The density function for atoms in second quantization, addressing the symmetry

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It is first stressed that the density function for a well defined atomic state is not *a priori* spherically symmetric in the general open shell case. The specific angular content of the density function is investigated [1] and ways of building it as a spherical symmetric function are discussed, from which the radial electron density function emerges. This function is written in second quantized coupled tensorial form for exploring the atomic spherical symmetry. The presented formalism leads to an expression for the density function, which has been implemented in the ATSP2K package [2].

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Extremely sensitive coherent control of atomic processes

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Coherent control was introduced few years ago to control accurately the dynamics of a physical system excited by light. It relies on the interference effects produced by excitation with coherent fields. The control is performed by adjusting the relative phase between the exciting fields which steers the interference of the quantum paths involved in the process. Such control has been demonstrated in many contexts. Generally, the quantity of interest corresponds to a cross section or the population of an excited state and the sensitivity of the process to the relative phase is limited to a smooth variation that follows the optical variation of the total field with the relative phase. The originality in the present work is to show that much higher sensitivity can be obtained using different configurations. For instance, in an atomic driven system, we show that geometric phases like the Pancharatnam phase exhibit a highly sensitive dependence with the phase shift, much more pronounced than the population dynamics dependence [1]. In a non resonantly driven atomic system, non adiabatic transitions can lead to a significant population transfer if the pulse profile is asymmetric. We show that the interaction of two time delayed, phase-locked, and non-resonant pulses with an atomic system leads to an efficient control of non adiabatic coupling. The population transfer to excited states exhibits a very sensitive dependence with the relative phase that is a consequence of the high non linearity of the interaction [2]. Finally, in a double two-level excited by a sequence of two orthogonally polarized fields system, coherent control of the optical response of the medium can be achieved in both the long and short pulse regime [3, 4]. Depending on the relative phase between the two fields the system can be converted into an absorber or an amplifier and allows the medium to switch from slow to fast light medium as well. With the virtue of this increased sensitivity, these effects can lead to the improvement of the techniques based on interferometry and open large perspectives in the control of systems dynamics.

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Hyperfine structure of near-infrared transitions in neutral nitrogen revisited

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Doppler-free spectra of N I transitions on the $2p^2(^3P)3s\ ^4P \rightarrow 2p^2(^3P)3p\ ^4P^o$, $^4D^o$ multiplets have been recorded by Jennerich *et al.* [1] using saturated absorption spectroscopy. From these data, the authors extracted values for the hyperfine structure coupling constants for the various J levels of these multiplets, for both ^{14}N and ^{15}N. Isotope shifts of three transitions in each multiplet have also been measured, revealing a significant J-dependence of the shifts. These authors recommended a theoretical investigation of the underlying cause of this unexpected phenomenon.

We present *ab initio* calculations of hyperfine structure and specific mass shift parameters using the ATSP2K package of Froese Fischer *et al.* [2]. Elaborate correlation models within a systematic approach are used for assessing the reliability of the *ab initio* parameters. The strong disagreement between theoretical and experimental hyperfine constants is confirmed by more elaborate calculations performed on the ^{4}P term, suggesting serious problems in the interpretation of the observed spectra. The latter is currently under investigation, on the basis of our *ab initio* results. The eventuality of the J-dependency of the specific mass shifts is also considered.

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A theoretical study of the isotope shift on electron affinity of chlorine

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If the electron affinity (EA) is well known for most of the elements, it remains a challenging quantity to calculate. On the experimental side, the measurements of isotope shift (IS) on electron affinity are limited by both resolution and sensitivity. In this case, theory can eventually be of some help even though correlation plays a dominant role in negative ions structure and, particularly, in the calculation of specific mass shift (SMS).

We report Multiconfiguration Hartree-Fock calculations on isotope shift in electron affinity of chlorine. The present study solves the longstanding theory-observation sign discrepancy between the calculated and measured specific mass shift contributions on electron affinity of chlorine for the isotopes 37 and 35 [1].

Table 1: Electron affinities and isotope shifts calculated and measured using our calculated field shift -0.003 (20) GHz.

Model	EA (eV)	$\mathrm{SMS}^{37/35}$ (GHz)	$\mathrm{IS}^{37/35}$ (GHz)
Theory [1]		+0.50	1.24
Theory (this work)	3.663	−0.495	0.253(20)
+ relativistic correction from [2]	3.611		
Experiment [1]	3.613		0.22(14)

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Nonresonant corrections for the optical resonance frequency measurements in hydrogen atom

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The deviation of the natural spectral line profile from the Lorentz shape for the optical resonant frequency measurements is considered. This deviation leads to an asymmetry, which is mainly due to nonresonant correction to the resonant Lorentz profile. The nonresonant corrections are studied for the different types of the atomic resonant experiments [1,2]. The most accurate recent optical resonance experiments [3,4] are analyzed, i.e. the two-photon $1s$–$2s$ resonance excitation of the hydrogen atom with the delayed decay in the external electric field. The description of the nonresonant correction in the latter case requires the employment of QED with different in- and out-Hamiltonians.

The nonresonant corrections for this experiment are investigated and found to be about 10^{-5} Hz, while the recent experimental uncertainty is 34 Hz and in the near feature is expected to be few Hz. The projected $1s$–$2s$ resonance excitation experiment with the three-photon ionization detection (which is now in progress) is also considered.

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Interatomic Coulombic decay of the Ne^{2+}(2s^{1}2p^5)Ar states populated via the K-LL Auger decay of Ne

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Interatomic Coulombic decay (ICD) [1] is known to be the dominant relaxation pathway of the one-site inner-valence ionized states of complexes. In ICD the relaxation of the initially ionized state results in the emission of a low energy electron from the neighboring subunit. As a consequence of ICD a Coulomb explosion takes place leading to a damage of the complex.

In the present work we report a theoretical analysis of ICD of the Ne^{2+}(2s^{1}2p^5)Ar states populated via the K-LL Auger decay of Ne. For this purpose, we have computed the relevant potential curves of the NeAr system and the corresponding decay rates using accurate ab-initio methods as described in [2,3]. The electron spectra were computed within the framework of the time dependent theory of wave packet propagation, similarly as performed in [4]. As seen in Fig. 1, the strongest ICD spectrum corresponds to the Ne^{2+}(2s^{1}2p^5 ^{1}P)Ar → Ne^{2+}(2p^{-2} ^{1}D)Ar$^+$(3p^{-1}) transition. The spectra for the Ne^{2+}(2s^{1}2p^5 ^{1}P)Ar → Ne^{2+}(2p^{-2} ^{1}S)Ar$^+$(3p^{-1}) and Ne^{2+}(2s^{1}2p^5 ^{3}P)Ar → Ne^{2+}(2p^{-2} ^{3}P)Ar$^+$(3p^{-1}) transitions are slightly weaker and appear at lower electron energies. The ICD is ultrafast: it lasts only about 30 fs for the singlet Ne^{2+}(2s^{1}2p^5 ^{1}P)Ar state.

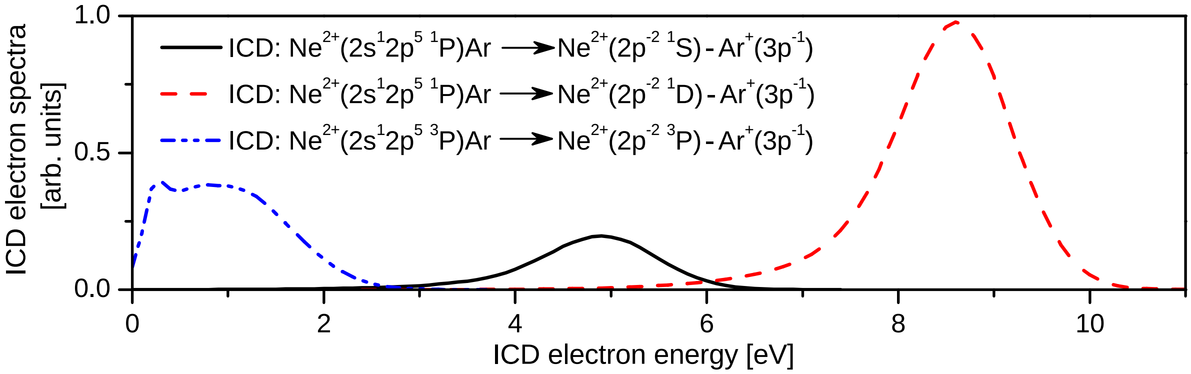

Figure 1: ICD electron spectra resulting from the Ne^{2+}(2s^{1}2p^5)Ar states.

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New view on the description of the hyperfine structure of free atoms and ions. Case of the model space $(5d + 6s)^3$ of lanthanum atom

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On the basis of our earlier works, both experimental and theoretical [1,2], as well as numerous works by other authors we feel qualified to submit a proposition, that the existing theories, which provide a semi-empirical description of hyperfine interactions in the structure of a complex atom, are not sufficiently precise to yield a correct interpretation of the measured hyperfine splittings within the up-to-date experimental accuracy.

In our group a procedure of analysis of experimental data concerning the structure of complex atoms, was developed. In the updated procedure the segment "parametrization of one- and two-body hyperfine interactions" was improved with respect to the earlier applied method [2,3] through inclusion of full parametrization of the excitations from closed shells to open shells, as well as generalization allowing parametrization of two-body hyperfine interactions in all really existing configurations up to three open shells.

In the case of lanthanum atom, the configuration system $(5d+6s)^3$ is well separated from the other perturbing configurations. This fact allows to analyse alternative models of second order perturbations, taking into account "open shell - empty shell" or "closed shell - open shell" excitations.

By comparison of the results of both models for the fine and the hyperfine structure, we can verify correctness of description of atomic structure and precisely determine information included in the radial parameters calculated on the basis of experimental data [4,5].

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Search for the frequencies for the nuclear optical clock with the use of information from the analysis of the fine structure of high lying energy levels in Th$^+$ ion

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The nucleus of ^{229}Th has the very low energy (7.6 eV) of excitation [1]. Therefore, it is possible to use this system to establish nuclear laser spectroscopy and eventually to built a nuclear optical clock of very high accuracy [2,3].

The Th$^+$ ion has a very high density of electronic states. According to suggestion of prof. E.Peik, the electronic excitation can be used as a kind of "antenna" to increase the coupling of laser light to the small nuclear moments (nuclear excitation via electron transition)[4]. The efficiency of these processes depends on resonance conditions, i.e. the availability of electronic states near the nuclear excitation. Available information on energy levels and lines of Th$^+$ is restricted to values below 60000 cm^{-1}, based on the analysis of 13 three-electron configurations involving 5f, 6d, 7s and 7p electrons [5].

In our semiempirical calculations, based on the experimental data, we determine the even and odd parity level scheme of Th$^+$ ion in the range up to about 75000 cm^{-1}, taking into account higher excited electron configurations. Using the fine structure eigenvectors, determination of the transition probabilities for the allowed transitions will be possible.

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Recoil by Auger electrons: theory and application

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Translation-momentum coupling between electrons and nuclei in a molecule ejecting high energetic photoelectrons may result in internal excitations of the molecule [1]. This effect has been recently verified by observing photoelectron recoil-induced vibrational excitations in molecules [2]. The study of recoil by high energetic photoelectrons increases the experimental efforts, since photoionization cross sections typically fall off at high energies. Alternatively, one can study the Auger decay after the K-shell photoionization, where the photoelectron is only slightly above the 1s-threshold and the recoil momentum is provided by the fast Auger electron.

The simple scheme to account for the momentum coupling between electrons and nuclei suggested in [1] has been extended to describe the recoil of nuclei by a fast Auger electron in diatomic molecules. The key for obtaining transparent equations is to represent the occupied orbitals as a LCAO and the fast continuum electron by a plane wave. This allows one to change the integration variables from the molecular frame to the laboratory one in the analytical evaluation of the Coulomb integrals.

As an application, the impact of recoil by the fast Auger electron on the interatomic Coulombic decay (ICD) following the K-LL Auger decay in the Ne dimer has been investigated theoretically. ICD is a process where the transfer of relaxation energy from one site of a weakly bonded complex leads to the emission of a low-energy electron from a neighboring site [3]. The ICD after Auger decay in Ne_2 has been predicted theoretically in [4] and was recently verified experimentally [5]. A detailed theoretical interpretation is presented in [6].

The present computations are performed within the framework of the time dependent theory of wave packet propagation. Our calculations illustrate an enormous effect of the recoil of the nuclei on the computed wave packets propagating on the potential curve populated by the Auger decay. The corresponding final state of the Auger process decays further by ICD. We show that the recoil momentum imparted differently onto the nuclei modifies the computed ICD spectra considerably.

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Influence of the UV laser light on the brightness characteristics of AC electroluminescence structures

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The alternating current electrolumiscent (AC EL) displays are multilayer structures with a wide application in color information representation. These displaer structures consist of an electrolumiscent (EL) layer on the base of ZnS luminophore and a protective non-organic or organic layer [1, 2].

The improvement in the brighness on this type of structures attract our interest. Our recently investigations connected with illumination of the one of the layers with non-polarization monochromatic light with $\lambda = 365nm$ emitted by a Hg spectral lamp show increase the integral brighness of the EL structure.

In the present experiment we investigate the influence of the N_2 laser light on the brighness of EL structure with different color of luminiscence.

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Level shift and electron-impact excitation of H-like ions in dense plasma

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Plasma screening effect on atomic structures have been subject to extensive studied during the last decades[1,2]. In the present work, the plasma effects on level shift and electron-impact excitation (EIE) have been analyzed by including the Debye-Hückel potential into the self-consistent Dirac-Fock equations. The wave functions of the target states are generated by the modified package GRASP92[3]. Table 1 presents the level shift of H-like Ar^{17+} ion in several electron densities for $T_e = 48$ eV. Figure 1 show the total EIE cross sections (a) and the magnetic sublevels EIE cross sections (b) of Lyman α_1 transition of Ti^{21+}. As a comparison, the theoretical results of Reed *et al.*[5] is also included in the figure. For total cross section, from the figure we can see that our results are in very good agreement with result of Reed *et al.* For excitation to the magnetic sublevels, it is clear that the m = 0 sublevels is preferentially populated in electron-impact excitation. However, for incident electron energies lower than 3 time of the theoreshold energy, there is a significant discrepancy between the two results, this difference also result in a large difference of polarization.

Table 1: Level shift (eV) for Ar^{17+} for different electron densities

$n_e(cm^{-3})$	1s	2p	3p	4p
1×10^{23}	34.74	34.50	34.00	33.31
5×10^{23}	77.40	76.22	73.79	70.54
1×10^{24}	109.16	106.83	102.06	95.82
5×10^{24}	241.32	230.37	208.06	181.01

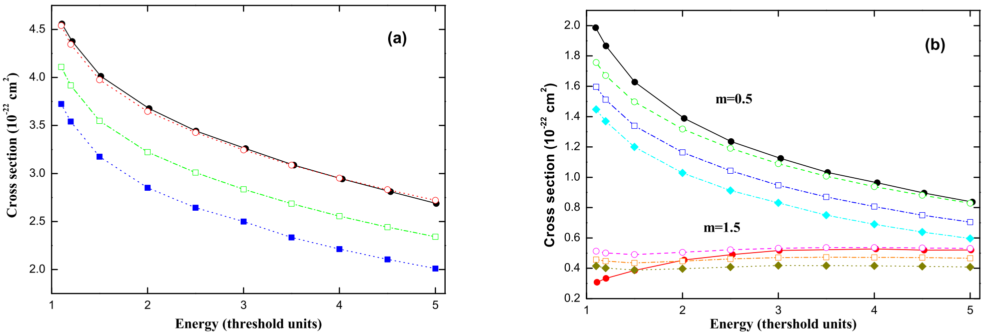

Figure 1: Total electron impact excitation cross sections (left) and magnetic sublevels cross sections (right) of the $1s \rightarrow 2p_{3/2}$ of Ti^{21+}. Solid line: theoretical values of Reed *et al.*[5], open circles: DW calculations for free ion, open square: DW calculation at $\lambda = 3$, Diamond: open square: DW calculation at $\lambda = 1.5$

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Two-electron-one-photon M1 and E2 transition between $2p^3$ and $2s^22p$ configuration of B-like ions

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In the past years, there are many studies on energy structures, transition probabilities and relevant atomic properties of B-like ions. On the one hand, there exist strong configuration interactions between the $2s2p^2$ configuration and the $2s^2ns$ and $2s^2nd$ Rydberg series. It is interesting to explore electron correlation, Breit interactions and quantum electrodynamical (QED) effects in the B-like ions [1,2]. On the other hand, B-like ions widely exist astrophysical [3] and laboratory plasma like EBIT or thermal nuclear fusion device [2,4]. Therefore, the transitions within the $n = 2$ complex including forbidden and resonance lines play key roles in diagnose of temperature, density and abundance of plasma [5].

More recently, a large scale spectrum calculations on energy levels, specific mass shift parameters, hyperfine interaction constants, Landé g_J factors and transition probabilities for C II, N III and O IV have been carried out by us [6] using GRASP2K package [7] based on multiconfiguration Dirac-Fock method. In this paper, we further calculated tow-electron-one-photon (TEOP) M1 and E2 transitions between $2p^3$ and $2s^22p$ configuration of B-like ions with $18 \leq Z \leq 74$ [8]. The influence of Breit interaction and QED effect on concerned TEOP M1 and E2 transitions energies and probabilities were analyzed in detail. It was found that the contributions of Breit interaction to the TEOP transition can not be neglected especially for M1 decay.

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Hyperfine quenching of $3s3p\ ^3P_0,\ ^3P_2$ level of Mg-like ions

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Theoretical investigations on hyperfine quenching of metastable levels $3s3p\ ^3P_0$ and $^3P_2$ of Mg-like ions between $Z = 13 - 78$ have been performed [1, 2] using Grasp2K package [3] based on the multi-configuration Dirac-Fock method. Electron correlation, Breit interaction and QED effects were taken into account systematically. Hyperfine quenching rates of $3s3p\ ^3P_0$ level were compared with other theoretical [4, 5] and experimental values [6]. The present calculated probability of $4.327 \times 10^{-2} s^{-1}$ for $^{27}\mathrm{Al}^+$ is in good agreement with recent the experimental measurement of $4.854 \times 10^{-2} s^{-1}$ [6]. Furthermore, a fitting formula scaling in Z was obtained, which was presented in Fig.1 (a). In addition, it was found that the lifetime of $3s3p\ ^3P_2$ level is sensitive to the hyperfine quenching at the beginning of the isoelectronic sequence as shown in Fig.1 (b).

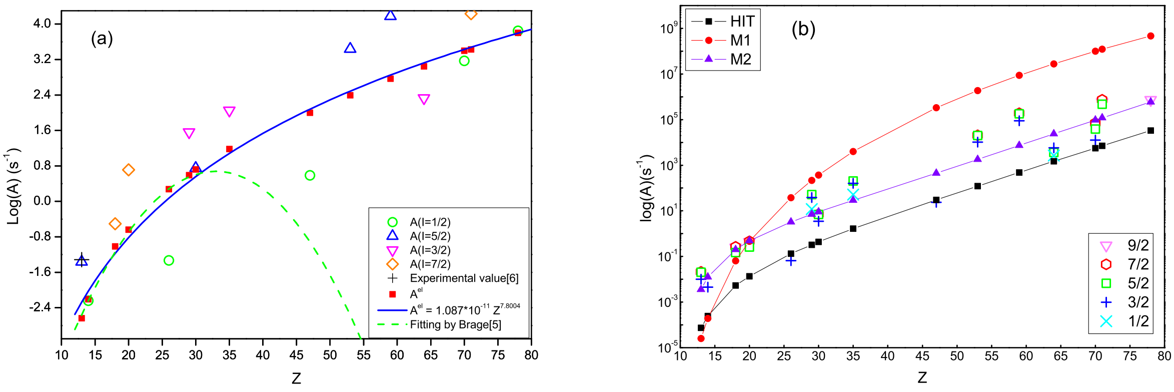

Figure 1: Logarithm of hyperfine induced transition rates A together with reduced hyperfine induced transition rates A^{el}. (a): hyperfine quenching of $^3P_0$ level, other theoretical and experimental results were shown; (b): hyperfine quenching $^3P_2$ level compared with other main decay rates.

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Interference spectra involving doubly excited states $[1s2p](^3P)3p^2$ (J=1) in 1s photoionization of Ne

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Combining the multiconfiguration Dirac-Fock (MCDF) method and the Fano technique [1], the interference effects between photoionization and photoexcitation autoionization involving doubly excited $[1s2p](^3P)3p^2$ (J=1) states of neon have been studied theoretically. The resonant excitation energies from the ground state $1s^22s^22p^6\ ^1S_0$ to the doubly excited states $[1s2p](^3P)3p^2$ (J=1) and the relevant bound/continuum-bound transition matrix elements have been calculated by using RATIP package [2-4] and RERR06 code [5-6] and then the Fano parameters q and ρ^2 can be obtained. In Fig. 1, the fine structure of the calculated interference spectra is compared with the available experiment [7], and the dominant contribution to the strength and profile resulting from some individual resonances are shown.

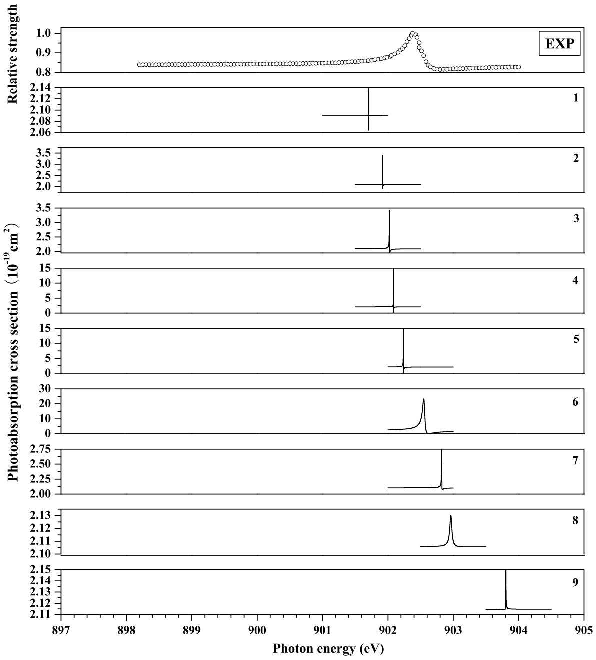

Figure 1: Comparison between the experimental spectra [7] and the calculated individual interference profile in Babushkin gauge. The theoretical energies are shifted by +2 eV for comparison.

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Luminescence of exciton-impurity complexes in binary argon-xenon clusters

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Observation of luminescence from volume and surface excitons in free xenon clusters was first reported in Refs. [1, 2]. Here we study the influence of an impurity embedded in xenon clusters on the excitonic luminescence spectra. Argon was chosen as impurity substance to enable tracing the evolution of luminescence spectra upon the process of decay of the mixed xenon-argon system into pure components resulting in formation of a xenon core covered by an argon shell.

Experiments were made on clusters formed in supersonic jets expanding into vacuum through a supersonic nozzle. The pressure and temperature of the primary gas mixture at the entrance of the nozzle were kept constant with the values p_0=1 atm and T_0=190-200 K, respectively, the only thing varied was xenon concentration (1.8% through 4.7%). Luminescence spectra were measured from a cluster beam excited with 1-keV electrons, the spectroscopic measurements being supplemented by electron diffraction study of the cluster structure.

For xenon clusters with a low number of argon atoms (distributed all over the cluster volume without forming any argon shell), we clearly observed the volume exciton luminescence band at 8.35 eV, a band of a surface polariton at 8.38 eV, and two surface-allowed excitonic bands at 8.23 and 8.31 eV. It was rather unusual to find out that the bands are clearly observable in noncrystalline clusters having the structure of multilayer icosahedron. This fact still needs to be studied theoretically, yet it may be due to the small exciton radius, which is less than the lattice parameter of xenon. When changing concentration of argon impurity in xenon clusters, a shift to lower frequencies (from 8.355 to 8.341 eV) was observed for the first time for the volume exciton band. The most pronounced shift of the band accompanied by its quenching took place for clusters with an argon shell under formation.

In our opinion, the shift of the excitonic band and the impurity-dependent behavior of its intensity are due to the formation of exciton-impurity complexes. The quenching of the excitonic band may be due to lowering of barrier height for exciton trapping into molecular centers with strong argon enrichment of surface layers.

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The kinetics of cluster formation during the phase transition gas-liquid in alcohols

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The processes of the molecular cluster formation of monohydric alcohols (from methanol to hexanol) were investigated by FTIR using the matrix isolation technique in Ar matrices. The transformation of FTIR bands of free hydroxyl groups (3600–3800 cm^{-1}) into diffuse bands (3000–3600 cm^{-1}), which were assigned to the stretching vibrations of the H-bonded O–H groups in various clusters, was monitored in its initial stage softening the matrices by heating from 20 K to 50 K. The band shape analysis was carried out for all investigated systems. The FTIR bands of alcohol molecules trapped and solidified in the matrices without annealing were found very close to be Gaussian-shaped. The magnitude of inhomogeneous broadening due to the matrix effect was evaluated. The values of hydrogen bond dissociation time of alcohols trapped in matrices were evaluated from the bandwidths of dimers, trimers and higher aggregates after broadening factor was taken into account. These data correlate with those directly measured in ultra fast infrared experiments of alcohols in solutions.

A 465 nm laser, based on sum frequency mixing in PP-KTP, for investigations on metastable $^3He_2$* molecules

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A single-frequency tunable laser has been developed to probe the 465 nm molecular absorption lines of helium plasmas [1] in order to study the influence of helium metastable molecules (He_2*) on metastability-exchange optical pumping of ^3He [2] under various conditions [3]. The generation of blue light is based on sum frequency mixing of two infra-red laser beams at 923 nm and 937 nm (from 100 mW DFB laser diodes) in a non-linear PP-KTP crystal. The overlapping of the IR beams in the crystal is obtained using a set of 3 dispersive prisms. A conversion efficiency of 2.9 % $W^{-1}cm^{-1}$ is achieved, with a maximum output power of 175 μW of blue a in single-pass configuration of pump beams through the crystal. The specified range for temperature control of the IR laser diodes provides a tuning range of 1.3 nm around the central wavelength 465.4 nm. It is thus possible to probe the electronic transitions for branches Q(1-8), P(2) and R(0) of metastable $^3He_2$* molecules.

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QED theory of laser-atom and laser-nucleus interaction: Stark effect and multi-photon phenomena

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QED theory is developed for studying interaction of atoms and nuclei with an intense and superintense laser field. In order to describe multi-photon phenomena we present an advanved energy approach. The method is based on a description of system in the field by the k- photon emission and absorption lines. The lines are described by their QED moments of different orders, which are calculated within Gell-Mann and Low adiabatic formalism [1,2]. The analogous S-matrix approach is developed for consistent description of the multi-photon resonances in nuclei. We have studied the cases of single-, multi-mode, coherent, stochastic laser pulse shape. Results of the calculation for the multi-photon resonance and ionization profile in H, Cs, Tm, Gd atoms and Sn, Fe nuclei are presented. Strong field (DC, AC) Stark effect for nuclei, atoms, including Rydberg atoms, is studied within the above cited energy approach and relativistic operator perturbation theory [1,2]. We present here the calculation results of the Stark resonances energies and widths for a number of atoms (H, Li, Tm, U etc.) in the ground, low-lying and Rydberg excited states. We discovered and analyzed the weak field effect of drastic broadening of widths of the Letokhov-Ivanov re-orientation decay autoionization resonances in Tm, Gd, U atoms. The similar phenomenon in nuclei is also discussed. In particular, the AC Stark effect for nuclei is described within the operator perturbation theory and the relativistic mean-field (RMF) model [3] for the ground-state calculation of the nuclei.

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Bound beta-decay and decay of isomeric states for fully ionized atoms and astrophysical nucleosynthesis

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Many attempts have been made to influence on the nuclear decay rate by varying the temperature, chemical environments or by applying strong fields. The situation iscompletely different in hot stellar plasmas where the ions are partially or fully ionized. In this case it can be expected that the rates of nuclear β decay and electron capture, as well as internal conversion, are strongly affected in comparison to those of neutral atoms [1]. In our paper the relativistic many-body perturbation theory [2] is used to define β decay parameters for a number of β-transitions. We studied the electronic rearrangement induced by nuclear transmutation in decay of ^6He-^6Li. We calculated the probabilities of excitation to final discrete states of $^6Li^+$ (including to doubly excited autoionizing states) as well as the total probabilities for single and double ionization. We have calculated beta decay parameters for a number of transitions: ^{33}P-^{33}S, ^{35}S-^{35}Cl, ^{63}Ni-^{63}Cu, ^{241}Pu-^{241}Am etc and show that the theoretical values agree quite well with some available experimental data. We also studied the chemical environment effect on parameters of beta transitions, in particular, $^{63}Ni^{(0)}$-$^{63}Cu^{(+1)}$, $Ni^{(+2)}$-$Cu^{(+3)}$, $^{241}Pu^{(0)}$-$^{241}Am^{(+1)}$, $Pu^{(+2)} - Am^{(+3)}$ and found a little modification of β decay parameters. It is connected with account of the changing the integration limits in the Fermi function integral, energy corrections for different chemical substances as well as the possibility of bound or other decay channels. The half-life period for decay of the tritium atom (ion) has been estimated with taking into account the bound β decay channel correction and some other accompanying effects (population of bound states of ^3He, population of the continuum states with exchanging orbital electron by the electron, the charge screening effect due to the orbital electrons etc). The estimates for a ratio λ_b/λ_c of bound-state (λ_b) and continuum-state (λ_c) beta decay rates for the case of bare $^{207}Tl^{81+}$ions and isomeric states of fully ionized ^{144m}Tb etc are given. The similar effects are also studied for ^{187}Re. The effects studied are responsible for creation of elements in space and astrophysical plasma.

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Raman scattering of the light on metastable levels of diatomics

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Laser action on molecules leads to different non-linear processes, including multi-photon phenomena, light scattering. The intensities and polarization of lines in the spectra are defined by polarizability and derivative on inter-nuclear distance. We study the Raman vibration scattering of the light on metastable levels of molecules (H_2, HD, D_2, Cs_2, Fr_2). New numerical method for construction of the Green electron functions for optical electrons and electron wave functions is developed within the pseudo-potential approach in the spheroid coordinates system that allows to take into account non-spherical character of molecular field [1,2]. We have carried out the calculations of molecular polarizability, its derivative on inter-nuclear distance, depolarization degree under Rayleigh and Raman light scattering on the frequencies of the *Rb*, Nd lasers. Analysis of results of the calculation of a polarizability, its derivative on inter-nuclear distance, for example, for excited triple metastable $c^3\Pi_n$, states of the H_2, HD, D_2 molecules on the frequencies of the *Rb* (1.78eV) and Nd (1.18eV) lasers shows that the main contribution into polarization of the cited metastable molecules is provided by changing the electron shell due to the laser field action. An influence of the nuclear motion terms is quite little. Relativistic generalization of proposed approach is carried out too.

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Large scale CIV3 calculations of fine-structure energy levels and lifetimes in Al-like Vanadium

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We have performed large scale CIV3 calculations of excitation energies from ground states for 97 fine-structure levels as well as of oscillator strengths and radiative decay rates for all electric-dipole-allowed and intercombination transitions among the fine-structure levels of the terms belonging to the $(1s^22s^22p^6)3s^23$p, $3s3p^2$, $3s^23$d, $3p^3$, 3s3p3d, $3p^23$d, $3s3d^2$, $3p3d^2$, $3s^24$s, $3s^24$p, $3s^24$d, $3s^24$f, and 3s3p4s configurations of V XI, using very extensive configuration-interaction (CI) wave functions [1]. The important relativistic effects in intermediate coupling are incorporated by means of the Breit-Pauli Hamiltonian which consists of the non-relativistic term plus the one-body mass correction, Darwin term, and spin-orbit, spin-other-orbit, and spin-spin operators [2]. The errors, which often occur with sophisticated *ab initio* atomic structure calculations, are reduced to a manageable magnitude by adjusting the diagonal elements of the Hamiltonian matrices. In this calculation we have investigated the effects of electron correlations on our calculated data, particularly on the intercombination transitions, by including orbitals with up to n=5 quantum number. We considered up to three electron excitations from the valence electrons of the basic configurations and included a large number of configurations (1164) to ensure convergence.

Our adjusted excitation energies, including their ordering, are in excellent agreement with the recommended data by the National Institute of Standard and Technology (NIST). In this calculation the mixing among several fine-structure levels is found to be very strong. Due to this strong mixing sometime it is very difficult to identify these levels correctly. In our CIV3 calculation we identify the levels by their dominant eigenvector [3, 4]. We believe that our very extensive calculations may assist the experimentalists in identifying these strongly mixed levels. From our transition probabilities, we have also calculated radiative lifetimes of the fine-structure levels in V XI. Significant differences between our calculated lifetimes and those of Froese Fisher et al. [5] for several fine-structure levels are discussed. We predict new data for several levels where no other theoretical and/or experimental results are available.

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Energy levels, oscillator strengths and lifetimes in Ge XXI

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Emission lines from multiply charged Mg-like ions are frequently observed in the spectra of astrophysical plasma and laboratory plasmas. Accurate absorption oscillator strengths for these ions are needed in astrophysical observations and in the study of laboratory plasmas both for diagnostic purposes and for the determination of the effects of impurities on controlled thermonuclear fusion.

We have calculated excitation energies from the ground state for 53 fine-structure levels as well as oscillator strengths and radiative decay rates for all electric-dipole-allowed and intercombination transitions among the fine-structure levels of the terms belonging to the$(1s^2 2s^2 2p^6)3s^2$, 3s3p, 3s3d, 3s4s, 3s4p, 3s4d, 3s4f, $3p^2$, 3p3d, 3p4s and $3d^2$ configuration of Mg-like Germanium. These states are represented by extensive configuration-interaction (CI) wave functions obtained using the CIV3 computer code of Hibbert [1]. The important relativistic effects are incorporated through Breit-Pauli Hamiltonian [2]. Small adjustments to the diagonal elements of the Hamiltonian matrices have been made. These adjustments improve the accuracy of the mixing coefficients b_{ij}, which depend in part on the accuracy of the eigenvalues. This is a fine-tuning technique [3] that has been further justified in a paper on Na III [4] and most recently on Cl I [5].

Our excitation energies, including their ordering, are in excellent agreement with the available experimental results [6]. The enormous mixing among several fine-structure levels makes it very difficult to identify them correctly with the result that their positions in other calculations are interchanged compared to our results and the experimental values. We identify these strongly mixed levels by their dominant eigenvector [7]. From our transition probabilities, we have also calculated radiative lifetimes of some fine-structure levels. Our calculated oscillator strengths and the lifetimes are found to be in good agreement with the experimental and other theoretical results (wherever available). In this calculation we also predict new data for several fine-structure levels where no other theoretical and/or experimental results are available. We believe that the new oscillator strengths will be useful in many astrophysical applications and in technical plasma modeling.

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Energy losses of fast structural multicharged ions at collisions with polyatomic molecules and nanotubes

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In this paper the nonperturbative theory of energy losses by fast structural multicharged ions (projectile) in a collisions with polyatomic molecules and the nanotubes (target) is developed. In calculating the energy losses of ions at collisions with molecules, in contrast to the case of collisions of ions with single atoms, it is necessary to take into account the effects due to multiple collisions [1] and the orientation of the axis of the target molecules. Energy losses $\kappa^{(p)}$ of fast structural ions on the excitation of their electronic shells (with an arbitrary fate of the target) at collisions with diatomic molecules were considered in [1]. Summarizing the results of [1] to the case of N-atomic targets for energy losses $\kappa^{(p)}$, with a fixed orientation of the target, we can write

$$\kappa^{(p)} = \frac{N_p}{2} \int \Big(\sum_{m=1}^{N} \mathbf{q}_m \Big)^2 d^2\mathbf{b} = \kappa + \Delta\kappa \, , \tag{1}$$

where N_p – number of projectile's electrons, $\mathbf{b}$ – impact parameter of ion, $\kappa = \sum\limits_{m=1}^{N} \kappa_m^{(p)}$, $\kappa_m^{(p)} = \frac{N_p}{2} \int \mathbf{q}_m^2 d^2\mathbf{b}$ – energy losses of ion in a collision with an isolated m-th target atom, $\Delta\kappa = \frac{N_p}{2} \int \sum\limits_{m,n=1}^{N} (\mathbf{q}_m \mathbf{q}_n) \, d^2\mathbf{b}$ – the correction to the energy losses due to multiple collisions, and $\mathbf{q}_m$ – the momentum transferred to each projectile's electron in a collision with m-th target atom. The Dirac-Hartree-Fock-Slater model [2] is used to describe the distribution of electron density in target atoms.

Under this theory, we carried out calculations of energy losses of fast ions in collisions with various polyatomic molecules, as well as with nanotube C_{300}. Calculations showed that the correction $\Delta\kappa$ substantially depends on the orientation of the target's axis relative to the direction of movement of ions, and takes larger values when two or more atoms in a target located along one or more straight lines, parallel ion velocity. Thus, for example, the average energy losses of ions, colliding with the nanotube C_{300} at the energy 1000 MeV/nucleon, increased by 8,6 times with the changing orientation of the nanotube's axis from perpendicular to parallel relative to the direction of movement of ions. Furthermore, under the parallel orientation of the nanotube's axis the resulting energy losses $\kappa^{(p)}$ are 9,1 times as large than the total energy losses κ on the individual atoms of nanotube.

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Predominant dissociation of the $\mathrm{CO}^* \left(\mathrm{D}\,^2\Pi\right) n(\mathrm{d/s})\sigma$ Rydberg states into the $\mathrm{C\,I}^*\ 2\mathrm{s}^2 2\mathrm{p}^1 n(\mathrm{d/s}) + \mathrm{O}$ fragments

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Superexcited states of a molecule serve as doorway states for the effective formation of neutral fragments above the first ionization potential [1]. It was surprisingly obtained in [2], that the $(\mathrm{c}\ ^4\Sigma_u^-)\, n(\mathrm{d/s})\sigma_g(v)$ states of the O_2 dissociate predominantly into the $\mathrm{O\,I}^*(2\mathrm{p}^3\ ^4\mathrm{S})n(\mathrm{d/s})$ states conserving the effective principal quantum number n^* of the Rydberg electron. In the present work we apply photon-induced fluorescence spectroscopy [3] to investigate fluorescent fragments populated via the neutral dissociation of the vibrationally excited $\mathrm{CO}^*\,(\mathrm{D}\,^2\Pi)\, n(\mathrm{d/s})\sigma(v)$ states [4].

Cross sections for fluorescence from fragments were measured at the undulator beamline U125/1 at BESSY II, Berlin, in the spectral range of 115–135 nm as a function of the exciting-photon energy between 20–25 eV. First experimental indications were found for a predominant dissociation of the $\mathrm{CO}^*\,(\mathrm{D}\,^2\Pi)\, n(\mathrm{d/s})\sigma$ states into the Rydberg states of the C I atom conserving the n^* of the Rydberg electron.

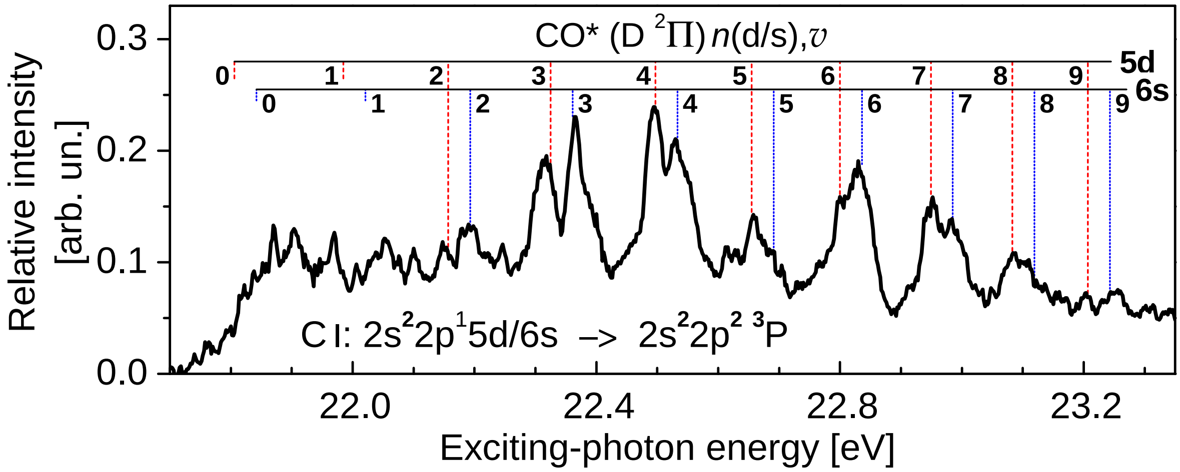

Figure 1: Cross section for the C I: $2\mathrm{s}^2 2\mathrm{p}^1(^2\mathrm{P})5\mathrm{d}/6\mathrm{s} \rightarrow 2\mathrm{s}^2 2\mathrm{p}^2\ ^3\mathrm{P}$ fluorescence.

The latter fact is illustrated in Fig. 1. One can see, that the most prominent resonant features observed in the cross section for the $2\mathrm{s}^2 2\mathrm{p}^1(^2\mathrm{P})5\mathrm{d}/6\mathrm{s} \rightarrow 2\mathrm{s}^2 2\mathrm{p}^2\ ^3\mathrm{P}$ fluorescence in the C I were assigned to the $\mathrm{CO}^*\,(\mathrm{D}\,^2\Pi)\,(5\mathrm{d}/6\mathrm{s})\sigma(v)$ vibrational progressions. Results of the present measurements are interpreted with the help of the theoretical potential energy curves of the CO^+ ion and the molecular orbitals of Rydberg electrons computed within the single center (SC) approach.

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Electron stereodynamics in multiple ionization of rare gas dimers by slow highly charged ions

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Much attention has been called to multiple ionization dynamics of molecules by impact of highly charged ions. For diatomic molecules, the angular and charge state distributions of Coulomb explosion fragments have been intensively measured for 'fixed-in-space' molecules with the momentum imaging technique. In contrast to covalent molecules, however, rare gas dimers have been little investigated, where the dynamics is expected far different due to electron localization character.

In the present work, we address multiple ionization (actually electron transfer) with slow ($v < 1$ au) highly charged ions by modifying the three-center Coulombic over-the-barrier model developed by the present authors [1]. In particular, we clarify electron stereodynamics peculiar to rare gas dimers (*e.g.* Ne_2) and analyze how it manifests itself in the orientation-dependent charge-pair distribution [2].

The outermost electrons at two atomic sites, B and C, in a target BC are assumed to successively form a quasimolecule with the projectile ion A^{q+}, where the target ion-core state is labeled by a pair of charge states, which evolves in respective steps as $(q_\mathrm{B} - 1, q_\mathrm{C}) \to (q_\mathrm{B}, q_\mathrm{C})$, or as $(q_\mathrm{B}, q_\mathrm{C} - 1) \to (q_\mathrm{B}, q_\mathrm{C})$. It is assumed for simplicity that the electron never returns to the target once trapped in the quasimolecule. Three ion cores $(q_\mathrm{A} = q, q_\mathrm{B}, q_\mathrm{C})$ induces a three-center Coulombic potential, which necessarily has two saddle points. Hence an orientation-dependent critical distance for the quasimolecule formation is determined by equating the electron energy localized at B or C with either of the two saddle energies according to the configuration of three ion-cores. The critical distances of all active electrons make a mosaic pattern of spacial regions for fragment charges $(r_\mathrm{B}, r_\mathrm{C})$ produced in a collision. This is in sharp contrast to a target of covalent molecule (*e.g.* N_2), where emerges a regular shell pattern with the number $r = r_\mathrm{B} + r_\mathrm{C}$ of total removal electrons.

We have applied this model to collisions of $\mathrm{A}^{8+} + \mathrm{Ne}_2$ with four active electrons and calculated orientation-dependent partial cross sections $\sigma(r_\mathrm{B}, r_\mathrm{C}; \theta)$ of the charge-pair production. It is found that symmetric charge states as $r_\mathrm{B} = r_\mathrm{C}$ (so that $r =$ even) are dominantly populated when the target dimer is oriented in a parallel direction to the incident beam, while asymmetric charge states are dominant in a perpendicular direction. Final states with $|r_\mathrm{B} - r_\mathrm{C}| \geq 2$ are little produced.

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Electron stereodynamics in charge-asymmetric Coulomb explosion of N_2 molecules with slow highly charged ions

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This investigation is motivated by a triple coincidence measurement [1] with the momentum imaging technique for collisions of slow (10 — 200 eV/amu) Kr^{8+} ions with N_2 molecules. In a coplanar geometry are detected a dissociating ion pair ($\mathrm{N}^{Q+}, \mathrm{N}^{Q'+}$) in transverse to the beam axis ($\vec{v}$) and a scattered ion in forward left and right directions. A remarkable result thereby was unequal strengths of charge-asymmetric fragmentation between the *near* and *far* sites relative to the projectile trajectory. For a given nonequivalent charge pair $Q \neq Q'$, the asymmetry parameter is obtained as $A(Q, Q') = (P_> - P_<)/(P_> + P_<)$ through $P_>$ and $P_<$, where $P_>$ ($P_<$) denotes a coincident population for $Q_{\text{far}} > Q_{\text{near}}$ ($Q_{\text{far}} < Q_{\text{near}}$), with Q_{far} and Q_{near} being the far and near fragment charges. The experiment indicated a striking positive asymmetry A; the far site is populated more by a higher charge than by a lower charge. This result was interpreted [1] to come from target electron polarization by the projectile charge during a collision.

In previous works [2], we have analyzed the observations by developing three-center Coulombic over-the-barrier models. Although leading to a correct sign of A, the polarization effect was found negligibly small with a two-step picture, *i.e.*, 'electron removal followed by Coulomb explosion'. Hence, we extended the model so as to describe an *inseparable* process, *i.e.*, formation of a three-center quasi-molecule and its decay into three (one scattering and two dissociating) moving atomic ions. It was suggested that large asymmetry arose from rapid bond elongation during a collision for small impact parameters as $b < 5$ au, where all 10 valence electrons form the quasi-molecule.

In the present contribution, we further analyze the charge-pair distributions by applying the model above. The electron localization probabilities are estimated at configurations of three ion cores determined for respective electrons (rank $t = 1 \sim 10$) with respective impact parameter vectors $\vec{b}$ ($\perp \vec{v}$). We thereby calculate the parameter A of asymmetric population and compare it with the experimental result.

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Optical lattice clock without atom-motion-dependent uncertainties

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Excellent controllability of system parameters for atoms in optical lattices has found broad applications in condensed matter physics, quantum information science and metrology. Polarization gradient lattice led to efficient laser cooling mechanisms and controlled atomic transport. The long coherence times of atoms in far-detuned intensity lattices make them attractive for precision measurement. In these applications, so far, the lattice potentials are well characterized by the electric dipole (E_1) interaction, hence, the higher order multipole interactions, such as the magnetic-dipole (M_1) and electric-quadrupole (E_2) interactions, are rarely discussed as an experimental concern. Besides controlling atomic motion, engineering light shift potential of a far-detuned intensity lattice opens up possibilities for novel atomic clocks. Optical lattice clocks are attracting growing interest as candidates for future redefinition of the second. It was pointed out, that different spatial distributions of multipolar (E_1,M_1,E_2) atom-field interactions may critically affect the uncertainties of highly accurate clocks based on atoms in an optical lattice of a "magic" wavelength [1], introducing difficulties in canceling out the light shift in clock transitions. There are two possibilities to overcome this problem: (i) to use an optical lattice, where the spatial distribution of the E_1 Stark effect coincided with the distributions of the M_1 and E_2 Stark energies; (ii) to shift the magic wavelength so, as to equalize the spatial distributions of the Stark-effect corrections to the energies of atoms in their excited and ground states, which for equal amplitudes E_0 of the waves is:

$$\triangle E_{St}^{g(e)}(\mathbf{r}) = -\frac{E_0^2}{2}\left[\alpha_{E_1}^{g(e)}(\omega) g_{E_1}(\mathbf{r}) + \alpha_{M_1}^{g(e)}(\omega) g_{M_1}(\mathbf{r}) + \alpha_{E_2}^{g(e)}(\omega) g_{E_2}(\mathbf{r})\right] \tag{1}$$

where $\alpha_{E_1}^{g(e)}(\omega)$, $\alpha_{M_1}^{g(e)}(\omega)$, $\alpha_{E_2}^{g(e)}(\omega)$ are the polarizabilities of the ground-state (excited) atom at the frequency ω , and the factors $g_{E_1}(\mathbf{r})$, $g_{M_1}(\mathbf{r})$, $g_{E_2}(\mathbf{r})$are the spatial distribution factors of the corresponding light shifts. A thorough analysis demonstrates, that 2D and 3D lattices exist with standing waves produced by running waves with mutually orthogonal polarization, where the E_1 distribution $g_{E_1}(\mathbf{r})$ could coincide with either $g_{M_1}(\mathbf{r})$ or $g_{E_2}(\mathbf{r})$. E.g., in a 3D lattice with running waves polarized along the standing-wave axes Ox, Oy and Oz the M1 and E1 distributions coincide: $g_{E_1}(\mathbf{r}) = g_{M_1}(\mathbf{r}) = 3 + \cos k(x+y) + \cos k(x+z) + \cos k(y+z)$, while $g_{E_2}(\mathbf{r}) = 6 - g_{E_1}(\mathbf{r})$. In the case of polarization at the angle $\pi/4$ to the axes the E2 distribution coincides with that of the E1: $g_{E_1}(\mathbf{r}) = g_{E_2}(\mathbf{r}) = 3 + 2\sin kx \sin kz + 2\cos ky \cos kz$, while $g_{M1}(\mathbf{r}) = 6 - g_{E_1}(\mathbf{r})$. In every case, the position-dependent Stark shift of the clock frequency may be eliminated by corresponding choice of the magic wavelength, while the residual position-independent multipole offset may be correctly taken into account.

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Non-linear magneto-optical resonances at D_1 excitation of atomic rubidium in ordinary and extremely thin vapor cells

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Non-linear magneto-optical resonances (NMOR), which are associated with coherences among ground state sublevels, have been known and generally understood for some time. In most alkali systems, adjacent transitions are not resolved under Doppler broadening. Therefore, to study NMOR in alkali vapors, one can develop a detailed theoretical model that takes into account Doppler broadening in ordinary vapor cells [1]. Alternatively, one can perform experiments in extremely thin cells (ETCs) [2], whose width is on the order of the wavelength of the light, and which offer sub-Doppler spectral resolution. However, in the ETCs interactions with the cell walls alter the characteristics of the resonances [3]. In order to understand the NMOR in the ETCs, we have studied such resonances in ordinary vapor cells and in an ETC for the D_1 transition of ^{87}Rb and ^{85}Rb experimentally and described the experimental results with a detailed theoretical model. The cells were placed at the center of a three-axis Helmholtz coil system, which canceled the ambient magnetic field. The magnetic field was scanned from negative to positive values along a direction that was perpendicular to both the polarization direction and propagation direction of the laser radiation. Laser induced fluorescence was observed in the direction of the magnetic field. We have collected a large amount of data for all the hyperfine transitions in the system and for various laser power densities, beam diameters, and laser frequencies for both the ordinary cell and the ETC, and we have studied the NMOR for different values of the wall separation in the ETC. Detailed comparison of experimental results and calculations based on the optical Bloch equations for a wide range of experimental situations allowed us to understand the influence of transit relaxation time, laser power density, and Doppler broadening and to characterize the manner in which these effects play a role in the ETC.

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Non-linear magneto-optical resonances and cascade coherence transfer at $6S_{1/2} \rightarrow 7P_{3/2}$ excitation of cesium

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Non-linear magneto-optical resonances have been studied experimentally and theoretically at $6S_{1/2} \rightarrow 7P_{3/2}$ excitation of atomic cesium. Unlike in previous studies (see, for example, [1] and references therein), we have observed the resonances in laser induced fluorescence (LIF) from the $7P_{3/2}$ state as well as from intermediate states $6P_{1/2}$ and $6P_{3/2}$ that were populated by cascades (see. Fig. 1(a)). The experiment was performed with cesium vapor in a sealed glass cell at a room temperature. A three-axis Helmholtz coil system compensated the ambient magnetic field and scanned the magnetic field in the observation direction. Cesium atoms were excited to the $7P_{3/2}$ state by linearly polarized laser radiation at 455.5 nm with its polarization vector perpendicular to the scanned magnetic field. Three interference filters were used to select different transitions for observation. The two orthogonal LIF polarization components (parallel I_{par} and perpendicular I_{per} to the laser polarization direction) were detected simultaneously with photodiodes while the magnetic field was scanned. Figure 1(b) shows the dependence of the polarization degree on the magnetic field observed in the fluorescence to the ground state from two different states, $7P_{3/2}$ and $6P_{3/2}$, when the original excitation took place from two different hyperfine levels of the ground state to the $7P_{3/2}$ state. Work is in progress to describe the signals with a detailed theoretical model based on the optical Bloch equations.

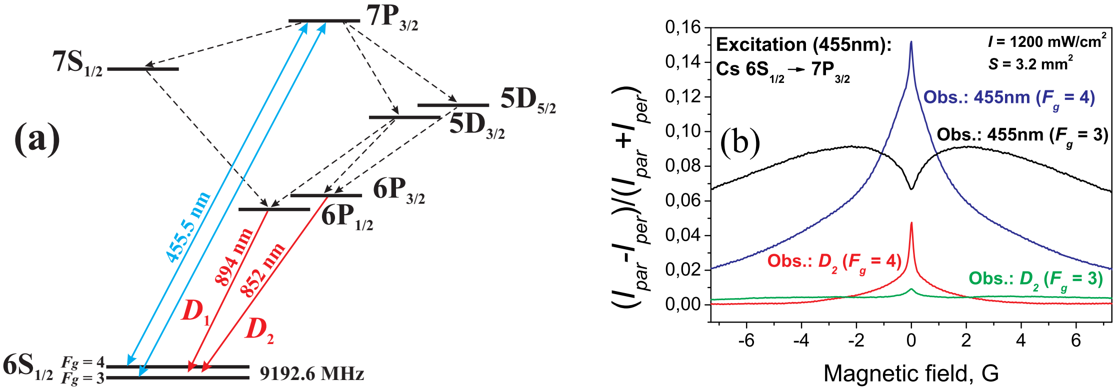

Figure 1: (a) Energy levels of ^{133}Cs, (b) polarization degree vs. magnetic field.

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Investigation of the 3 i 4 $^1\Pi_u$ states in Li_2 using polarisation labelling spectroscopy

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Absorption spectra of the $3\,^1\Pi_u$ and $4\,^1\Pi_u$ states of the lithium dimer were measured — primarily $^7Li_2$, but also $^7Li^6Li$. Polarisation labelling spectroscopy was used to simplify measured spectra, limiting visible transisitions to one or more progressions of PQR triplets [1].

Assigned transitions are consistent with previous measurements [2], but span a much greater range of rotational-vibrational quantum numbers. The positions of energy levels were found to be heavily perturbed: by nearby Σ states, but also by the electrostatic interaction between the two Π states.

A deperturbation analysis was performed by extending Inverted Perturbation Approach with simultaneous treatment of two electronic states. The results of an attempt to reproduce spectral measurements from a model with two potential wells and parameters describing the electrostatic perturbation are shown.

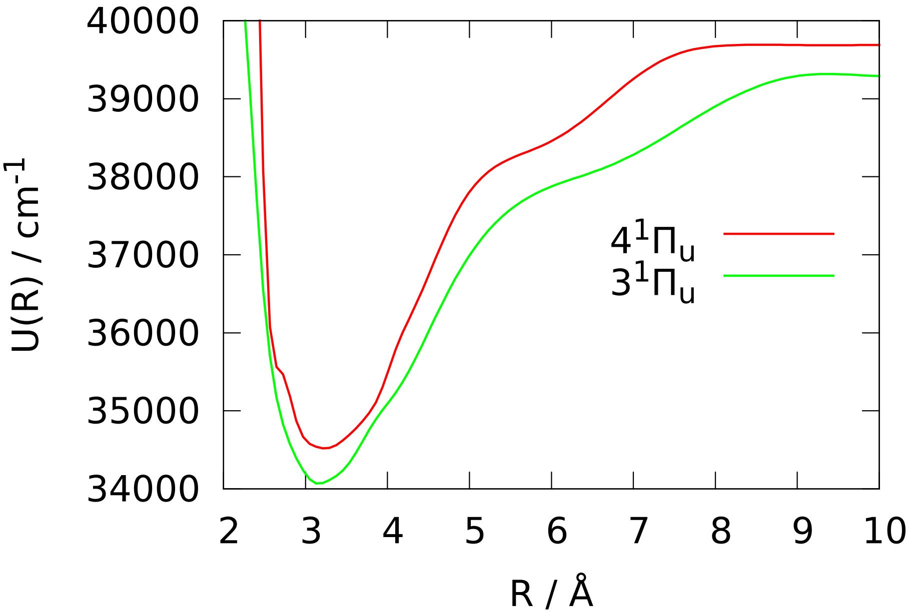

Figure 1: Potential energy in the $3^1\,\Pi_u$ i $4^1\,\Pi_u$ states of the $^7Li_2$ molecule.

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Determination of ground and excited state dipole moments of 4,5’-diamino [1,1’:3’,1”-terphenyl]-4’,6’-dicarbonitrile using solvatochromic method and quantum-chemical calculations

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Electronic absorption and fluorescence spectra of 4,5’-diamino[1,1’:3’,1”-terphenyl]-4’,6’-dicarbonitrile were recorded at room temperature in several solvents of different polarities. The results of spectroscopic measurements are analyzed using the theory of solvatochromism, based on a dielectric continuum description of the solvent and the classical Onsager cavity model. The difference in the excited and ground state dipole moment ($\mu_e - \mu_g$) of molecule under study was estimated using methods applied by: Bayliss, Ooshika, McRae, Lippert, Mataga, Bakhshiev and Kawski. Finally, the influence of polarizability on the determined change of the dipole moment was discussed. Austin model 1 (AM1) semiempirical molecular calculations were carried out to estimate the ground state dipole moment.

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The MBPT study of electrons correlation effects in open-shell atoms using symbolic programming language MATHEMATICA

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Atomic Many-Body Perturbation Theory (MBPT) allows systematic study of correlation effects in atoms and ions. In order to generate the atomic datum of high accuracy it is necessary to include the third and higher orders of MBPT. However, the calculations of correlation corrections in the third-order turns into a very complicated task due to the large number of MBPT expansion terms. Especially difficult computational problem arises for the open-shell atoms. Then one needs to calculate the matrix elements of n-particle operators ($n \geq 2$) in many-electron case.

In the present paper we develop technique for the generation of MBPT expansion terms for open-shell atoms using symbolic programming language MATHEMATICA [1]. The generalised Bloch-equation is used [2] to determine correlation corrections for atomic state wave function and energy levels. To demonstrate this technique, the expansion terms (diagrams) of the second-order wave operator and effective operator [2] are generated with authors produced package *NCoperators* (which is based on MATHEMATICA). The special attention is paid to the angular reduction of the expansion terms because for the open-shell atoms the efficiency of calculations depends on the way the valence electrons (the electrons in the open-shells) are considered [3]. In the present paper the second quantisation method, keeping in mind tensorial properties of creation and annihilation operators for valence electrons, is used.

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Above threshold two photon transition in H-like ions

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Exact calculation of laser-induced processes with H-like ions have attracted considerable attention over the last decades. These research has additional interest due to highly precision spectroscopic measurements of fundamental constants with the bound system experiments. Such investigations are sensitive enough to relativistic, radiative, retardation and QED – effects. On this reason exact fully relativistic calculations of the two photon transition amplitudes in hydrogen-like ions have some interest last years [1,2]. Among the different kinds of the two photon transitions like Raman and Rayleigh scattering particular interest play the two photon transitions when the energy of photon $\hbar\omega$ is above threshold of the one photon ionization I for Dirac state $|njm>$.

At present report the polarizability of $1s$, $2s$, $2p_j$ Dirac states of H-like ions with nuclear charch $Z = 1..130$ and photon energy from I to $10I$ were calculated using the Coulomb Green function $G(E)$ method [3] to sum intermediate states. The total matrix element to calculate polarizability may be presented in the form"

$$<njm|r_\mu G(E_{nj} \pm \hbar\omega) r'_\mu|njm>= \alpha_s(\omega) + \alpha_v(\omega)m\mu + \alpha_t(\omega)(3\mu^2 - 2)[3m^2 - j(j+1)], \quad (1)$$

where α_s, α_v and α_t are scalar, vector and tensor parts of polarizability accordingly. All this coefficients α_n are complex for energy photon above the one photon ionization.

The exact numerical results of calculation are presented both in the exact table data and in the following convenient analytical form:

$$\alpha_n = \alpha_n^{ner}\left[1 + c_n\,(\alpha Z)^2\right]. \quad (2)$$

Here $n \in s, v, t$, and α_s^{ner} and α_t^{ner} are well known nonrelativistic expressions $\approx Z^4$, but α_v^{ner} is the main part of $\alpha_V \approx (\alpha Z)^2$, α – is a fine structure constant. For example, in α_s case $c_s = -0.84626$ and α_s^{ner} has known real and imagine part dependent from photon energy. In general the accuracy of approximated results (2) are $\approx 10^{-4}$ for $Z = 1..100$, and $\hbar\omega$ from I to $10I$.

On the base of optical theorem the photoionization and photorecombination cross-section are calculated in numerical and approximated form like this one

$$\sigma_{phot} = \frac{4\pi}{c}\omega\,\mathrm{Im}\,\alpha_s = \sigma_{phot}^{ner}\left[1 - b_{nj}(\alpha Z)^2\right]. \quad (3)$$

Here σ_{phot}^{ner} is a nonrelativistic photoionization cross-section, and b_{nj} depends from the Dirac state $|njm>$. Retardation effects are discussed and calculated too.

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Elastic electron scattering by fullerenes and carbon tubes

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Fullerenes and carbon nano tubes have attracted intensive attention since its discovery. But the studies of the simplest collision processes for such atomic clusters are limited. Some experimental and Born approximation theory at high impact energies are presented in [1]. The high-level computational study of the low-energy elastic cross section on C60 presented in [2]. The calculation of cross section for elastic scattering of low-energy electrons by fullerene C60 within the static-exchange approximation are carried out in [3]. Properties of clusters like fullerenes and carbon nano tubes explain the transition from single atoms and molecules to the solid state. One can observe in clusters the appearance of new physical features such as plasmon excitation, supercoductivity, super liquidity and so on most of its exist in solid state and absent in single atom. Theoretical studies of electron interactions with C60 have mostly based on simplified models like Hartree-Fock jellium one. Such models approve that in fullerenes the delocalization of electrons take place on the surface in the vicinity of fullerenes cage and when considering electron collision the valence delocalized electrons play the most important role in the formation of the cross section.

At present work the cross section of elastic scattering of fast electron on C60 and simple carbon nano tubes calculated in Born approximation

$$\frac{d\sigma}{d\Omega} = \frac{4m^2e^2}{\hbar^4 q^4}\left|\int \rho(\vec{\mathbf{r}}) exp\left(i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}\right) dv\right|^2, \tag{1}$$

where $\vec{\mathbf{q}} = |\vec{\mathbf{k}} - \vec{\mathbf{k}}'|$ is the electron wave vector transfer and $\vec{\mathbf{k}}$, $\vec{\mathbf{k}}'$ are the wave vectors of electron in the initial and final state respectively, $\rho(\vec{\mathbf{r}})$ is the charge density of cluster

$$\rho(\vec{\mathbf{r}}) = \sum_{k=1}^{N} Z_k e\delta(\vec{\mathbf{r}} - \vec{\mathbf{r}}_k) - en(\vec{\mathbf{r}}). \tag{2}$$

Here Z_k is the nuclear charge of k-atom in cluster, $\vec{\mathbf{r}}_\mathbf{k}$ is a position of k-nuclear in cluster and $n(\vec{\mathbf{r}})$ is the total electron density. The calculation of $n(\vec{\mathbf{r}})$ was carried out on base of Gaussian03 program in different basis sets. Final results were obtained using 6-31G(d) basis set for fullerenes and density functional B3LYP method for carbon nano tube. The three-dimensional quadrature is carried out to calculate the form factor.

The results are presented in the table form for the different electron energy (500-5000 e.v.) and scattering angle $\theta = 10^0..150^0$ and clusters symmetry axis.

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Spin-exchange cross sections at the interaction between ground state sodium and metastable helium atoms

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At the interaction between spin-polarized excited atom and ground state alkaline metal atom in gas discharge elastic and inelastic processes take place simultaneously. In such a case these two processes influence on each other giving rise to a change of the cross section's value for the elastic process. It means, that besides the chemiionization of the ground state atom at the expense of the atom's excitation energy (inelastic process), an exchange of electrons was shown to be possible without a great depolarization (s.c. spin exchange, or elastic process) [1].

Up to the present there were only two experimental works where the spin-exchange and chemiionization cross sections were measured. The experiment have been done for $He^* - Cs$ and $He^* - Rb$ systems [1,2]. In order to determine interesting us cross sections we have to separate two simultaneously occurring spin-dependent processes. In the experiment on optical polarization of the helium metastable atoms these atoms may be aligned or oriented along a static magnetic field. It can be shown that the rates of distruction of the orientation $< S_{He} >_z$and alignment $< Q_{He} >_{zz}$ of metastable atoms depend on chemiionization and spin-exchange processes as follows:

$$1/\tau_{or} = \pi\delta f_{or} = N(1/3C_{ci} + 1/2C_{se}), \tag{1}$$

$$1/\tau_{al} = \pi\delta f_{al} = N(1/3C_{ci} + 3/2C_{se}), \tag{2}$$

here N is the alkali metal atom concentration, C_{ci} and C_{se} are the chemiionization and spin-exchange rate constants, δf_{or} and δf_{al} are the widths of the orientation and alignment signals,$1/\tau_i$ is the rate of the decay of the metastable atom's orientation or alignment. As one can see from Eqs., the contribution to the width of the magnetic resonance line for aligned helium atoms should be different from that of oriented atoms. This difference makes it possible to determine the rate constants of the two simultaneously occurring processes.

In this work the experiment on optical orientation of atoms has been done for He*-Na system. It was established that the rate constant for spin exchange (C_{se}) in collision of metastable 2^3S_1 helium atom with a Na atom in $3^2S_{1/2}$ ground state equals $(23 \pm 11)10^{-10} cm^3 s^{-1}$. The rate constant for chemiionization of rubidium atoms by metastable helium atoms (C_{ci}) was determined at the same time to be $(29 \pm 14)10^{-10} cm^3 s^{-1}$.

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Chemiionization and spin exchange in collisions of triplet metastable atoms in a mixture of helium isotopes

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It is known that, in a collision of two triplet metastable atoms of helium a quasimolecule, He_2^* is formed that breaks down via the reaction:

$$He^*(2^3S_1) + He^*(2^3S_1) \to He_2^* \to ions \tag{1}$$

The quasi-molecule formed in the collision can be in one of three states with a total spin S = 0, 1, and 2. These spin values correspond to three molecular states $^1\Sigma^+$, $^3\Sigma^+$ and $^5\Sigma^+$, which can be described by the singlet (V_s), triplet (V_t), and quintet (V_q) molecular terms. On conservation of the total spin of a system, ionization is only possible from the states of low multiplicity, i.e., from the singlet (cross section σ_s) and triplet (cross section σ_t) states, since in this case, the total spin is the same at the exit and entrance of reaction. At the same time, in collision of triplet metastable atoms of helium with atoms possessing electronic paramagnetism, process (1) is accompanied by the spin-exchange process, i.e., the colliding atoms exchange valence electrons. Such processes accompanied by chemiionization, in particular, the interaction of triplet metastable atoms of helium with alkali-metal atoms in the ground state, were studied both theoretically and experimentally. Indeed, the following process occurs in the collision of two triplet metastable atoms of helium:

$$He^*(2^3S_1, m_1) + He^*(2^3S_1, m_2) \to He_2^* \to He^*(2^3S_1, m_1') + He^*(2^3S_1, m_2') \tag{2}$$

Spin-exchange process can be described by three cross sections. σ_1 is governed by interference of elastic scattering from the triplet and quintet terms, σ_2, from the singlet and quintet terms, and , σ_3 from all the three terms.In collision of different isotopes of helium (^3He and ^4He) or in collision of two ^3He atoms, all three cross sections present in can be observed. In the collision of two even helium isotopes (^4He and ^4He), only the spin-exchange cross section σ_2 can be observed in an experiment. In addition, the identity of colliding particles is important only at very low temperatures, and it can be taken into account by introducing a factor of $(-1)^l$ into formulas for the cross sections. Thus, we can introduce the cross section σ^{abs} and σ^{tr} which, characterize the decay of orientation and alignment of colliding particles as a result of chemiionization and spin exchange in the optical orientation experiment as follows:

$$\sigma_{or}^{tr} = 1/3\sigma_1^{tr} + 1/3\sigma_2^{tr} + 2/3\sigma_3^{tr} \tag{3}$$

$$\sigma_{or}^{abs} = 1/9\sigma_s^{abs} + 1/3\sigma_t^{abs} \tag{4}$$

$$\sigma_{al}^{tr} = \sigma_1^{tr} + \sigma_2^{tr} \tag{5}$$

Cross sections of spin exchange and chemiionization in collisions of two triplet metastable helium atoms have been calculated for different isotopes of helium. The data on the spin exchange cross sections for the systems studied are reported for the first time.

Spin-exchange frequency shift in the system triplet metastable helium atom-ground state lithium atom.

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It is well known that, apart from polarization transfer between colliding particles, spin-exchange collisions lead to a magnetic resonance frequency shift [1]. A frequency shift occurs during collisions between atomic particles, as well as during collisions of atomic particles with electrons. Magnetic resonance frequency shifts associated with spin exchange produce an appreciable negative effect (in particular, in operation of quantum electronics devices based on the optical orientation of atoms). If a spin-exchange process is accompanied by an inelastic process, the magnetic resonance frequency shift noticeably changes [2]. Following [2], we write the expression for the cross section of the frequency shift in the spin-exchange process in the form

$$\sigma_{sh} = \pi/k^2 \sum_{l=0}^{\infty}(2l+1)\exp(-2\lambda_l^d)\sin 2(\chi_l^d - \eta_l^q) \tag{1}$$

This expression differs significantly from the expression for the frequency shift in the case of a "pure" spin exchange. In our case, expression (1) contains the factor $\exp(-2\lambda_l^d)$ associated with the ionization process. Here, $\eta_l^d = \chi_l^d + i\lambda_l^d$ is the scattering phase in the doublet term and is the scattering phase in the quartet term. The presence of the imaginary part in indicates that the doublet term may contain ionization (i.e., a decrease in the number of particles) apart from scattering. It can be seen from formula (1) that with increasing ionization probability (i.e., for $\lambda_l^d \to 0$), the magnetic resonance frequency shift tends to zero. Thus, taking into account expression (1) for the cross section of the shift, the magnetic resonance frequency shift can be written in the form

$$\delta\omega_i = 2/3N_i < S_i >^z \pi/k^2 \sum_{l=0}^{\infty}(2l+1)\exp(-2\lambda_l^d)\sin 2(\chi_l^d - \eta_l^q) \tag{2}$$

As a result of the spin-exchange and chemiionization processes in the system formed by a metastable helium atom and a lithium atom in the ground state, not only polarization is transferred between the partners, but a magnetic resonance frequency shift is observed due to the spin-exchange process. It was established that the cross section is a negative value. A negative value of the cross section indicates that the magnetic resonance frequency is shifted towards lower values (relative to the exact value). With increasing temperature in the absorption chamber, the resonance frequency is shifted toward higher values (relative to the exact value). Using the values of cross sections obtained here, we can estimate the magnetic resonance frequency shifts due to spin exchange accompanied by chemiionization both for metastable helium atoms and for lithium atoms in the ground state.

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Shape resonances for electron scattering on N_2 and CO_2 in modified effective range theory

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$^2\Pi$ temporary negative ion states in N_2 and CO_2 at 2.1 eV and 3.8 eV [1] respectively, are the best known examples of so-called shape resonances, in which the incoming electron is captured into the potential well of the target, rather than to a specific electronic orbital. In the previous work [2] the modified effective-range theory using analytical solutions of the Schrödinger equation with the polarization potential has been applied to positron scattering on Ar and N_2 up to 2 eV energy. In this work [3] we apply a similar procedure for electron scattering on N_2 and CO_2. The modified effective range analysis have been performed explicitely for the two lowest partial waves, using experimental integral elastic cross sections in the $0.1 - 1.0$ eV energy range. The parameters (i.e. the scattering length and the efective range for the two partial waves) of the scattering potential obtained are used again for the scattering problem at higher energies. Both for N_2 and CO_2 resonant maxima appear in the few eV energy range, sligthly higher than well known experimentally resonances in total cross sections. Agreement with the experiment can be improved by assuming the position of the resonance in a given partial wave. These observations allow to classify the structures in N_2 and CO_2 cross sections as pure shape resonances, i.e. occuring due to a particular shape of the scattering potential rather than to presence of virtual orbitals in the electronic structure of the target.

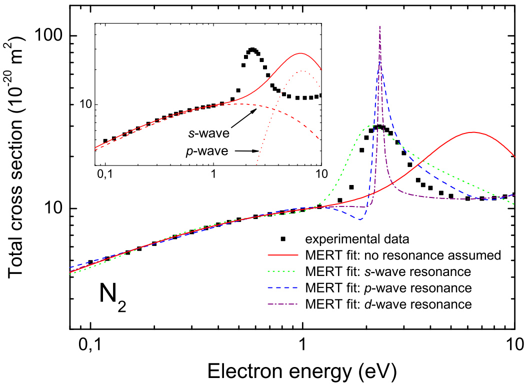

Figure 1: Total cross-section for the scattering of electrons on N_2 versus the energy. Depicted are: recommended experimental data from review [4] (stars), the theoretical fits based on MERT, assuming the resonance at 2.1eV in s wave (dotted line), p wave (dashed line), and d wave (dot-dashed line), and without assumption with respect to the position of the resonance (solid line). The inset shows in addition the s-wave and p-wave contributions to the MERT fit not assuming the position of resonance.

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Optical diagnostics on WEGA stellarator using Ar and Xe C-R models

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Non-intrusive emission spectroscopy diagnostics has been used to obtain local electronic temperature T_e and density n_e of the WEGA stellarator plasmas when fed with Ar or Xe. The WEGA stellarator is operated at IPP Greifswald and is mainly used for basic research in plasma-physics, educational training and for testing of new diagnostic equipment. For the evaluation of the experimental results Collisional-Radiative (C-R) models [1] for the Ar/Xe plasmas have been used, taking into account all the present species, both neutral and ionized, together with their excited states (including their structure and the involved transition probabilities) and also the rates of the contributing processes. Such models, valid for T_e going from a fraction of the eV up to several eV were developed previously and used in diagnosing and modeling of Ar and Xe plasmas in various devices [2]. The higher limit copes with situations where the available energy suffices to remove the totality of the six outer $3p$ electrons of the Ar or of the Xe atom. Spectra of neutral and lowly ionized Ar and Xe species have been previously registered in various WEGA discharges [3]. Notably, ions which cannot be simultaneously present in an homogeneous plasma with a sole Te have been observed. In the case of the WEGA separatrix and/or limiter plasmas a "temperature mixing" altering the total radiated energy may explain the simultaneous detection of signatures of all of the ionized species on the top of the neutrals. Typical Ar and Xe I-IV spectral lines have been identified. The main features of the relevant spectra will be shown and commented at the conference. In order to investigate the real presence and percentage of each ionized species and judge about the form of T_e in connection with deviations from the pure Maxwellian distribution, a detailed comparison with the theoretical spectra coming from the C-R models has been made. The present results contribute to develop a modeling taking into account the atomic properties as described by the C-R models and the traveling of the species through a model based in existing codes [4].

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Atomic parity nonconservation in heavy atoms and observing P and PT violation using NMR shift in a laser beam

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During the past decade, the optical experiments to detect atomic parity nonconservation (PNC) have progressed to the point where PNC amplitudes can be measured with accuracy on the level of a few percents in certain heavy atoms [1]. Nowdays the PNC in atoms has a potential to probe a new physics beyond the standard model. Promising idea (Forston) is to apply the techniques of laser cooling and ion trapping to measurement of the PNC in $6s^2S_{1/2}$-$5d^2D_{3/2}$ transition of the Ba^+. In our paper we systematically apply the QED many-body perturbation theory [2] to precise studying PNC effect in heavy atoms with account for nuclear, QED corrections. We present the calculation results for energy levels, hyperfine structure in-tervals, $E1-$,$M1-$transitions amplitudes in heavy atoms of ^{133}Cs, $^{137}Ba^+$, ^{119}Sn. As example, let us present below the calculation result for the parity non-conserving $6s-7p$ dipole amplitude in Cs. Our calculation gives the value: $D=< 6s|Dz|7s >=-0.903i|e|a(-Q_w/N)$. The received data are compared with known earlier and recent results by Dzuba etal (Novosibirsk), by Bouchiat etal (Paris), by Johnson et al (Indiana), by Johnson-Sapirstein-Blundell (Notre Dame). We discuss a new improved possibility for observing P and PT violation using a nuclear magnetic resonance (NMR) frequency shift in a laser beam (c.f.paper by Sushkov [1]). This shift is provided by a correlation of a nuclear spin with the momentum of photon (Ik).

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New optimal laser photoionization schemes for separating and sensing isotopes and nuclear reactions products

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Laser photo-ionization (LPI) method is one of the most perspective methods for sensing and separating isotopes, isomers, nuclear reactions products etc [1]. The proposed optimal LPI scheme is based on laser excitation of atoms into excited Rydberg states and further autoionization or collisional ionization. To carry out computer modelling the optimal LPI scheme parameters we used the operator perturbation theory [2], the Focker-Plank stochastic equation method and density matrices formalism [1,3]. We studied laser separating and sensing Na, U, Cs (Cf) isotopes. In experiments by Letokhov (Russia) and Moor (USA) two dye-lasers are used for Na separation. The 1-st laser provided a saturation of the resonant Na transition: $3s^2S_{1/2} - 3p^2P_{1/2}$. The wavelength of 2-nd laser is tuned in region of 4210-4490A. The excitation cross section for Na isotope at first step of the scheme is σ=10^{-12} cm^2; the ionization σ from excited $3p$ state 10^{-17} cm^2, from ground state 10^{-19} cm^2. Obviously, the relation of these σ is 10^5, 10^7. This provides the known non-efficiency of the standard scheme. Using above indicated mechanisms (+ ionization by electric field) on the last stage is more effective from energetic point of view. Our estimate shows that the stochastic ionization σ=$4,8 \cdot 10^{-14}$ cm^2. The similar data are obtained for U isotopes. The LPI scheme includes the steps: i). Excitation of the ^{235}U isotopes from the ground $5f^3 6d7s^2 -^5 L_6^0$ state and low lying metastable $5f^3 6d7s^2 -^5 K_5^0$ state with energy 620.32 cm^{-1}; ii). Transition to Rydberg state and then autoionization (laser field) or collision ionization. A scheme for sensing the nuclear reaction products is considered on example of the fusion ^{252}Cf isotope on the unsymmetrical coils (Cs etc). LPI sensing the Cs isotopes is based on resonant excitation of Cs ($6s^2S_{1/2}2 - 7p^2P_{3/2}$, 4555A and $6s^2S_{1/2} - 7p^2P_{1/2}$, 4593A) and further autoionization (laser or electric field). Sensing nuclear reaction products results in detecting Cs atoms as spontaneous nuclear fusion coils.

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Novel nanosensors for environmental and medical sensing using ultra-sensitive mass, chemical and biological detection methods based on carbon nanostructures

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Nanotechnology has emerged as one of the most active facets of scientific research and technology development. In our talk we will discuss two areas were the fundamental research could be used for environmental and medical applications.

Developing field-capable sensors that can be used to characterize and assist in the remediation of environmentally polluted sites is vital. To properly understand, monitor and characterize the impact of nanotechnology on the environment, ultra-sensitive sensors that outperform the current state-of-the-art are required. For instance, to monitor the effect of nanoparticles, sensors that are capable of detecting miniscule amount of nanoparticles will be necessary. To this end, we intend to fabricate and develop ultra-sensitive sensors based on suspended carbon nanotubes and graphene. These devices have a resonant frequency that depends on the total mass of the suspended part; thus the adsorption of molecules can be detected through shifts in the resonant frequency. Since both carbon nanotubes and graphene are extremely light-weight, they can be exceedingly sensitive, e.g. suspended nanotubes have been demonstrated to detect the arrival of single atoms [1, 2]. In our recent work [1], we used individual single-walled carbon nanotube resonators to detect and weigh adsorbed atoms. Our work also constitutes the first demonstration of using nanotubes' single-electron transistor properties to self-detect the nanotube vibrations, which yields greatly enhanced displacement sensitivity. We expect to develop mass sensors and optimize and characterize their performance.

In the second part of our talk we will discuss using biosensors based on carbon nanotube and graphene devices for the early detection of melanoma and other cancers.

Melanoma (the 5th and 6th most common cancer in Caucasian males and females, respectively), is the most severe form of skin cancer, which is often fatal if recognized in its advanced stage. Clinically, it is very difficult to correctly differentiate nevi with atypical features or dysplastic nevi, and nevi of special sites from melanoma. Clearly, new, more powerful, less invasive, time consuming and expensive tools are needed for an early and accurate detection of melanoma. In order to address this need, we will discuss a development of a new set of tools, namely, carbon-nanotube and graphene based biosensors for the early and accurate detection of melanoma. Once successful, we will modify and apply this new technology to early and accurately detect other types of cancer.

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Coincidence investigation of e-He inelastic scattering

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Electron-photon coincidence technique has been for many years successfully employed in studies of inelastic electron-atom collisions and on many occasions allowed for quantum-mechanically complete experimental determination of excitation amplitudes [1]. Electron impact excitation of 2^1P_1 state of He has been the first collisional process investigated using the method (1973) [2]. Since then, similar studies have been carried out for other collisional systems and stimulated a progress in both theoretical and experimental studies of electronic collisions [1].

Feasibility of application of magnetic angle changer (MAC) [3, 4] in coincidence experiment has been demonstrated recently [5], which extended range of experimentally accessible scattering angles up to 180°. The first coincidence experiment in full range of scattering angles has been performed for electron impact excitation of 2^1P_1 state of He atoms by 100 eV electrons [6] using angular correlations technique with application of MAC. The experiment is being continued for lower impact energies (80 eV). The experimental data for the electron impact energies of 100 and 80 eV will be presented and discussed.

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Coincidence investigations of zinc 4^1P_1 excitation by electron impact – feasibility study

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The atoms with two valence electrons outside a relatively inert core i.e. alkaline earths elements and associated group of atoms like Zn, Ca, Cd and Hg are still a challenge for both theoretical and experimental investigations of electronic collisions [1]. Electron – photon coincidence experiments are well known for providing more detailed information about atomic scattering than any earlier technique and have stimulated studies of increasingly complex collision systems.

The photon polarization analysis version of the method has been applied to study electron impact excitation of zinc atoms. The geometry of the experiment is typical for a coherence analysis technique with electron beam cross-fired with a beam of Zn atoms propagating inside a vacuum chamber. 213.8 nm photons resulting from the a radiative decay of the 4^1P_1 state excited by electron impact are detected in a direction perpendicular to the scattering plane and analysed (in coincidence with scattered electrons) for either linear or circular polarisation.

The present work is a continuation of our previous coincidence studies of electron scattering on Ca, Cd and He atoms [2,3,4]. We present first complete experimental results for the electron impact excitation of the 4^1P_1 state of Zn obtained for the incident electron energy of 100 eV.

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Electron ionization of Dimethylphenylsilane – appearance energies of selected ionic fragments

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Several studies, including electron ionization techniques have been performed to describe electron induced chemistry of Dimethylphenylsilane [1]. The techniques used didn't determined the appearance energies of particular ions. In present study, quadrupole mass spectrometer equipped with trochoidal electron monochromator (more details in [2]) was used to solve this particular task.

The study is continuation of our collaboration with UT Brno [3], where PECVD (Plasma Enhanced Chemical Vapour Deposition) of organosilicone films is systematically studied. Detail knowledge of electron ionization process in gas phase is fundamental for understanding and further development of this plasma chemistry application.

In mass spectra measured at 70 eV more than 40 cations have been observed. Surprisingly only five of them shows significant intensities (more than 5%) m/z=121, m/z=105, m/z=58, m/z=53 and m/z=43. These were chosen for further measurements of electron energy dependent ion yields. Additionally cations formerly studied in computational experiment of Cho[1c] were measured. Appearance energies (AE) were than acquired from near threshold measurements of energy dependent ion yields for particular reaction channels and are summarized in Tab 1.

Table 1: Appearance energies of selected ions

m/z	expected ion	AE(eV)	ΔE(eV)	ΔE(eV) Ref.[1c]
136	$DMPS^+$ $[C_8H_{12}Si^+]$	**9.04±0.06** 8.92±0.15[1b] 8.72±0.2[1a]	0	-
135	$(DMPS\text{-}H)^+$ $[C_8H_{11}Si^+]$	**10.42±0.09** 10.43±0.04[1b]	**1.38**	1.17
121	$(DMPS\text{-}CH_3)^+$ $[C_7H_9Si^+]$	**10.52±0.13**	**1.48** 1.34[1a]	1.16
106	$C_6H_6Si^+$	**9.6±0.2**	**0.56**	-
105	$C_6H_5Si^+$	**13.47±0.02**	**4.43**	-
78	$C_6H_5{}^+$	**10.7±0.2**	**1.66**	2.43
58	$(DMPS\text{-}C_6H_6)$ $[C_2H_6Si^+]$	**10.26±0.14**	**1.22**	1.11
53	$C_6H_6Si^{2+}$	**19.5±0.2**	**10.46**	-
43	CH_3Si^+	**13.9±0.2**	**4.86**	-

$\Delta E_{ion} = AE_{ion} - IE$, data from ref.[1c] converted 1kJ/mol=0.0103642eV

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Angular distribution of fluorescence from sub-valence shell ionized alkaline atoms by electron impact

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The interaction of atoms with collimated beam of charged particles introduces a large degree of anisotropy in atomic system. The electron-impact ionization of inner-shell electrons produces fluorescence radiation. Its characteristic feather is non-uniform angular distribution and high degree of polarization. The general expression for the cross section of fluorescence radiation induced by ionization of polarized atoms by polarized electrons is derived by applying method [1] alternative to density matrix formalism. Plane wave Born (PWB) and two-step approximations are used. Some special cases suitable for specific experimental conditions are studied as more simple cases of the general expression. The asymmetry parameter of the angular distribution (β) and degree of linear polarization (P) of fluorescence radiation are calculated in the case of sub-valence np-electron ionization from Na, K, Rb and W^{37+} atoms (see Table 1).

Table 1: The asymmetry parameter of the angular distribution (β) and degree of linear polarization (P) for sub-valence np-electron ionization from Na, K, Rb and W^{37+} atoms for selected electron impact energies E (in eV)

	Na		K		Rb		W^{37+}		
E	β	P	β	P	β	P	E	β	P
42	−0.08	0.11	−0.12	0.18	−0.20	0.28	2000	0.01	−0.02
50	−0.16	0.23	−0.14	0.21	−0.23	0.30	2500	−0.03	0.01
100	−0.34	0.44	−0.24	0.32	−0.31	0.40	3000	−0.01	0.20
150	−0.44	0.54	−0.33	0.43	−0.38	0.48	5000	−0.17	0.43

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Investigation of lowest autoionizing states of Cs

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For the identification of recently measured ejected-electron excitation function for the $5p^5 n_1 l_1 n_2 l_2$ LSJ autoionizing levels [1] of Cs atoms exited by electron impact, the calculations of the energy levels, excitation cross sections, autoionization probabilities as well as probabilities of the radiative transitions to the ground and among autoionizing states were made. In the case of Cs, the relativistic effects play more important role in comparison to the lighter atoms Na and K. Therefore, quasi-relativistic (Cowan) [2] and multiconfiguration Dirack-Fock (FAC) [3] computer codes were used. The structure of energy spectrum reveals the overlap of the lines arising from $5p^5 6s^2$, $5p^5 5d6s$, 5p56s6p and $5p^5 6s7s$ configurations. The lowest energy levels calculated by using configuration interaction (CI) approximation are presented in Table 1.

Table 1: Energy levels (in eV) of the lowest states $5p^5 6s^2 LSJ$ and $5p^5 5d(L_1 S_1)6sLSJ$ for Cs with respect to the ground state.

LSJ	FAC	Cowan	Exp [1]	LSJ	FAC	Cowan	Exp [1]
$6s^2\ ^2P_{3/2}$	12.24	12.23	12.31	$(^3P)\ ^4P_{5/2}$	13.09	12.94	13.20
$(^3P)^4P_{1/2}$	12.75	12.54	12.78	$(^3F)^4F_{7/2}$	13.11	13.06	
$(^3P)^4P_{3/2}$	12.91	12.68	12.93	$(^3P)^4S_{3/2}$	13.15	12.99	13.34
$(^3F)^4F_{9/2}$	13.08	12.94		$6s^2\ ^2P_{1/2}$	14.10	14.04	14.07

Acknowledgment

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Investigation of the hyperfine structure of Scandium atom

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Description of atomic structure with the use of semi-empirical methods proved to be very successful in cases of many elements. However the quality of such analysis strongly depends on the number of experimental data.

The experimental knowledge of scandium atom's hyperfine structure of the levels is very scarce. Although first observations of the spectrum of scandium were performed by Popow [1] in 1914 and by Catalan [2] in 1923, hyperfine splitting constants only for several tenths of levels were hitherto measured.

In the work of Dembczyński *et al.* [3] an extensive semi-empirical analysis of the electron structure of scandium atom was performed.

Measurements of the hyperfine structure of the levels of scandium atoms were performed by means of laser-induced fluorescence in a hollow cathode discharge. The experimental setup was described in detail in [4].

In several cases of relatively strong absorption transitions saturation effect was observed and a Doppler-free saturation spectroscopy could be applied to record the hyperfine structure spectra.

New experimental results were included in a renewed parametric fit. Preliminary results suggest the improvement of the fit quality [5].

Acknowledgment

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Injection locking of a single ion regenerative oscillator

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Injection locking (or entrainment) of oscillators has important and widespread technological applications. We present a study of injection locking in a particulary clean and well controlled representation of an oscillator, a regeneratively oscillating single trapped ion. In a first step we optically excite a regenerative oscillation of a $^{24}Mg^{+}$ ion [1] using both a blue and a red detuned laser beam. By controlling the detunings and intensities of the beams we can vary the oscillation amplitude and quality factor of this oscillator. In a second step we inject a RF signal using an auxillary electrode and phase-sensitively detect fluorescence photons by gating our single photon camera accordingly. The phase sensitive images allow to directly measure the average phase-lag of the ion relative to the injected signal. We studied the locking range and relative phases for a variety of parameters and find excellent agreement with the Adler [2] equations that describes injection locking, both inside and outside the locking range.

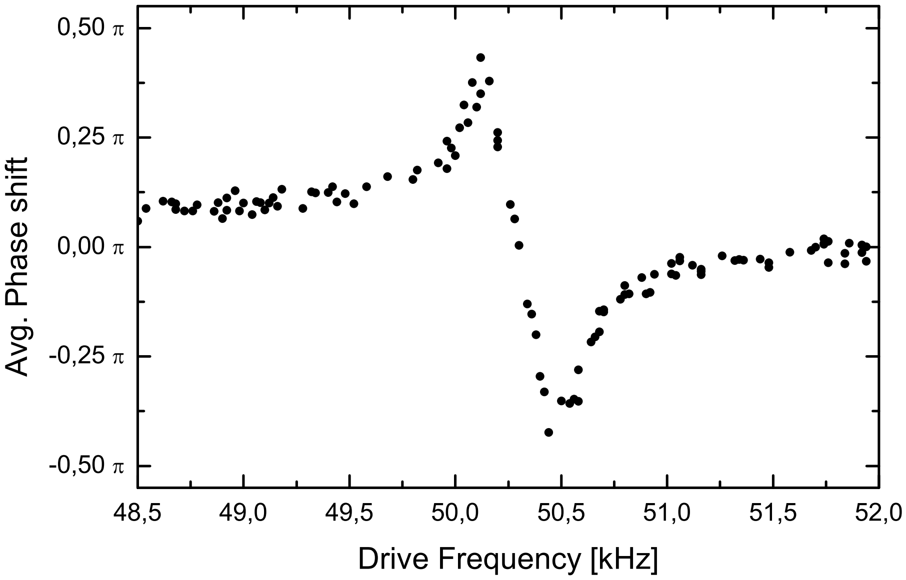

Figure 1: Average phase of a regenerative oscillating ion vs the injected frequency. Note the locking range enclosed by the two extrema.

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Towards a Raman quantum memory with Bose-Einstein condensates

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Bose Einstein Condensation allows preparing cold and dense atomic samples, providing conditions very favorable to strong coupling between light and matter. The high optical depth and an medium favorable to the decoupling between internal and external variables gives hope for implementing new quantum memory protocols in the near future [1].

Quantum memories with atomic ensembles are based on a collective atomic spin state and a light state, both showing a strong component along one direction and weak quantum fields along the others. The interaction is then engineered such as the quantum quadratures of light are mapped into long-lived atomic states. The Faraday type memory, already demonstrated for hot atoms [2], maps one light quadrature directly, while the second one needs to be transferred by a measurement and a feedback sequence. But ultracold atoms constitute an environment suitable for a pure Raman interaction scheme, which allows mapping both quadratures directly.

We are implementing a Raman type protocol, based on the two ^{87}Rb ground states (F=1, m_f=-1) (F=1, m_f=+1), and red-detuned from the D1 line. The elongated shape of the condensate (Fresnel number close to 1.4), together with a number of atoms close to 10^6, provides an on resonance optical depth of several thousands along the long axis (in trap), enabling thus a strong coupling regime. We will first report on experiments we performed ([3]) in order to check the effectiveness of the decoupling between variables (superradiance scattering ([4])) in our condensates. This scattering regime corresponds to the limit where macroscopic momentum is transferred to a part of the BEC, we investigated it as a harmful process, competing with a functional memory. We will also present the successful loading of our BECs in a far red-detuned dipole trap, necessary to create a trapping potential that is ground state insensitive. We will finally report on preliminary Faraday rotation measurements with BECs in the dipole trap.

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Ion beam purification by selective photodetachment in a gas filled ion guide

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There is a need for pure negative ion beams both in fundamental studies of negative ions and in their applications in for example tandem accelerators. Beams containing unwanted isobars or excited ions can result in interfering signals or disturbing backgrounds. As proposed by Berkovits *et al.*[1] it is possible to use photodetachment to remove a component of an ion beam that have a smaller binding energy than the desired component.

We have used selective photodetachment in combination with an ion beam cooler developed by Liu *et al.*[2,3] to investigate ion beam purification. The cooler is a gas filled radio frequency quadrupole ion guide that was used to contain an ion beam with energies of less than 50 eV. The radiation from a 1064 nm Nd:YAG laser was overlapped with the slow moving ion beam, and in this way long interaction times were achieved. To measure the effect of the depleting laser, a pulsed laser (1064 nm) was used to probe the ion beam after the cooler. The number of detected neutrals originating from the probing photodetachment served as a measure of the remaining impurities in the ion beam.

Production of ground state negative ion beams was investigated for $C^-$and Si^-. The loosely bound excited state in $C^-$was detached almost completely by the collisions in the cooler. The ^2D state in Si^-, on the other hand, survived the collisions, and laser light was applied to investigate its depleting effect. The excited state population as a function of laser power followed an exponential behavior on top of a constant background. With a laser power of about 50 mW half of the population was removed and with 0.5 W a depletion of about 85 % was achieved. We draw the conclusion that the background was caused by repopulation of the excited states in the re-acceleration region after the ion guide.

A second experiment was performed with the same setup, investigating depletion of Co in a beam of Ni. The problem is interesting for the production of radioactive ^{56}Ni beams and have ben previously investigated [1,3]. The present experiment demonstrated a 99.995 % depletion of the Co beam while less than 20 % of the Ni beam was removed. The result was reached with 0.7 W laser power, although powers up to 3 W was used.

From the presented experiments we can draw the conclusion that photodetachment in a gas filled ion beam cooler can be a very effective tool to purify ion beams.

Photodetachment studies of systems interesting for mass spectrometry, where interfering isobars exist, are under way and will be discussed.

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Differential cross sections for electron impact vibrational excitation of nitrogen in the angular range 10^o-180^o

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Absolute differential cross sections (DCSs) for vibrational $v = 0 \rightarrow 1$ excitation of the $X^1\Sigma_g^+$ ground state of N_2 have been measured at electron incident energies between 5eV and 20eV and in the scattering angle range $10^o - 180^o$. At 20eV the $v = 0 \rightarrow 2$ DCS has also been determined. Measurements were performed with crossed electron-molecular-beam spectrometer [1] equipped with a magnetic angle-changer which has been used to access backward scattering up to 180^o. Absolute DCSs were derived from energy loss spectra recorded at fixed scattering angles. The ratios of vibrational to elastic intensities were obtained and normalised against our DCSs for elastic scattering [2].

Figure 1a presents DCSs for $v = 0 \rightarrow 1$ excitation at 20 eV. This energy is close to the centre (23 eV) of the $^2\Sigma_u^+$ shape negative-ion resonance which is the d-wave resonance with a contribution of the p-wave. The present results are compared with the more recent results of Tanaka *et al.* [3] and Middleton *et al.* [4]. The present cross section shows a minimum near 85^o which is reproduced well in the calculations of Gillan *et al.* [5] and Onda and Truhlar [6]. These results, however, greatly underestimate absolute values of the DCS. The present DCS for $v = 0 \rightarrow 2$ excitation at 20eV (figure 1b) shows very similar angular dependence to that of the $v = 0 \rightarrow 1$ excitation confirming its resonance character.

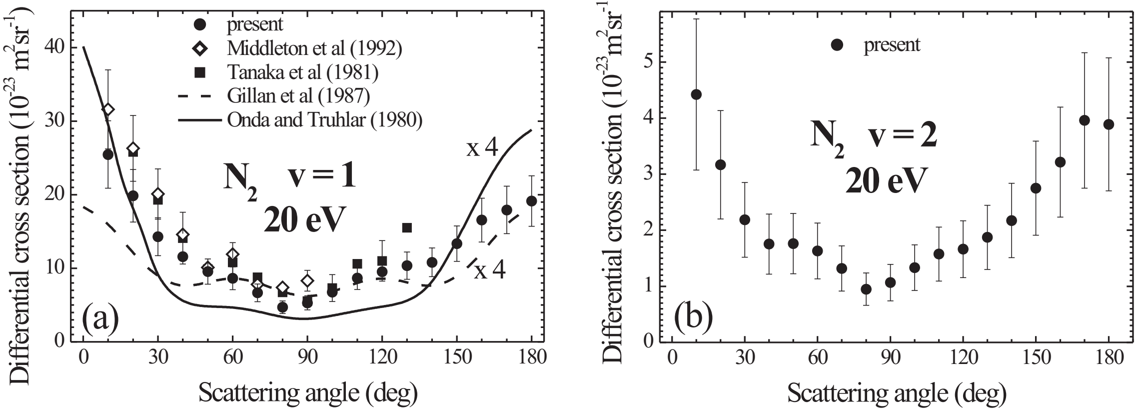

Figure 1: DCSs for excitation of the vibrational, (a) v = 1 and (b) v = 2 levels of molecular nitrogen at incident electron energy of 20eV.

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Nuclear quantum effects in Hydrogen storage materials

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We present the structural properties of Lithium Imide (Li_2NH) and Amide ($LiNH_2$), investigated by means of Path Integral Molecular Dynamics (PIMD [1, 2]). This kind of complex hydrates have higher gravimetric hydrogen density than conventional hydrogen storage materials, due to its composition from light atoms (a capacity of $11.5wt\%$ is reported [3]). These materials are, however, still not well understood [4]. Experiments suggest different H adsorption sites [5, 6], but they mostly cannot give a definitive answer to the storage mechanism. The potential energies for the protons is relatively flat which can lead to quantum delocalization, as Hydrogen can behave non-classically. Specifically for Li_2NH, the symmetry of the material and the proximity of several possible sites within a flat potential energy surface can lead to quantum delocalization of the protons over six octahedral equipotential sites around each Nitrogen. We aim at a deeper understanding of this phenomenon, by means of ab-initio PIMD simulations.

In this study all atoms in the material are treated as quantum particles, while in standard ab-initio calculations only electrons are treated to that accuracy. The results for different initial structures and levels of quantum description are compared. NMR spectra are calculated and compared with experimental solid state NMR results, showing good agreement. The results show that protons tend to be bond to Nitrogen atoms while showing a degree of delocalization (fig. 1).

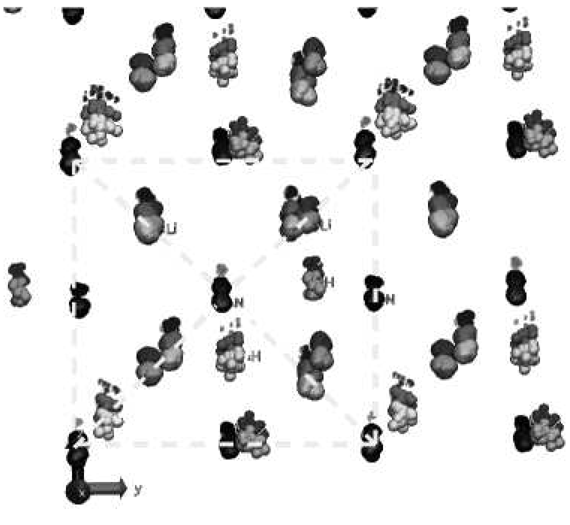

Figure 1: Structure of crystalline Li_2NH. Proton clouds (light gray) represent their quantum delocalization.

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Radiative lifetimes and transition probabilities in Hf I and Hf III

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Hafnium has been observed in the spectra of some stars, in particular in mild barium star HD 202109 (ζ Cyg), Sirius A and in the photosphere of δ Scuti (the prototype of the class of pulsating variables). Hf is also of astrophysical interest as a chronometer for stellar and galaxy evolution. This stimulated the present investigation of radiative lifetimes and transition probabilities in Hf I and Hf III.

In the present work radiative lifetimes of 9 odd excited levels in Hf III (5d6p $^3P_{0,1}$, $^1D_2$, $^3D_{1,2,3}$, $^3F_{2,3,4}$) and of 2 odd levels in Hf I (5d^{2}6s6p z $^3D_{2,3}$) are reported. They were measured using a time-resolved laser-induced fluorescence (TR-LIF) technique [1]. The investigated levels in Hf I were excited in a single-step process from the ground term (5d^{2}6s^2 a ^{3}F), whereas in Hf III, we started from the low-lying 5d6s ^{3}D and ground 5d^2 ^{3}F terms.

Free hafnium atoms and ions were generated by laser ablation in a vacuum chamber with 10^{-6}-10^{-5} mbar background pressure. For the ablation, an Nd:YAG laser with 10 ns pulse duration was used. The laser system for the excitation of the Hf I and Hf III levels consisted of a dye laser which had a pulse duration of about 1-2 ns.

For all of the investigated levels the lifetimes have been measured for the first time. The error bars are in the interval 10-25%. A multiconfigurational relativistic Hartree-Fock method (HFR) (as described by Cowan [2]), including core-polarization effects, has been used to compute radiative lifetimes and branching fractions of 15 Hf III levels, including those measured in this work. A first set of transition probabilities is also proposed for 55 transitions of Hf III. The results are compared with the experimental data.

Acknowledgment

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A coherent multi-mode light-matter interface based on a ion Coulomb crystal in an optical cavity

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Cavity Quantum Electrodynamics (CQED) is a powerful platform for the realization of efficient light-matter quantum interfaces at the single photon level. Laser-cooled, trapped ions offer many attractive features for CQED, namely long coherence and trapping times, low densities and excellent localization. Using a linear rf-Paul trap incorporating a high-finesse optical cavity along its rf-free axis [1] we have realized such an interface with an ensemble of cold ions, cooled to a self-organized Coulomb crystal structure. This has previously allowed us to observe for the first time collective strong coupling between cold ions and a cavity field at the single photon level [2].

Our recent results explore further the coherent coupling of ion Coulomb crystals to various transverse modes of the cavity field. These results take advantage of some of the attractive features of ion Coulomb crystals mentioned above. First, the high degree of spatial localization of the ions makes it possible to use a thin needle shaped Coulomb crystal for precise reconstruction of the spatial profile of different transverse cavity modes by measuring the ion-light coherent coupling. Second, the stationarity and uniform density of large crystals ensures that identical coupling strengths are achieved with different transverse modes. These results, combined with the long coherence times of ion Coulomb crystals[2], are promising for high efficiency generation and storage of single photons into different transverse modes.

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Electron collisions with cyclopropane

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Electron interactions with alkyl groups are important for a number of applications. The cross sections of the prototype compounds, the alkanes, do not show pronounced resonant structure, however, only extremely broad humps covering the 2-15 eV region [1]. This is somewhat surprising, alkanes have many empty orbitals, which could give rise to shape resonances.

In cyclopropane, however, the high symmetry has the consequence that one virtual orbital couples only to f-wave and not to lower l waves, thus retarding the 'leaking out' of the electron through the centrifugal barrier in the corresponding a'_2 shape resonance at 5.5 eV [1]. As a consequence, this resonance is exceptionally narrow for a shape resonance in a saturated hydrocarbon (Fig. 1), an effect which could be called 'symmetry-induced narrowing'. The present work characterizes this resonance and generally electron collisions with cyclopropane by measuring the absolute differential cross sections for elastic scattering and for vibrational excitation. Since the resonance is, in chemical terms, due to a temporary capture of the incoming electron in a C-C antibonding σ^* orbital, it excites primarily the symmetric ring breathing vibration ν_3. A representative cross section, drawn as a function of energy and of scattering angle, is shown in Fig. 1. The calculation of Čurík and Gianturco [2] are in good agreement with the present measurement.

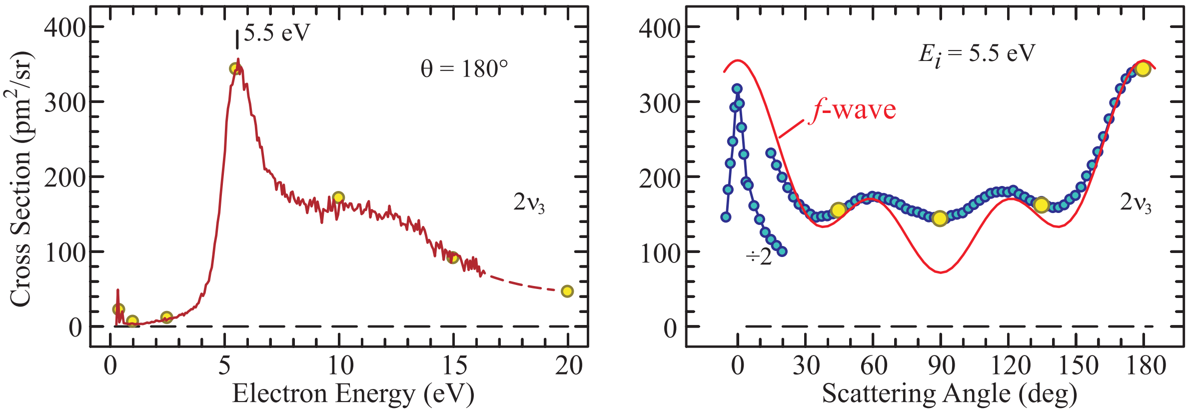

Figure 1: Cross section for exciting the first overtone of the ν_3 symmetric ring breathing vibration, shown as a function of the incident electron energy (left) and of scattering angle at the 5.5 eV resonance (right).

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Electron collisions with $Pt(PF_3)_4$

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The interest in electron interactions with $Pt(PF_3)_4$ stems from its use as a platinum precursor in Focused Electron Beam Induced Processing (FEBIP) [1]. It is a volatile platinum compound with a molar mass of 547 amu! For FEBIP it has the advantage of not causing carbon deposits. It is a tetrahedral d_{10} complex.

Representative vibrational energy-loss spectrum, recorded with about 10 meV resolution at an incident energy of 0.7 eV is shown in Fig. 1, with an assignment based on the vibrational frequencies from Ref. [2]. Cross sections were measured for elastic scattering and for vibrational and electronic excitation, both as a function of electron energy and as a function of scattering angle. The elastic cross sections have deep Ramsauer-Townsend minima and their angular distributions have interesting minima around 40° which drop to lower scattering angles with increasing energy. The cross sections for vibrational excitation, reveal five resonances, probably shape resonances.

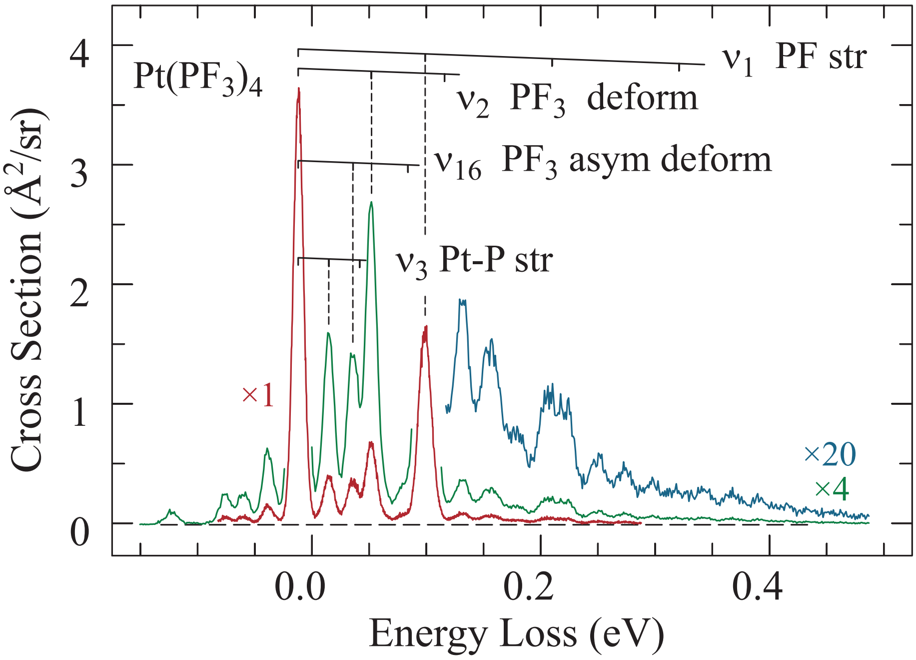

Figure 1: Electron energy-loss spectrum of $Pt(PF_3)_4$, recorded with an incident electron energy of 0.7 eV at a scattering angle of 45°.

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Isotope effect in dissociative electron attachment cross sections in acetylene

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We present absolute partial cross sections for dissociative electron attachment to C_2H_2 and C_2D_2 which have been measured using a new time-of flight ion spectrometer combined with a trochoidal electron monochromator. For C_2H_2 the new data is in good agreement with the total cross sections measured previously in our laboratory [1] and elsewhere [2] using the total ion collection principle.

The present measurement on deuterated acetylene reveals a pronounced isotope effect at the first dissociative electron attachment band at 3 eV, with the cross section for C_2D^-/C_2D_2 being 14.7 times smaller than that for C_2H^-/C_2H_2. The dramatic magnitude of the effect is attributed to slower motion of the D atom as compared to H atom, combined with unfavorable competition of the dissociation with autodetachment. The recent calculations by Chourou and Orel are in good agreement with our experimental values for C_2H^-/C_2H_2 but underestimate values for C_2H_2/C_2D_2, their ratio $\sigma(C_2H^-)/\sigma(C_2D^-)$ being 28.9 [2].

A second band is observed at around 8 eV corresponding to the light fragments H^- or D^- which dominate above the C_2^- fragment, in contrary to previous assignment. These bands exibit much weaker isotope effects, in agreement with their assignment to Feshbach resonances with narrow autodetachment widths.

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Fragmentation of multiply charged clusters

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A multiply charged cluster is stable if its size is larger than the appearance size. Otherwise, the cluster fragments automatically. The stability and fragmentation of van der Waals clusters have been discussed within the framework of the liquid drop model (LDM) [1]. Recently, the author has studied the role of geometrical shell effect to the appearance size of multiply charged clusters [2,3]. Here we discuss influences of the shell effect on the decay of multiply charged clusters. The shell energy is estimated from the calculation of the energy of Lennard-Jones clusters [4,5]. Fig. 5 shows the energy barriers for fragmentation, $\mathrm{Kr}_{53}^{+} \rightarrow \mathrm{Kr}_{\mathrm{k}}^{+} + \mathrm{Kr}_{53-\mathrm{k}}^{+}$ as a function of k. By taking account of the shell effect, the predicted decay pattern changes completely. Although the LDM predicts that fragmentation is possible for all k for $10 < k < 43$, only $k = 13$ (a magic number) is the energetically accessible decay channel if we consider the shell effect. This fact indicates us the shell effect plays a significant role in the decay of multiply charged clusters.

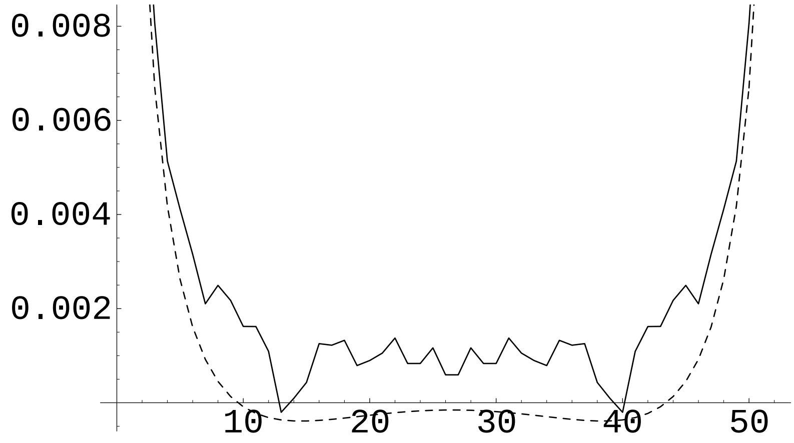

Figure 1: $\mathrm{Kr}_{53}^{+} \rightarrow \mathrm{Kr}_{\mathrm{k}}^{+} + \mathrm{Kr}_{53-\mathrm{k}}^{+}$. Solid line: calculation including shell effect; Dashed line: calculation with LDM

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Relativistic *ab initio* calculations of isotopes shifts

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When the effects of the finite mass of the nucleus and the spatial charge distribution are taken into account in an Hamiltonian describing an atomic system, the isotopes of an element will have different electronic energy levels. The first effect is called the *Mass Shift* (MS), the second the *Field Shift* (FS), both forming the *Isotope Shift* (IS). For systems with more than one electron, the *Specific Mass Shift* (SMS), that does not exist for hydrogenic systems, appears in the MS. Due to its low ponderation, the SMS parameter can be treated as a perturbation of the Hamiltonian and its estimation requires the calculation of Vinti integrals [1]. The computation of the SMS parameter in the full relativistic Dirac-Fock scheme, is possible in GRASP2K [2]. In the same relativistic framework, the *Multi Configuration Dirac Fock and General Matrix Element* (MCDF-GME) code [3], is often used by the atomic physics community but the current version of this code does not allow the calculation of SMS. GRASP2K and MCDF-GME use the Fano-Racah tensor algebra and the Slater determinant algebra, for performing the angular integration of the operators, respectively, with its own advantages and disadvantages. Recently, wishes of sharing expertise on both sides have been expressed and even materialized through some interesting common work (see for example [4]). In this line, we built the computer code interface dedicated to the estimation of the SMS from multiconfiguration MCDF-GME wave functions.

We report on our very first results in lithium-like atoms to illustrate and quantify the importance of relativistic effects when increasing the nuclear charge, by comparing systematically the non-relativistic Vinti integrals calculated with ATSP2K [5] and the relativistic ones estimated with our computational tool. This comparison is interesting enough at the non-relativistic one-configuration level of approximation. However, Hartree-Fock theory is not the end of the story for highly correlated systems and we will illustrate how the generalization of the interface with the MCDF-GME for correlated wave functions will be performed, taking advantage of the parallelism between the SMS and the Coulomb interaction operators.

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Metastability exchange optical pumping of ^{3}He gas at elevated pressure at 4.7 Tesla

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The results of metastability exchange optical pumping of ^{3}He gas in the 32-267mbar pressure range performed in the magnetic field of 4.7 Tesla are reported for the first time. Comparing to previous data, the present experiments extend the pressure range by factor of 4, and the magnetic field range by almost factor of 2.5, probing the large parameter space in serch for optimal operating conditions.The optical pumping efficiency as a function of magnetic field for two pressures: 32 and 64 mbars in the same operating conditions (pump laser power 0.5 W and weak discharge) is shown in Fig 1, where the data obtained before [1] and in the present work are compiled. After almost linear increase of the steady state nuclear polarization M with magnetic field up to 2 T, a plateau is reached and a limiting value of 0.62 and 0.6 for 32 and 64 mbar, respectively, is achieved.

The observed monotonic decrease of nuclear polarization with pressure is compensated by an increase of total magnetization, which to our knowleage is highest ever achieved by the method. This will put less demanding requirement for the final compresion stage, which is necessary in growing applications of highly polarized ^{3}He gas in magnetic resonance imaging of human lungs.

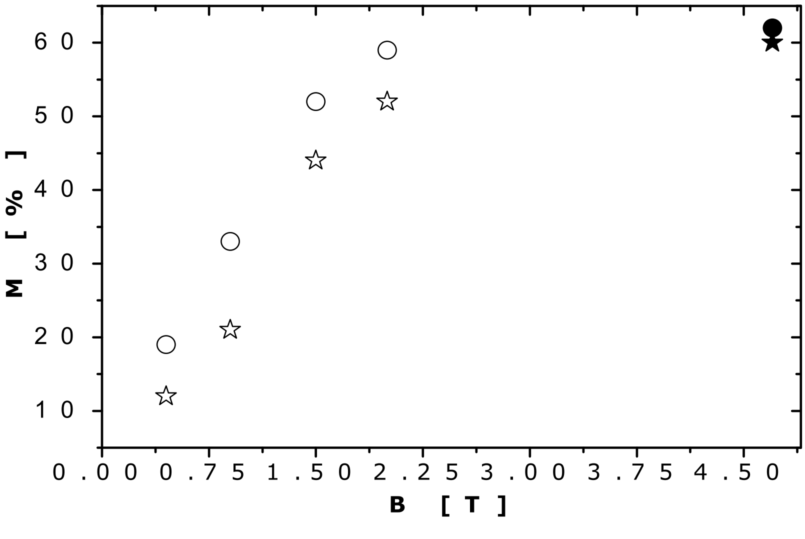

Figure 1: Steady-state polarization as a function of magnetic field B.

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Precision spectroscopy on a fast lithium ion beam for a time dilation test

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In Ives-Stilwell-type experiments, fast atomic ions containing a well-known transition are used as moving clocks, and time dilation as well as the velocity are derived from the simultaneous laser-spectroscopic measurements of the Doppler shifts with and against the direction of motion. In order to accurately measure these Doppler shifts, the Doppler broadening caused by the ions' velocity distribution needs to be overcome. We performed laser spectroscopy on $^7\mathrm{Li}^+$ ions in the $2\mathrm{s}^3\mathrm{S}_1$ metastable ground state at the GSI in Darmstadt. The ions were stored in the Experimental Storage Ring (ESR) at a velocity of $0.338c$, and optical-optical double resonance spectroscopy on a closed Λ-type three-level system was performed with two laser beams propagating parallel and antiparallel, respectively, to the ions. The used laser setup (shown in Fig. 1 left) allows for a frequency accuracy of $\Delta\nu/\nu < 10^{-9}$ by stabilizing the lasers to atomic and molecular references. Analyzing the emerging fluorescence signal (Fig. 1 right) and taking all statistic and systematic uncertainties into account, the current experiment sets an upper bound on hypothetical deviations from the predictions of special relativity of the order 7×10^{-8}, which is comparable to the so far leading experiment [1], but an improvement of this limit by an order of magnitude seems to be feasible in future measurements.

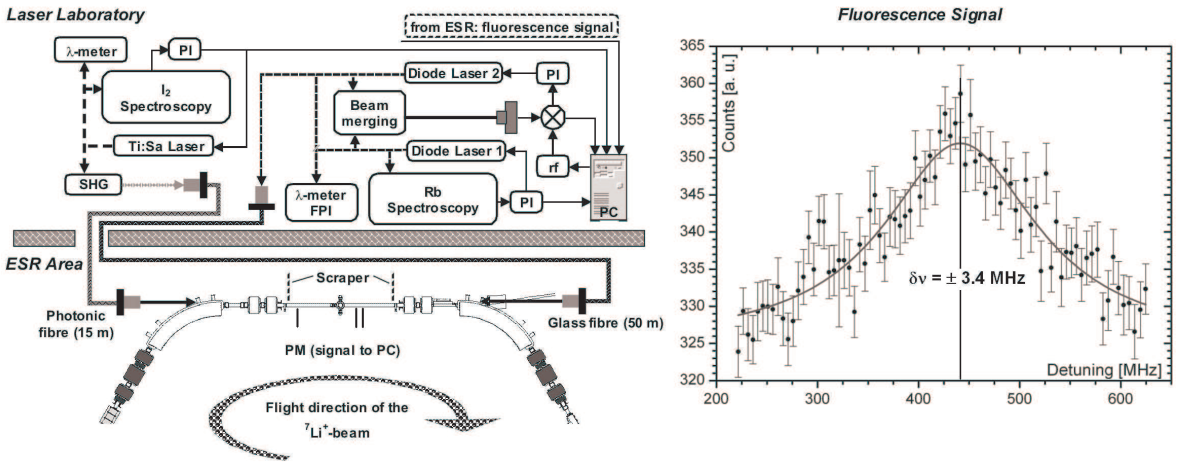

Figure 1: Left: Experimental setup (PI: proportional-integral controller, PM: photomultiplier, SHG: second harmonic generator, rf: radio-frequency source, FPI: Fabry-Perot interferometer). Right: Example signal from optical-optical Λ-type spectroscopy.

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Perturbed molecular lines of N_2^+ for plasma diagnostics

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Plasma diagnostics is an important tool for any plasma sources applications, both scientific as technical. In temperatures higher than 8̃000K the diagnostics can be performed by using intensities of the atomic lines, but in lower temperatures already the existence of temperature can be doubtful as the equilibrium between the energy subsets starts to break down. In such a plasma the temperature that can be still relatively safely assumed to exist is the one derived from Maxwell translational energy distribution for the heavy particles. Measuring this kind of energy distribution can be done by using the atomic lines' profiles, but this requires using either lasers, or very, very precise Fabry-Pèrot spectrometers. The other method of calculating this parameter is by using the Boltzmann plot of the rotationally resolved molecular lines, as the Boltzmann distribution of the rotational energy can be assumed to be in equilibrium with the translational energy distribution. Unfortunately, in many cases the rotational spectra are difficult to resolve, and the lines that overlap originate from very different energy levels, making the classical method of modeling the molecular spectra to fit the observed ones [1] very imprecise, as the molecular spectrum shape can change very slightly for higher temperatures.

One of the very widely used molecule is N_2^+, as this molecular ion can be found in most of the plasmas, even without nitrogen added explicitly, as it is an often found impurity. This spectrum, for example the 0-0 band of B→X transition around 390 nm, can be used with very good precision for temperatures from hundreds to about 3000 K, even unresolved, as the profile of this spectrum changes very strongly in this region. Unfortunately, for temperatures 4000K and higher the fit starts to exhibit big uncertainties, because the P and R branches of the spectrum begin to overlap, masking the temperature dependence. There is, nevertheless, one interesting point in the spectrum where they do not, because the rotational levels for the upper level are disturbed by high rotational sublevels of the A N_2^+ level [2]. Perturbation of the levels shifts the lines in this region enough so the P and R branches are not overlapping and the lines' intensities can be measured precisely, and used for determining the temperature.

Unfortunately, for determining the temperature, the transition probabilities of the observed lines have to be determined. Theory gives the transition probabilities (or at least their dependence on the rotational number) as the Hönl-London factors [3]:

$$S_J^R = \frac{(J''+1) - \frac{1}{4}}{J''+1} \quad S_J^Q = \frac{2J''+1}{4J''(J''+1)} \quad S_J^P = \frac{J''^2 - \frac{1}{4}}{J''} \tag{1}$$

which in case of the perturbed lines is not true. In this report the measured transition probabilities are given, and the dependence of line intensities on plasma parameters are presented and discussed.

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EIT in Rb admixture noble-gas

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Electromagnetically induced transparency (EIT) [1,2] has now been over the last decade subject of many studies, both theoretical and experimental but numerical modeling is still required to describe and analyse results of experiments carried out for complex systems significantly differing from a basic three-level lambda set of atomic levels.

We present results obtained with a model developed for analysis of EIT properties of a sample of hot rubidium atoms contained in a resonance cell filled with a buffer gas. The model has been elaborated specifically for D1 transitions induced in ^{87}Rb ($5^2S_{1//2}$, F=1,2 → $5^2P_{1//2}$, F'=1). It involves 11 hyperfine states and accounts for most of the effects and interactions that may influence EIT properties of the ensemble of Rb atoms.

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Resonances in electron scattering by molecules

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Scattering states properties of three-body resonantly interacting particles are considered and are shown to be independent of a form of two-body forces, being determined only presence of resonances. The resonances produce an effective long range interaction between three particles [1].

The methods of the quantum theory few-body scattering based on the Faddeev-Yakubovsky equations [1] in momentum and configuration space are present [2,3] and applied to the calculation of the dissociative electron attachment to hydrogen and hydrogen-halide diatomic initial rovibrational exiting molecules H_2, N_2, Li_2, Na_2, HCl, DCl, HBr, DBr, HJ, DJ.

The results of this calculations are compered with available experimental data [4] and other calculation [2-3].

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Vibrational exiting in collision electrons and atoms with molecules

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The transfer of vibrational energy has been the topic of active experimental and theoretical study for many years. Increasing technological progress has recently made possible the study of such processes on the microscopic, molecular level. It is becoming feasible to characterize the detailed rare constants from a given internal level of the reactants to a given internal level of the products [1].

The methods of the quantum theory few-body scattering based on the Faddeev-Yakubovsky equations [1] in momentum and configuration space are present [2,3] and applied to the calculation of vibrational exiting in collision electrons and atoms with molecules H_2, N_2, Li_2, Na_2, HCl, DCl, HBr,DBr, HJ, DJ.

The results of this calculations are compered with available experimental data [1,4] and other calculation [2-4].

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Evimov states and ultra cold collisions helium atoms with helium molecules

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Results of the calculations of the Efimov states [1] in molecular systems based on the three body approximation are present [2-4]. A mechanism of appearance and disappearance of the Efimov states of the helium trimer $^4He_3$ in three-body approximation is present when the force of interatomic interaction is changed. It is shown that these states arise from virtual levels which are in turn formed from quasiresonances settled on the real axis. The resonances including virtual levels are calculated by the method based on the solution of the boundary value problem at complex energies based on the Faddeev differential equations. All calculations are performing with the well known interatomic potential [3,4] in which a strong repulsive component at short distances between helium atoms is approximated by a hard core. Geometric structure of the helium trimer are presented. A special attention is devoted to the substantiation of the method used for calculations resonances and to the investigation of its applicability range.

The calculations of the scattering and bound states of He_3 were performed on the basis of the most advanced few-body calculation techniques both in boundary condition model (BCM) [2-4] approximation and without BCM approximation. In all considered pair waise potential support only two bound states approximately, but the properties of these states are very different:

- the ground states is strongly bound, whereas the binding energy of the excited state is comparably with binding energy of dimer;
- the sizes of these two states also very different.

The characteristic size of the ground state estimated by $< r >$ or $< r^2 >^{1/2}$ is approximately 10 times less than the size of dimer molecule, but the size of the excited state has the same order magnitude of the dimer's one.

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Collision of slow electron by hydrogen halide molecules in few-body approximation

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The electron scattering by hydrogen halogen molecules has been the subject a large number of experimental and theoretical papers [1,2]. If the energy of scattering electron is slow hydrogen halogen molecules HX (X is halogen atom) may be considered consisting of an proton and negative ion of halogen because electron affinity halogen atom is much more than the affinity of hydrogen atom [2]. In this assumption the processes of the collisions slow electron with hydrogen halogen molecules is treated as four-body process:

$$e + (H^+, X^-) \rightarrow \begin{cases} e + (H^+, X^-) & (1) \\ e + (H^+, X^-, (v,j)) & (2) \\ H + X^- & (3) \\ H + X + e & \\ H^+ + X^- + e & (4) \end{cases}$$

The interaction of the electron with the hydrogen halogen molecule is replaced approximately by the pair-wise interaction with each component consisting hydrogen halogen molecule (H^+, X, e) as if they are simple field centers. In this case two-body potentials have form of sum the long-range part and short-range one. In this approach we consider all processes of the scattering of the electron by molecule such as elastic scattering (1), ro-vibrational excitation (2), dissociative attachment (3), ionization (4) simultaneously.

This approximation seems reasonable as long as the energy of incident electron is below the threshold of electronic excitation of hydrogen hyalogen molecule.

To calculate the cross section of the processes (1)-(4) we use the modified Faddeev-Yakubovsky equations (FYE) [3]. It is well known that the FYE are the most consisting and concise way of treating multiple scattering effect in few-body problems as well as the resonances connected with arbitrary number and location of the centers [4]. For the numerical solution of FYE we used the technique developed in [3,4]. Using this model the calculations of the electron scattering HF, DF, TF, HCl, DCl, TCl, HBr, DBr, TBr, HJ, DJ, TJ molecules of the processes (1)-(4) are presented and discussed. The results of this calculations are compared with the available experimental data and other calculations [1,2,4].

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Few-body approximation in atomic and molecular physics

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The main difficulties in the research of few-body problems are bounded with the really many-channels and multidimensional nature of the these problem, impossible applied many well known theories such as adiabatic, impulse, coupled channels, etc.

For this reason we proposed new method for the investigation of the different few-body processes used the mathematically rigorous formalism based on the treatment of collision processes as many body processes, using Faddeev-Yakubovsky equations [1] (FYE) in integral and differential forms. In particular techniques based on FYE have been used successfully in studies of the dynamics of few-particle systems (bound-state properties and elastic, reactive and breakup scattering) [2]. The following results are presented and discussed [2]. Calculation of low-energy characteristics in scattering processes like scattering length, effective range parameter, amplitude, cross section etc. in processes $p + d$, $n + d$, $p + He$, electron + molecule etc. for the verification of the fundamental principal of the atomic and chemical interaction. The theoretical investigation of the quasibound, virtual and resonances states in few-body systems such as $p+d$, $n+d$, $e+H$, $e+He$, $p+H$, $p+He$. Scattering the electrons, protons on the few-centers targets (atoms, molecules etc.) and the estimation the role of many center scattering in these cases. The calculations of the excitation, rearrangement and ionization H and He atoms and its ions by the electrons and protons impact. The investigation of the influence of the long range part of pair-wise potentials in FYE on the scattering in few-body systems. The study on the correlation between low-energy characteristic in few-body scattering. Scattering electrons by two atomic (H_2, HD, D_2, N_2, Cl_2, F_2, Br_2, J_2, HF, DF, HJ, DJ, HCl, DCl, HBr, DBr,$RbCl$, $RbBr$, $CsCl$, $CsBr$, KI) and few atomic molecules (CO_2, O_3, NF_3). The investigation the theory of quasimolecule (electron + molecule), the ionization mechanism in quasimolecule and the main characteristics of quasimolecule autoionization states, determination of the bound between these states, the resonance states, potential energy surface (PES) and dynamics of the chemical reaction. The scattering atoms with two ($O + CS$, $H + H_2$, $O + N_2$, $O + O_2$) and few atomic ($O + CF_3J$, $O + CS_2$, $O + OSC$, $HCl + HCl$) molecules, the many particles interactions, orientations of the reacting molecules etc. on the reactions dynamic, the confection between the interactions in FYE and PES, the investigation of the resonances, virtual states and threshold phenomena in chemical reactions. The studding the unusual dynamical threshold phenomena in chemical reactions such as Efimov states based on FYE. This research may be obtain the information of the reaction mechanism, PES etc. and may have a strong influence on the scattering observable. The investigations of the possibility of the analytical solution of FYE in the different approximations, the construction of the solvable model in FYE approach are presented.

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Multiple scattering approximation in atomic and molecular physics

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The multiple scattering approximation based on the modified Faddeev-Yakubovsky equations [1] for charged particles is applied to the calculation of the scattering amplitudes and cross sections of the different processes ion-atom, ion-molecular and atom-molecular collisions. In three-body approximation the amplitude may be written in the form [2]: $f_{2-2} = f_c + \Psi_{2-2} v_1 (G_2V_2 + G_3V_3 + G_2V_2G_3V_3 + G_3V_3G_2V_2)\Psi_{2-2}$ - for elastic scattering and $f_{2-3} = \Psi_{2-3} v_1 (G_2V_2 + G_3V_3 + G_2V_2G_3V_3 + G_3V_3G_2V_2\Psi_{2-2}$ - for break-up processes, where $f_c = \eta \exp(-i\eta \ln \sin^2\theta/2 + 2iarg\Gamma(1+i\eta))/2(\mid k \mid \sin^2\theta/2)$ - Coulomb amplitude; $\cos(\theta) = (\vec{k},\wedge \vec{k'})$; $\Psi_{2-2} = \varphi_{2-2}(x)\psi_c(y,p); \psi_c(y,p) = e^{-\pi\eta/2}\Gamma(1+i\eta)\Phi(-\eta, 1, i \mid p \mid\mid \xi \mid)$; $\eta = n/2 \mid p \mid$; $\xi = \mid y \mid - (y,p)$; $\Psi_{2-3} = \varphi_{2-3}(x,k)\psi_c(y,p)$; $v_i = n_i / \mid x_i \mid + v_i^s(x_i); n_i = \gamma Z_i Z_j / \sqrt{2\mu_{ij}}$; $\mu_{ij} = m_i m_j/(m_i + m_j)$; $V_i = V_i^1 + V_i^2; V_i^1 = v_i^s + n_i \chi_i(x_i, y_i, \nu)/ \mid x_i \mid$; $V_i^2 = (1 - \chi_i(x_i, y_i, \nu)) n_i / \mid x_i \mid$; $x_i, y_i, k_i, p_i, m_i, Z_i$ - coordinate, momenta and charge of i-particle; ψ_{2-2},ψ_{2-3} -wave functions of the bound and continuous states two particle subsystems; G_i, χ_i - Green and cutoff functions defined in [1]. The parameters ν, x_i, y_i chosen such that χ tends to unity in the limit $x_i << y_i \rightarrow \infty$ and vanishes when $x_i \sim y_i \rightarrow \infty$, thus proving asymptotic decoupling of the scattering channels. f_c -coulomb amplitude. This expression is agree with expression for neutral particles which is get in multiple scattering approach [3], if take it into account that $V_i G_i = G_0 T_i$. The present model obviously take into account the long range interactions and allows to take the multiple scattering into account in explicit fashion, as well as the resonances connected with it for arbitrary number and location of the scattering centers. In this approach the elastic, inelastic (rearrangement, charge-exchange) and ionization processes considered simultaneously. Using the eikonal approximation of Green function explicit expressions for the differential cross section in case three-body scattering are presented. The characteristic features in the ionization spectrum at forward angles (the continuum electron capture and binary encounter peak) and different mechanism of this processes are discussed. Under conditions in which such features play a dominant role by determining the order of magnitude of the cross sections of the processes in which we are interested, the use multiple scattering approach allows us to obtain a simple and effective estimate of the cross section. The results of these calculations are compared with the available experimental data and other calculations such as quasiclassical, (saddle point mechanism), classical, multiple-scattering treatment, Born and impulse approximation, semiclassical Faddeev-Watson approximation.

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Study of charge transfer excitation in collisions of nitrogen ions with carbon dioxide molecules

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Numerous papers were dedicated to the CO_2-molecule reactions in the past four decades [1], primarily due to an increase of interest in laser technology and natural phenomena in the ionosphere, solar corona and planetary atmospheres. Most attention has been paid to measurements of cross sections [2, 3] for charge transfer excitation but recently emphasis was placed on determination of vibrational state distribution of excited electronic states of CO_2^+ ions. Experimental vibrational state distributions were compared with those predicted by theory, especially Franck-Condon and curve-crossing models [4].

In the present work, collision-induced charge transfer experiments for $N+(^4S) + CO_2$ were performed in a beam-gas arrangement under single-collision conditions. A detailed description of the experimental setup has been given elsewhere [5]. Briefly, a beam of mass-selected nitrogen ions collides with target gas. Luminescence is detected with optical system consisting of optical spectrometer with a photon counting system. The collision energies were in the 6-1000 eV_{lab} range, target gas pressure was 15 mTorr.

The $A\ ^2\Pi_u$ - $X^2\Pi_g$ and $B\ ^2\Sigma_u^+$ - $X^2\Pi_g$ of CO_2^+ luminescence spectra were recorded and excitation functions for the charge-transfer reactions have been obtained.

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Nonrelativistic energies for lithium-like systems with exponentially correlated functions

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The analytical evaluation of four-particle integrals, performed in 1987 by Fromm and Hill [1], opened up possibilities for high-precision variational calculations of four-particle systems in a basis of exponential functions of all interparticle distances. These ideas were explored later by several authors [2, 3] with a moderate success.

We are going to present effective algorithm for the four-body system, based on the combination of the integration by parts technique [4] and numerical integration methods [5]. We determined accurate non-relativistic wave functions and energies for the Li atom and the Be^{+} ion with an uncertainty of 10^{8} using only 96 basis functions.

Apart from the nonrelativistivc energy, these functions can be used in matrix element calculations. They are very useful especially for operators at higher orders of the perturbative NRQED theory. Together with our high-precision methods in Hylleraas basis [6], we are aiming to determine $m\alpha^6$ and $m\alpha^7$ effects in the hyperfine structure of lithium-like systems.

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Importance of polarization potential and PCI in the (e, 2e) processes on alkali and alkali earth targets at low energies

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The study of electron impact ionization of atoms and molecules has been of interest, since the early days of atomic and molecular physics, since the kinematics of this process are easily controlled, and the electrons or ions resulting from the reaction can be observed with relative ease. The electron impact ionization of atoms is a three body problem governed by the Coulomb force acting between incident electron, target electron and residual ion. Fundamentally an (e, 2e) process is one where an electron of well defined energy and momentum is incident on a target, ionizes it and the outgoing electrons are detected in coincidence with their energies and angles resolved. Ionization is a technique which is used as a tool to probe target wave functions. Study of ionization process in different geometrical arrangements offers a help to understand the reaction mechanism better. Through the careful choice of geometrical arrangement and the energies of incoming and exiting electrons one can predict the physics which will dominate the shape and magnitude of the triple differential cross section. The calculation of triple differential cross section opens up a whole new area of theoretical study and offers a direct insight into the subtleties of spin-dependence and other purely relativistic effects etc. Since the first coincident measurement of (e, 2e) process on atoms by Erhardt *et al*[1] and Amaldi *et al.* [2] extensive theoretical and experimental investigations have been done to measure the TDCS. There has been recent interest to study (e, 2e) processes on alkali and alkali earth atoms initiated by measurements of Murray [3]. Recently U Hitawala *et al.* [4], Srivastava *et al.* [5] and Bray *et al.* [6] have reported the results of (e, 2e) triple differential cross sections for alkali atom Na and K. We present in this communication the results of our distorted wave Born approximation (DWBA) calculations of TDCS for the ionization of alkali atoms Na and K and alkali earth atoms Mg and Ca. We also include correlation-polarization potential in DWBA formalism as a function of density function. We discuss the salient features of our DWBA results which are different from the results of earlier workers. We will also discuss the effects of incident electron energy, distortion, nuclear charge, correlation-polarization, post collision interaction etc. on the trend of TDCS for alkali and alkali earth targets.

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Exploration of possibilities of quasirelativistic Breit-Pauli approach within oxygen isoelectronic sequence

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Calculations of energy spectra of atoms and ions within Breit-Pauli approach have certain advantages: the energy spectra are obtained within LS-coupling comfortable for interpretation of the experimental data and the methods for extended calculation of the correlation corrections are well- developed and require moderate computational resources. However, application of the traditional Breit- Pauli approach is limited for heavy atoms and highly charged ions. The possibilities to extend the framework of Breit-Pauli approach by using the quasirelativistic radial orbitals are investigated within the oxygen isoelectronic sequence ($Z = 9 - 34$).

The quasirelativistic Hartree-Fock equations have been formed anew seeking to avoid any unjustified simplifications and solved taking into account the finite size of the atomic nucleus [1]. The total energy corrections of Breit-Pauli formalism are rewritten in correspondence with the properties of the quasirelativistic radial orbitals [2]. The calculations are performed applying the configuration interaction technique on the basis of the transformed radial orbitals with variable parameters. In order to evaluate the influence of the quasirelativistic radial orbitals on the accuracy of the results the same calculations are reduplicated within the usual Breit-Pauli approach on the basis of non-relativistic functions taking into account the correlation effects in the same way as with the quasirelativistic functions.

The energy levels of the $n = 2$ complex of O-like ions as well as transition characteristics have been calculated by two mentioned methods. The transformed radial orbitals have been formed using the excitations into the virtual states with $4 \leq n \leq 8$ and all possible values of l and configuration interaction have been performed within this basis. The results obtained are compared with the available experimental data [3]. The relative accuracies of the calculated values to the experimental ones are compared for two approaches used and plotted for every energy level throughout the isoelectronic sequence. The comparison of the results shows how relative deviations of the energy values calculated within the usual Breit-Pauli approach increase as ion nuclear charge grows while relative deviations of the energies calculated within the quasirelativistic Breit-Pauli approach change weakly within the explored isoelectronic sequence.

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Investigation of spectral characteristics of W II

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Investigation of tungsten properties is of major interest for construction of modern fusion devices, such as ITER – a joint international research and development project that aims to demonstrate the scientific and technical feasibility of fusion power. Tungsten is planned to use as a plasma facing material. Due to the high specific radiation losses if the element penetrates into the central plasma region, its fractional abundance in the plasma of a fusion device should be carefully controlled. Relevant spectroscopic data are necessary to investigate behavior of tungsten and its ions in the plasma.

The *ab initio* study of spectral characteristics of W II has been performed within the configuration interaction approach in the basis of transformed radial orbitals with a variable parameter for wide account of the correlation effects. The relativistic corrections have been taken into account within the Breit-Pauli formalism using quasirelativistic functions. The quasirelativistic radial orbitals are obtained solving quasirelativistic Hartree-Fock equations with all relativistic corrections up to the square of the fine structure constant α included and taking into account the finite size of the atomic nucleus [1]. The radial integrals of the Breit-Pauli energy operator are refined according to the properties of the quasirelativistic functions [2].

The quasirelativistic Hartree-Fock equations have been solved for inner shells and active shells with $n = 6$ and $l \leq 2$ of investigated configurations. Then using this basis of quasirelativistic radial orbitals the transformed radial orbitals with $7 \leq n \leq 12$ and $l \leq 8$ have been formed using the excitations into the virtual states. In order to perform configuration interaction 721 even and 890 odd admixed configurations have been selected. The energy spectra of ground configuration $5d^4 6s$ and excited configurations $5d^5$, $5d^3 6s^2$, $5d^4 6p$, $5d^3 6s6p$ and $5d^2 6s^2 6p$ are obtained and compared with the available experimental data [3]. It is problematic to interpret the obtained results because the mixing of energy levels is very strong and LS-coupling is not valid in this case. The wavelengths and transition characteristics have been calculated using obtained quasirelativistic multiconfiguration wave functions. The characteristics of the strongest transitions are presented.

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A brief review of recent experiments undertaken at FLASH

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FLASH (Free electron LASer in Hamburg) operates on the principle of Self Amplified Spontaneous Emission (SASE) and produces coherent, bright and ultrashort eXtreme-UV (XUV) pulses [1]. By synchronizing FLASH with an independent optical laser, it is possible to induce and control coherent processes in superimposed, intense XUV and NIR fields. One such process is photoelectron sideband generation [2]. In this class of experiment, photoelectrons are ejected by XUV radiation and simultaneously subjected to the intense field of an optical laser with which they can exchange photons. In effect, they absorb/emit photons with energy corresponding to $\hbar\omega$ i.e. that energy of the optical laser photons [3,4]. As a consequence the photoelectron spectrum is no longer comprised of a single feature corresponding to the main photoline but is straddled by additional photoelectron lines separated by $\hbar\omega$ – it is these features that are referred to as sidebands. By controlling the relative polarization angle between the FEL beam (pump) and the optical laser (probe) and recording the magnitude of the sidebands one can measure the contribution each partial wave has on the outgoing electron. This was recently demonstrated in [5] using atomic He, and a similar scan has since been sucessfully undertaken where sidebands have been unambiguously identified on the ^{3}P and ^{1}D photoelectron lines of Ne$^+$.

The use of a highly developed EUVL Si-Mo multilayer mirror allows one to focus the FEL beam, resulting in ultrahigh intensities on the order of 10^{-16}Wcm^{-2} [6]. This intensity, coupled with a low FEL wavelength (13nm) makes it possible to induce non-linear inner shell ionisation processes. For the first time using photoelectron spectroscopy, a signal has been detected resulting from the direct two photon inner shell ionisation of an atom, in this case of the 4d subshell of xenon.

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Effect of atom substituents on absorption and fluorescence properties of tetracyclic phenazine derivatives

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In our work we study effect of substituents on pentacyclic ring on spectroscopic properties of the tetracyclic uncharged phenazine derivatives (Fig.1). Investigation was carried out by the methods of absorption and polarized fluorescence spectroscopy in organic solvents of different polarities and proton donating abilities, as well as in aqueous solutions of different pH. The energies of the electronic $S_1 \leftarrow S_0$ transition and the changes in molecular dipole moments upon the optical excitation were determined. In aqueous buffered solutions the ranges of solvent pH, where individual ionic species of phenazines are predominant were determined. Their pK_a values were evaluated from experimental data. It was shown that donor-acceptor properties of the X-Y group substantially affect the values of the deprotonation constants and the character of chromophore protonation. It was found that only neutral species of the dyes fluoresces, the fluorescence quantum yield depends on substituent type, as well as on proton donating and hydrogen bonding abilities of solvent. The substitution of a hydrogen atom in the Z position by the sugar residue blocks the formation of the anionic species, and results in enhancement of the dye emission intensity. It was shown that F1rib and F4gl are the most promising compounds to be used as fluorescent probes for investigation of molecular hybridization of nucleic acids. The steep emission dependence for F1 and F1rib over pH range of 1-7 allows us to propose them as possible indicator dyes in luminescence based pH sensors for acidic region.

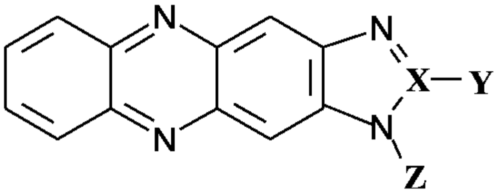

Figure 1: Molecular structure of phenazine derivatives. F1: X = C; Y = H; Z = H; F2: X = C; Y = CH_3; Z = H; F3: X = C; Y = CF_3; Z = H; F4: X = N; Y – absent; Z = H; F1rib: X = C; Y = H; Z = β-D-ribofuranose; F4gl: X = N; Y – absent; Z = β-D-glucopyranose.

Noise reduction in optically pumped magnetometer assemblies

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The ultimate sensitivity of an optically pumped magnetometer is limited by the shot noise of the photo receiver. In real measurement setups this shot noise limitation can not be reached, however. Noise contributions of the light source, the magnetic field and the signal electronics are superimposed. Whereas the latter should easily be cancelled, the other ones degrade the noise limited magnetic field resolution drastically in practice.

We look for methods to decrease the extra noise sources in order to approach the shot noise limit. The basic concept is to use gradiometer configurations. The subtraction of the signals of two adjacent magnetometers is not enough, however. Because of frequency mixing at the Larmor frequencies only direct noise contributions of the homogeneous magnetic field can be cancelled this way. Therefore the fluctuations themselves need to be reduced wherever possible. The pump laser frequency fluctuations, converted to amplitude fluctuations by the alkali vapour absorption, indeed could be reduced drastically by a subtraction of the photo diode signals of the two magnetometer channels, prior to the signal processing with the lock-in amplifiers. So, each of the lock-ins has to select its own Larmor frequency from the now common signal. This demands a magnetic field gradient between the two magnetometer cells, which has to be assured somehow.

In our investigations with two Cs cells from the University of Fribourg, Switzerland, we use an M_x measurement configuration. Homogeneous and gradient magnetic fields are generated in a large shielding barrel in order to get rid of environmental disturbances.

Inserting the magnetometer cells into the laser beams enhances the photo current noise by one order of magnitude as compared to the direct illumination without Cs vapour (where it was on shot noise level). In the result of the above sketched photo current subtraction this excess noise could be reduced again by a factor ample of about four. This directly reflects in the white noise levels of the magnetic field signals (measured in a field of 5 μT). The noise of the single magnetometers ($\sim$700 fT/$\sqrt{\text{Hz}}$) reduces to about 200 fT/$\sqrt{\text{Hz}}$. The remaining difference to the intrinsic noise of 60 fT/$\sqrt{\text{Hz}}$ will at least partially be due to the noise of the magnetic field sources. The common gradient measurement, realized by the subtraction of the two magnetometer signals, additionally results in a drastic reduction of the low frequency magnetic field noise.

Measurement of copper L shell x-ray production cross-sections induced by 2-30 keV electrons

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The ionization cross-sections or x-ray production cross-sections are required for various applications in atomic physics, plasma physics, space science, cosmic ray interactions, and radiation physics and for the characterization of materials. The L shell x-ray production cross-sections of copper induced by electrons in the energy range of 2 to 30 keV have been reported for the first time. Some measurements have been reported for some elements but in higher electron energy range [1,2,3]. The copper L x-ray lines lie in the energy range of 0.8 to 1.1 keV hence difficult to analyze and measure due to poor detector efficiency in this range. The present measurements are made in vacuum using EDS with 127 ev FWHM at 5.9 keV, attached with a Ziess SEM. The need of absolute efficiency of the detector is eliminated by measuring relative cross-sections. The thick targets are used in experiments to make the target absorption effects negligible at low x-ray energies of Copper. Since no other experimental data are available for comparison, the measured values are compared with those calculated using required parameters like fluorescence yields and Coster-Kronig transition probabilities in literature [4]. The energy dependence of the total L shell x-ray production cross-sections is investigated in this energy range and are found to show the similar trends but with some deviations in the lower energy range.

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Radiative correlated double electron capture (RDEC) in O^{8+}+C collisions at low energy

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Radiative double electron capture (RDEC) is a one-step process where target electrons are captured into bound states of the projectile, e.g., into an empty K-shell, and the excess energy is released as a single photon. This process provides insight into several very challenging problems in atomic physics, such as the electron-electron interaction in electromagnetic fields or the search for a proper description of a two electron-continuum wave function.

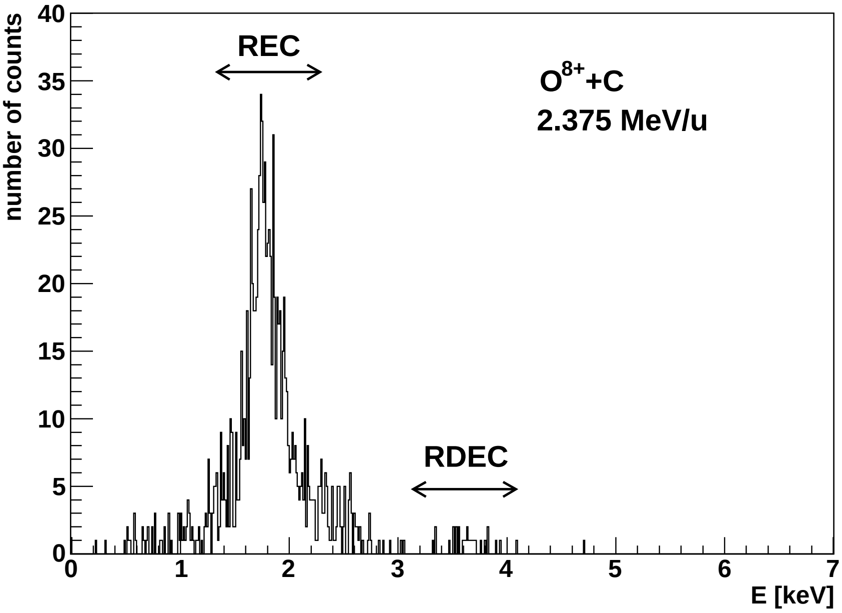

Figure 1: Sample X-ray spectrum registered in coincidences with double electron capture. Structure consistent with RDEC process is visible.

The choice of the collision system used in the presented experiment was based on the latest theoretical calculations of RDEC cross sections [1, 2, 3], which predicted enhancement of this process in low energy systems. The experiment was conducted at Western Michigan University using the tandem Van de Graaff accelerator. Bare oxygen ions with energies of about 2.375 MeV/u were collided with 2 μg/cm^2 carbon target and the x-ray spectra were registered in coincidence with single and double electron capture. Example of a spectrum registered in coincidence with double charge change is presented in Fig. 1. Here a peak structure near 3.5 keV consistent with RDEC is visible.

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Effective field theory for light transport in disorder atomic medium

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The character of light transport in disorder atomic medium is determined by the multiply elastic scattering of light. In a sample of randomly distributed scatters, the initial direction of the wave is fully randomized by multiple scattering, and a diffusion picture seems to be an appropriate description of light propagation in the case of small densities of scatters. Despite successful predictions, this theory does not take into account interference effects. In fact, wave interference affects the physics of light propagation and results in so-called weak or strong localization regime [1-2]. A system of randomly distributed atoms with an atomic transition frequency close to the light frequency provides necessary conditions for experimental observation of the interference and non-linear phenomenon. The photons can be transferred radiatively as well as non-raditiavely via the resonance dipole-dipole interaction in such a medium. The last is equivalent to including the longitudinal component of the electromagnetic field. Non-radiative transfer becomes more important with increasing the density of atoms, when a typical energy of dipole-dipole interactions is comparable with the excitation energy of atoms.

We have developed a field theory approach to light propagation in a gas of resonant atoms, where both the atoms and the electromagnetic fields have been represented by quantum fields throughout the analysis, and taken into account vector character of light. The atomic number density n is assumed to be low or moderate (i.e. $n\lambda^3 < 1$) and the atoms are treated as a $(1+3)$-level system, i.e. a resonant $s-p$ transitions in atoms are supposed to occur only. The dipole-dipole interaction between atoms is incorporated into the approach non-petrubatively and the relativistic effects are allowed for. Starting from the exact action included interatomic dynamics, atom-atom interaction and electric field atom interaction; we have derived the Green function and its derivatives for the dressed photon that describes both the inelastic processes like a spontaneous emission of the atoms and elastic scattering photon in gas with density-density correlations via resonant atom-field interaction. The applied approach is not restricted to the rotating-wave approximation. We have shown that the energy associated with transition between resonance states does not change for low atomic density where the coupling parameter is $(16\pi d^2\rho/\Delta)$ is small. Influence of short-range and long-range correlations of the atom densities on light propagation has been analyzed. Contrary to the case of short-range atom density-density correlations, the long-range correlations result in anisotropic spatial dispersion controlled by the direction of the wave vector. When the wave length exceeds the typical scale for density-density correlations, the anisotropy in spatial dispersion disappears, as it should be for the case.

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Mass-spectrometric studies of electron-impact dissociative ionization of glycine molecule

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We have developed a mass-spectrometric apparatus based on the magnetic mass-analyzer intended for studying ionization of atoms and single/dissociative ionization of polyatomic molecules by low-energy electron impact. A primary emphasis was given to the production of ionic fragments following dissociation of complex molecules, mainly those having biological relevance. Such data are of specific interest in view of tracing the possible effects occurring in the live tissue under the influence of ionizing radiation accompanied by the production of slow secondary electrons, which, in turn, cause a series of structural transformations in the cells resulted in degradation of constituent elements of human/animal body [1]. Amino acids, which glycine belongs to, are one of the basic building blocks of the live body. Moreover, recent investigations have shown that amino acids are present in various space objects (say, meteorites and/or comets), proving, thus, the idea of life "import" to the Earth [2]. Of special interest is the fact that such molecules take an active part in constructing live cells and repairing damaged tissues, in particular, in forming antibodies, which fight against the viruses and bacteria that destroy the immune system of living organism. Experiment was carried out using a crossed-beam technique combined with mass separation of electron-molecule interaction products. The measuring procedure was fully automated using the PC control. Besides measuring the mass-spectra of the initial molecule, we have determined the energy dependences of the ionized fragment yield with the 0.3 eV energy step and the $0.2 - 0.5$ eV (FWHM) energy resolution from the threshold up to 150 eV using a specially-designed electron gun instead of the conventional one used in the original version of mass-spectrometer ion source. It has been found that the main ionic fragments of the initial $C_2H_5NO_2$ molecule are CH_4N^+, CH_3N^+ and CH_2N^+, which can be produced in various isomer states. Since the initial molecule may undergo strong fragmentation due to the thermal processes, special studies of possible temperature-induced fragmentation of the glycine molecule were carried out allowing one to choose the regime of molecular beam generation, minimizing, thus, the influence of thermal effects. Application of special least-square fitting procedure [3] enabled the absolute values of the appearance potentials for the above fragments to be found. Out data demonstrate fairly good agreement with the results of recent photoioniozation studies [4]. More detailed analysis of experimental data and possible mechanisms of electron-impact glycine molecule fragmentation will be presented at the conference.

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Detection of fluorine with cavity ring-down spectroscopy

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Fluorine compounds play very important role for living organism and are of great importance for agriculture and industry. However a quick development of these activities leads to excessive emission of this element and its deposition to soil, water and atmosphere. There is a small difference among doses which are desirable for living organism and which are harmful. Therefore there is a need of trace determination of this element. Good opportunities are provided by contemporary laser spectroscopy techniques.

Our approach to the trace detection of fluorine consists in atomic spectroscopy in plasma which is doped by the investigated matter. The plasma dissociates the matter and produces free atoms. Due to collisions with electrons some atoms are excited to metastable levels which are detected using the absorption spectroscopy at 685.603 nm line corresponding to $3s^4P_{5/2} - 3p^4D^o_{7/2}$ transition. High sensitivities might be expected due large oscillator strength of this transition (0.36) and due to application one of the most efficient method of absorption measurement – Cavity Ring Down Spectroscopy.

The experiment was performed in a tube ended with two mirrors of high reflectivity. Time of the radiation imprisonment in such optical resonator reached about 1.5 μs. In central part of the tube the RF cavity was installed. It was supplied by 150 W generator providing the plasma column of 20 cm.

The investigated mixture was composed of helium at a pressure of several Torr with addition of evaporated XeF_2 or SF_6. The cavity was illuminated with of single mode radiation from cw diode laser working at 685.603 nm. We used off-axis illumination of the resonator. Due to that the beam is reflected by the mirrors in this way that the light spots do not overlap. It provides opportunity to avoid sharp resonances that usually occurs in the optical cavity in the case of on-axis illumination. The laser beam was amplitude modulated by AOM with frequency of 50 KHz.

The light leaving the cavity through the front mirror was registered by the photomultiplier protected by the interference filter against noises occurring due to plasma luminescence. Digital oscilloscope and lock – in amplifier measured the radiation decay time and phase shift of the signal which occur due to light imprisonment. Using them the cavity Q-factor and the atomic concentration of absorbing fluorine were determined. We stated that such system provides opportunity to detect fluorine at the level of about 100 μg/kg.

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The modified relativistic J-matrix method of scattering

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Since the J-matrix method, a numerical technique to solve quantum mechanical scattering problems has been developed [1,2], many modifications has been applied to the original, non-relativistic method [3,4]. These modifications were necessary, as the original method encounters convergence problems. It is because only the extensive matrix V_{nm} accurately represents the potential $V(r)$, in certain applications. Since the Schrödinger matrix is only tridiagonal after all potential matrix elements have died out, the internal region is very large, and only after determination of a large number of matrix elements and solving of an enormous linear system, a converged result is obtained.

In this contribution we present modifications of the relativistic J-matrix method [5]. Some preliminary applications of the original relativistic J-matrix method to scattering have been already presented for some square-type potentials [6]. These tests proved that the method correctly describes the scattering process, but the convergence problems are even more noticeable than in the non-relativistic case.

We present the technique to expand the relativistic scattering solution in the oscillator eigenstates, and to solve the resulting linear system. We have introduced modifications that speed up the convergence and extend the applicability of the method. As a result, problems that lead to large potentials matrices (e.g. long-range potentials) can be now solved with a relatively small computational burden.

We started with analysis of the projection integral of an arbitrary function on a high-lying basis state. Due to rapid oscillations of this state, different contributions of this integral cancel, and the integral can be simplified. The next step concerns a study of the behavior of the potential matrix element $\langle n|V|m\rangle$, also leading to a simplified formula. This, in turn, leads to adding some terms to the asymptotic recurrence relation, which summarize the asymptotic effects of the potential. In this way, solving a relativistic scattering problem is reduced to two simple tasks: solving a recurrence relation and a small residual linear system.

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The relativistic J-matrix method in elastic scattering of slow electrons from Argon atoms

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The J-matrix method is an algebraic method in quantum scattering theory. It is based on the fact that the radial kinetic energy operator is tridiagonal in some suitable bases. Non-relativistic version of the method was introduced in 1974 by Heller and Yamani [1] and developed by Yamani and Fishman a year after [2]. Relativistic version was introduced in 2000 by P. Horodecki [3].

Some preliminary applications of relativistic J-matrix method to scattering have been presented for some square-type potentials [4], using the newly developed Fortran 95 code JMATRIX [5]. These tests proved that the method correctly describes the scattering process.

The main advantage of the method is that it allows to calculate phase shifts for many projectile energies with relatively small computational time. Also, the non-relativistic limit in relativistic calculations is properly achieved. This fact was expected, since the basis sets used in relativistic calculations satisfied the so called kinetic balance condition.

In this contribution we present relativistic scattering phase shifts together with total and differential cross sections in elastic scattering of slow electrons from Argon atoms, calculated using the modified relativistic J-matrix method [6]. To improve convergence, some mathematical and numerical techniques has been applied. Scattering potential has been calculated using the well-known GRASP92 package [7], and the scattering solution has been written in terms of series od the Laguerre, Gaussian and complete oscillator basis functions. We compare the results with other theoretical (e.g. these obtained using the multiconfiguration Dirac-Fock method [8]) and experimental (e.g. measured at high scattering angles [9]) data.

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Ionization of Mg atom by electron impact in the region of autoinizing states excitation

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The method of interacting configurations in complex numbers representation (MICCNR) was created in [1-3]. Moreover, the calculations of the positions and total widths of AIS, converging to the N=3 threshold of helium atom, were done [1-3].

MICCNR has a high precision in the problem of determination of positions and widths of autoionizing states (AIS) in the processes of ionization of the atoms by photons, electrons and other particles. The method under consideration is the further development and generalization of the standard method of interacting configurations in the real number representation.

The advantages of this method are as follows. First it is the absence of difficulties with the identification of resonances (of AIS), further we may mark the possibility of finding here the widths of quasi-stationary states, which is a problematical task in other methods.

The program of application of MICCNR to the calculation of ionization processes for more complex (in comparison with helium atom) atomic structures is the actual next step. Below we apply this method to the problem of photoionization of Mg atom. The positions of lowest five ^{1}S, ^{1}P, ^{1}D, ^{1}F AIS of Mg in the problem of ionization of atom by electron impact will be presented in the special table. The indirect comparison with the similar states, which are generated in the problem of electron scattering on the Mg ion [4] will be fulfilled. In the paper [4] the calculations were made in the diagonalising approximation.

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Two electron positive ion response to an intense x-ray pulse

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Revolutionary x-ray free electron lasers (FELs) are currently under construction in the USA, in Europe and in Japan. One of the first proposed atomic physics experiments using the Linac Coherent Light Source x-ray FEL is the direct observation of double K-shell ionization. We present double K-shell ionization rates of two-electron positive ions exposed to an intense x-ray FEL pulse.

The foundation of our work is the direct numerical integration of the full six-dimensional time-dependent Schroedinger equation (TDSE) [1]. The numerical method is an extension of the existing computer code (HELIUM) that has been developed over the last decade to solve, in its full generality with quantitative accuracy, the TDSE governing the two-electron helium atom interacting with high intensity laser light in the optical and XUV wavelength ranges [2,3,4].

However as the laser wavelength approaches atomic dimensions the electric dipole approximation, used in HELIUM, may break down. To enable HELIUM to model the two-electron K-shell response to an intense x-ray FEL pulse we incorporate non-dipole Hamiltonian interactions. The non-dipole terms cause a jump from 5- to 6-dimensions in HELIUM; the resulting increase in computational demand is met by the highest performance computers currently available in the UK.

We report results pertaining to two-photon double ionization for the two-electron positive ions Ne^{8+} and Ar^{16+}. We present double ionization rates, energy spectra and probabilities of double core hole formation at laser frequencies of 55 au to 90 au (200 au to 300 au) and for intensities in the range 10^{17} to 10^{19} W/cm^2 (10^{19} to 10^{22} W/cm^2) for Ne^{8+} (Ar^{16+}). Furthermore at a laser frequency of 110 au, where single-photon double ionization is possible, we present double ionization energy spectra for Ne^{8+}. Finally we discuss the relevance of the non-dipole Hamiltonian terms.

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Atomic lifetime measurements affected by cascades from peculiarly long lived levels

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In various ion trap experiments, the lifetimes of levels in the ground configurations of multiply charged ions (which decay only by electric-dipole forbidden transitions) have been considered to be the only long lifetimes (in the millisecond to second range) present. If valid, such an assumption would correspond to decay curves that are dominated by a single exponential, and those are easy to evaluate. Recent high-precision lifetime measurements of ions using electron beam ion traps, however, disagree with theory at a multiple of the perceived experimental uncertainty. Some measurements of 3p level lifetimes of Fe group element ions at a heavy-ion storage ring have yielded seemingly single-exponential decays of a clearly wrong decay constant or signatures of slow cascades. Hence it is necessary to re-assess the occurrence of long-lived levels in electronic shells well above the ground configurations and the conditions under which such levels may be populated and to what degree. Theory provides several specific candidate levels, some of which may have a lifetime uncomfortably close to that of the level of primary interest. In some cases, isoelectronic variation in the experiment can be exploited to avoid those cases in which the cascade situation may be worst (for the data interpretation) and to target the best (offering a chance at a meaningful experimental data analysis). In addition, variations of experimental parameters such as the excitation conditions are called for.

For ions of the iron group, with 13 to 17 electrons (Al- through Cl-like spectra), there now are data from measurements using an ECRIS ion source and an electrostatic trap, foil-excited ion beams stored in a heavy-ion storage ring [1], and electron beam ion traps [2] that produce the ions from an arc discharge or from a gas inside the trap. The range of experimental parameters spanned in these measurements is considerable; an assessment of the accuracy of the data can thus help to identify sources of systematic error and point towards optimum parameters for future precision measurements that, for example, are sensitive to the QED correction of the magnetic dipole transition operator [3].

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High resolution laser spectroscopy of Cs vapor layers with thickness variation around the light wavelength

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The high resolution spectroscopy of thin vapor layers has been made possible through the development of unique optical cell, the so called Extremely Thin Cells (ETC) with thickness around one micron [1].

In the presented work we examined, both theoretically and experimentally, the sub-Doppler resonances in the transmission and fluorescence spectra on the D_2 line of Cs atomic vapor layers with thickness $L = m\lambda$ (where $m = 0.5, 1, 1.5, 2, 2.5, 3$), irradiated by tunable single-frequency diode laser light. For low laser intensities and $m = 0.5, 1.5, 2.5$, in the transmission spectra the coherent Dicke narrowing is observed [2, 3], while for $m = 1, 2, 3$ the hyperfine structure is not resolved. In the last case, under high-intensity irradiation narrow dips of reduced absorption are observed, related to velocity selective optical pumping and saturation. For $m = 1.5, 2.5$ and for the closed transition only, a small absorption peak appears superimposed on the velocity selective deep. The difference between the open and closed transition behaviour can be related to the fact that for the open transitions the slowest atoms are effectively transferred to the ground-state level non-interacting with the light. Thus, they are lost for the absorption and can not participate in the formation of the coherent signal responsible for the Dicke narrowing. The ETC fluorescence profiles are intrinsically narrower than the absorption profiles [4]. Nevertheless, well pronounced narrow saturation dips appear in the fluorescence profiles, for all open transitions. The dip amplitude increases with the ETC thickness. In the case of closed transition, non-suffering population loss a small feature in the fluorescence profile is observed [5]. The utilized theoretical model is based on the Optical Bloch Equations for two-level system (closed and open) [4]. For both absorption and fluorescence theoretical profiles, we have obtained a qualitative agreement with the experimental observations. Presented results contribute to the further advancement in fundamental studies of saturation and optical pumping in extremely thin vapor layers.

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Description of the Be ground state based on the interaction of separately optimized pair correlation functions

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It is well known that variational methods produce one-electron functions placing themselves for bringing the largest stabilizing contribution to the total energy. It is therefore possible to target specific correlation by tailoring the configuration expansion. We want to take advantage of this feature in using independent pair correlation functions (PCF) obtained by separate multiconfiguration Hartree-Fock (MCHF) calculations [1]. Each PCF is built to represent a specific correlation effect, i.e. valence, core-valence or core correlation. The so-optimized separate PCFs are coupled to each other by solving the associated generalized eigenproblem. But the independent optimization of one-electron sets of orbitals spanning the different PCFs gives rise to radial non-orthogonalities between the correlation subspaces. The evaluation of the Hamiltonian and overlap matrix elements in the PCF basis is realized through biorthonormal orbital transformations and efficient counter-tranformation of the configuration interaction eigenvectors [2]. The latter approach has been implemented in ATSP2K [1] and has been used successfully for the treatment of one-body transition operator. The present study constitutes the first robust tests of this method for the two-body Coulomb operator.

The ground state of Be atom has been used thoroughly for testing various computational strategies and correlation models [3,4]. For this four electrons system, we show that the energy convergence is faster with our simple interaction model than with the usual SD-MCHF method optimizing a common one-electron orbital basis spanning the complete configuration space. Beryllium is a small system for which basis saturation can be achieved through complete active space MCHF expansions. But for larger systems, describing electron correlation in all the space by optimizing a common orthonormal set becomes hopeless. Moreover, our independent optimization scheme can also be used for coupling - through any one- or two-body operator - different and independently optimized physical states, with their own representation. Although looking promising, it raises many questions, especially related in the choice of the zeroth-order model to be used when building the interaction matrix. The present study constitutes the very first step in the current development of a large extension [5] of the ATSP2K package that will adopt the biorthonormal treatment for energies, isotope shifts, hyperfine structures and transition probabilities.

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Novel concepts of quantum search with trapped ions

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The quantum search algorithm of Grover [1] has been one of the driving forces behind the rapid expansion of the field of quantum computation. The standard recipes demand the use of a large number of elementary quantum gates, which require a very high fidelity of each single gate for a reliable operation. We have proposed several novel implementations of Grover's algorithm in a linear chain of trapped ions, which use the intrinsic symmetries of the system to realize the Grover operations — the oracle call and the reflection about the mean – in much fewer physical steps than in the standard approaches [2,3,4]. The quantum register comprises all collective states with m ionic excitations, with examples for $m = 1, 2$ and $N/2$. The database is therefore nonclassical for its size scales as N^m; for $m = N/2$ the scaling is exponential vs N. The system is initialized in an even superposition of all register states, i.e. in the symmetric Dicke state with N ions sharing m excitations [5]. The reflection-about-the-mean operator is produced merely by global addressing of the ion string by an off-resonant pulse with a suitable area [6], whereas the oracle operator is a conditional phase gate. This simplification should allow a demonstration of quantum search in databases of hundreds to thousands of elements without needing to synthesize multiple multi-qubit quantum gates.

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Discreteness and chance in atomic physics

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The discrete structure of matter (atoms) and fields (quanta) implies that free atoms cannot be observed continuously. Rather, they are observed by detecting discrete *elementary events* triggered by spontaneous quantum jumps or particle impact. The occurrence of these elementary events is governed by the laws of chance.

In this contribution we discuss the fundamental change from continuity to discreteness and from determinism to chance, which characterizes the transition from classical to quantum measurements. The quantized structure of the process of observation opens a new perspective on the relation between classical and quantum physics. Since the process of observation is quantized, the objects of physics do not evolve purely dynamically, but are exposed also to influences occurring spontaneously. This influence of chance is fundamental. It gives rise to thermal and statistical noise in precision measurements, and in quantum physics it has to be taken into account by introducing quantum jumps.

A purely dynamic evolution is possible only, if idealized experimental conditions are assumed. In classical dynamics one assumes that the objects can be observed continuously. In this case, the objects are not disturbed by spontaneously occurring events. Quantum dynamics applies to the opposite extreme. Quantum objects are unobservable [1]. The quantum dynamic evolution breaks down, if the object interacts spontaneously with the environment and, hence, becomes observable. By accepting quantum jumps in theory and noise in experimental physics as fundamental ingredients, we are led to the conclusion that quantum and classical dynamics apply to opposite extremes on a scale of observability [2]. However, the two theories are related by correspondence rules.

In contrast to our conclusion, quantum dynamics is often considered as a generalization of classical mechanics [3], and one concludes that only the uncertainty relations give rise to experimental uncertainties, even if the measurements are performed on macroscopic (continuously observable) bodies [4]. From our point of view, this conclusion is wrong, because the presence of thermal and statistical noise due to the observability of the body is disregarded.

The new insight into the quantum-classical relation necessitates a revision of the world picture of physics. The unobservable objects of quantum dynamics have to be considered as unstructured entities embedded in an observable environment. Classical model systems are justified only within the framework of the correspondence rules. We conjecture that ultimately quantum dynamics has a purely mathematical foundation. The correspondence between the classical world of particles and fields moving in space and time and the quantum world may guide the way to the appropriate algebraic structure. Some speculative investigations on a metric quaternion algebra have been performed.

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Hyperfine splitting in hydrogen and lithium: QED effects and electron correlation

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The ground-state hyperfine splitting (hfs) in hydrogen is experimentally known with an outstanding accuracy of a part in 10^{12} for over of 3 decades. Its theoretical description, however, is still limited by the nuclear-structure effects, whose contribution of about 30 ppm cannot be accurately described at present. This difficulty can be partially avoided by studying the normalized difference of the nS and $1S$ hfs intervals, $\Delta_n = n^3\nu(nS) - \nu(1S)$. The nuclear-structure contribution to Δ_n is suppressed by a factor of $(Z\alpha)^2$ as compared to the hfs of a single level, which makes this difference well suitable for testing the magnetic sector of the bound-state QED. In this talk, a calculation of the self-energy correction [1] is reported for the Δ_2 difference of the hfs intervals in light H-like atoms, which removes an important source of uncertainty in theoretical values of Δ_2 in hydrogen and in the helium-3 ion and increases the accuracy of theoretical predictions by a factor of three.

The hfs of lithium is more diffucult to describe theoretically than that of hydrogen. The main problem here is to accurately treat the electron correlation, this task being complicated by the high singularity of the hfs interaction. Because of the high precision of experimental data available, the hfs splitting in lithium has become one of the standard test cases for different theoretical methods of atomic structure calculations. In this talk, I report a large-scale relativistic configuration-interaction calculation of the magnetic-dipole and the electric-quadrupole hfs splitting in ^{7,6}Li and ^{9}Be^{+} [2]. A discussion of various (QED, nuclear-magnetization distribution, recoil, and negative-continuum) corrections is given. This calculation is the first one complete to the relative order α^2 and improves upon the previous studies.

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Hyperfine structure and g factor in heavy ions: towards a test of QED in strong fields

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Investigations of the hyperfine splitting and g factor in highly charged ions give an access to a test of bound-state QED in strongest electromagnetic field available for experimental study. To date, accurate measurements of the ground-state hyperfine structure and of the g factor were performed in several H-like heavy ions and in H-like ^{12}C and ^{16}O ions, respectively. An extension of such kind of experiments to highly charged Li-like ions will provide the possibility to investigate a specific difference between the corresponding values for H- and Li-like ions, where the uncertainty due to the nuclear effects can be substantially reduced. Achievement of the required theoretical accuracy for the hyperfine structure and for the g factor in the case of Li-like ions is a very interesting and demanding challenge for theory.

The paper will focus on one of the most difficult correction, namely, the screened QED correction in the presence of a magnetic field. The state-of-the-art calculation of screened QED correction is based on the employment of a local screening potential. A report on a crucial step made towards the rigorous evaluation of the complete gauge-invariant set of the screened one-loop QED corrections will be provided. The calculations have been performed in both Feynman and Coulomb gauges for the virtual photon mediating the interelectronic interaction. As a result, we have increased the theoretical accuracy for the specific difference between the hyperfine splitting values of H- and Li-like ions as well as for the g factor of Li-like ions.

Relativistic R-matrix calculation for photoionizations of atomic magnesium

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The photoionization cross sections of the ground level ($3s^2\ ^1S_0$) of magnesium, in the energy region between the $Mg^+(3s)$ and $Mg^+(3p)$ threshold, has been calculated theoretically using the fully relativistic R-matrix method [1]. The resonance positions and widths have also been obtained and compared with a recent experiment [2]. Five Rydberg series of doubly excited states have been exhibited in Fig. 1, i.e., $3pns\ ^1P$, $3pnd\ ^1P$, $3pns\ ^3P$, $3pnd\ ^3D$ and $3pnd\ ^3P$, which are in excellent agreement with experimental measurements. As we know, it is the first time that the $3pnd\ ^3P$ were identified as the new fifth series.

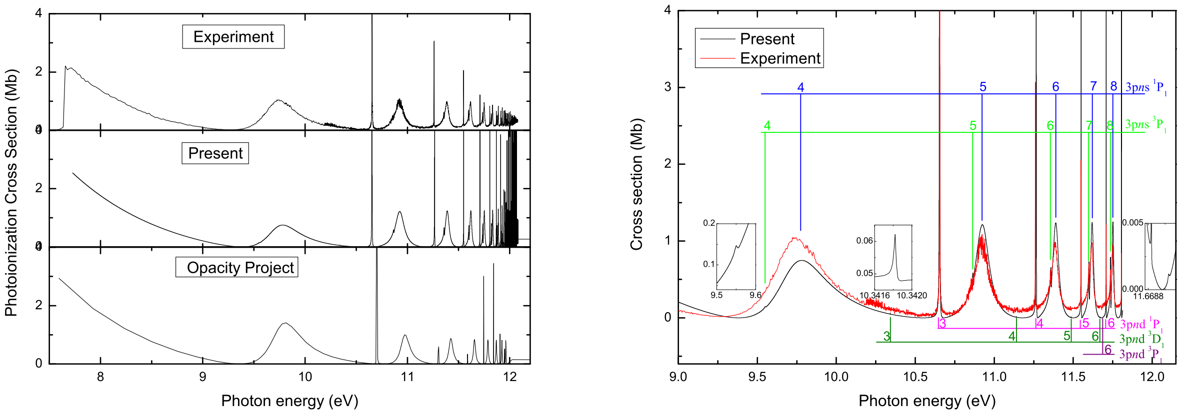

Figure 1: Comparison of present calculated cross sections with experimental results by Wehlitz *et al.* [2] and OP results by Butler *et al.* [3].

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Changes of the electron charge density of E1, M1, E2 and mixed type transitions of lead

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The isotope shift of atomic spectral lines consists of two contributions, this caused by the finite nuclear mass and that resulting from the field effect. In heavy elements (such as lead) the mass effect is negligible and the field effect, which increases with increasing Z, roughly accounts for the observed shifts. The field shift originates from the changes of the size and shape of the nuclear charge distribution when neutrons are added to the nucleus. As a consequence the binding energies of electrons which penetrate the nucleus differ among various isotopes. Thus the field shift is the result of multiplying a nuclear parameter and an electronic factor (F_i). The F_i depends on the changes of the electron charge density at the nucleus $\Delta\left|\psi(0)\right|_i^2$ in the i transition as follows:

$$F_i = \pi a_0^3 \Delta \left|\psi(0)\right|_i^2 f(Z)/Z \tag{1}$$

There are three ways by which this quantity can be obtained. It can be taken from experiments, but also it can be calculated theoretically by the use of both *ab initio* or semiempirical methods. Theoretical data available in literature for the $\Delta\left|\psi(0)\right|_i^2$ of the allowed and multipole lines of lead are scant. Calculations of the probability densities for the lowest configurations of Pb I have only been performed in [1,2]. To our knowledge there are no experimental data concerning this problem. So, the analysis of the 24 allowed (E1) [3] and forbidden (M1, E2 and M1+E2) [4] transitions of lead have been performed and the changes of the electron charge densities have been determined.

The measurement of the $\Delta\left|\psi(0)\right|_i^2$ can provide a test of theoretical wave-function calculations. These values can be also compared with the calculated screening ratios. In addition accurate knowledge of field shifts and the probability densities can be essential for future measurements of parity nonconserving optical rotation in lead.

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SWNTs in transverse electrostatic fields

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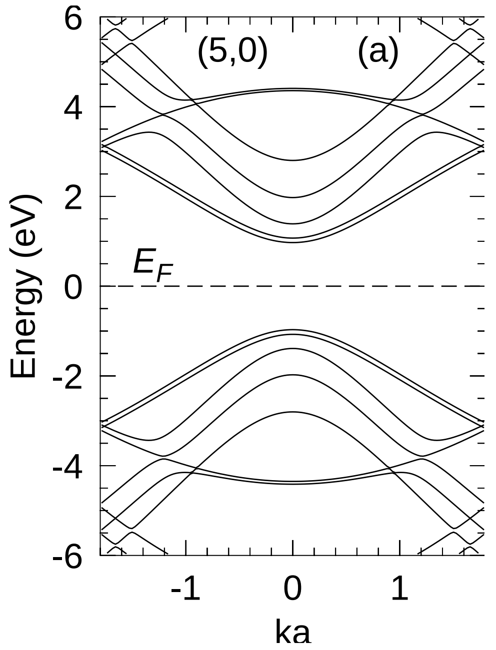
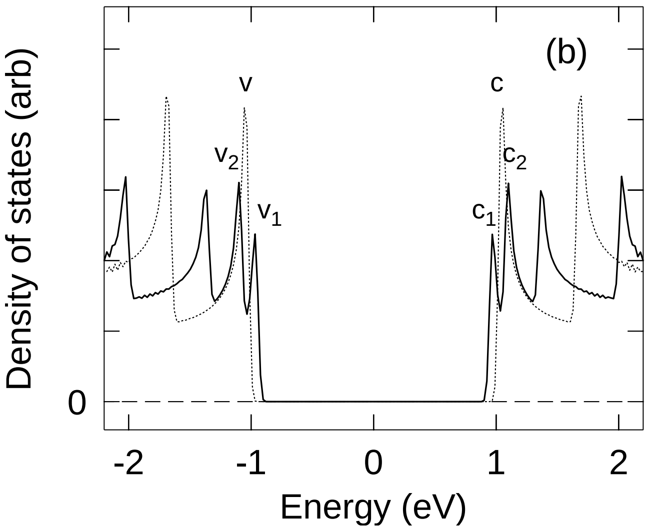
Previous theoretical calculations have shown that the electronic properties of single-walled carbon nanotubes (SWNTs) are very sensitive to their geometrical structure. Carbon nanotubes can be metals or semiconducters with a very sensitive energy gaps, depending on the diameter and helicity of the tubes. The main purpose of the present work is investigation of band structure of nanotubes in presence of transverse electrostatic fields. As an illustration we consider zigzag tubes and restrict ourselves the the π and π^* bands. Our calculations for single-walled carbon nanotubes was done using tight-binding approximation [1] modified to the case of external electric field. It is known if an atom is placed in an external electric field, its energy levels are altered. This phenomenon is known as the Stark effect. In our calculations we supposed that the electric field is weak and the displacement of the atomic energy levels is determined by a second-order effect with respect to the field ([2], page 285).

Below we illustarte our results for zigzag SWNT with chirality (5,0). In our calculations we used parameters $a = \sqrt{3}d_{cc}$, where $d_{cc} = 2.72$ au denotes distance between two neighbouring carbon atoms and tight-binding parameter $V_{pp\pi} = -2.7$ eV [3]. The dispersion curves are ploted in the left panel (a). The right panel (b) represents densities of states for isolated nanotube (thin dashed curve) and nanotube in the electric field (solid curve). We can see that van Hove singularities that reflect the quantized momentum component along the circumferential direction may split into two singularities.





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Shell model calculations for alkali halide molecules

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This work applies the shell model to study the behaviour of the internuclear interactions of diatomic alkali halide molecules from data given by the dynamical models for alkali halide crystals. Our interest is to test the breathing shell model when core holes have been introduced. This will provide another source of information on the nature of the interaction potential between anion and cation systems and give insight into the rate of relaxation in determining shifts in Auger and photoelectron spectroscopy.

It is well known that environmental shifts in photoelectron (PES) and Auger (AES) spectroscopies are due both to chemical shifts characterizing the initial state and to final state relaxation shifts. In specifying shifts in elemental solids and related compounds the free atom is often used as reference; then PES and AES are combined to isolate the so called extra-atomic relaxation, a quantity which is independent of experimental energy reference. The modified Auger parameter α' gives similar information. Alkali halide molecules are attractive systems for investigation, because the interatomic forces are well understood in the initial state, and it appears that chemical shift and relaxation are of comparable importance in their electron spectroscopy[1-3].

a) Rittner model

The influential Rittner potential [1] assumes the ions to be polarisable spherical charge distributions with full ionicity, and it is usually of the form:

$$U(r) = -\frac{1}{4\pi\varepsilon_0}\left[\frac{1}{r} + \frac{\alpha_+ + \alpha_-}{2r^4} + \frac{2\alpha_+\alpha_-}{r^7}\right] - \frac{C}{r^6} + R(r) \tag{1}$$

where α_+ and α_- are the polarisabilities of the alkali ion and halogen ion, respectively, $R(r)$ is a two parameter repulsion term (usually Born-Mayer). The second and third terms represent a dipole-dipole and a quasi-elastic energy stored in the induced dipole moments, and are valid for internuclear separation large cornpared with ion dimension.

b) The shell modell

The diatomic molecule is considered to contain a positive ion, which to first order can be considered as a point charge (+e)' and a negative ion contains a rigid shell of charge (Ye) and a core of charge (Xe), where $X + Y = -1$. In the presence of an electric field the shell centre will be displaced by distance ω, and the total potential $\Phi(R, \omega, \xi)$ can be described by the different contributions; electrostatic, polarization, deformation, and short range interactions:

$$\Phi(R, \omega, \xi) = \varphi_{es}(r, \omega) + \varphi_{pol}(\omega) + \varphi_{def}(\xi) + \varphi_{int}(R, \xi) \tag{2}$$

where $\varphi_{pol}(\omega) = 1/2k\omega^2$, $\varphi_{def}(\xi) = 1/2h_2\xi^2$, $\varphi_{def}(\xi) = 1/2G_2(\rho - \rho_0 - b)$ for anisotropic deformation and $\varphi_{int}(R, \xi) = B \pm \exp(-\alpha \pm r) - (C \pm r^6) - (D \pm r^8)$.

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Adiabatic potentials of single ionized diatomic potassium molecule

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We calculate adiabatic potential energy curves of the singly ionized potassium dimer. These curves are tabulated along the internuclear separation with the various step. Calculations are performed with the use of the MOLPRO package. Some comparisons are made with the available theoretical results and experimental data. In our effective one electron approach the core electrons are represented by pseudopotentials. This is quite analogous to the our previous calculations on single ionized lithium dimer [1]. Calculation methods and detailed results of the electronic ground state and several exited states will be presented at the conference.

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Highly-excited electronic states of the lithium dimer

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We report adiabatic potential energy curves for highly-excited electronic states of the lithium dimer. Calculated singlet and triplet, $\Sigma_{g,u}^{+,-}$, $\Pi_{g,u}$ and $\Delta_{g,u}$ states correlate to Li(2p)+Li(2p), Li(2s)+Li(3p), Li(2s)+Li(3d), Li(2s)+Li(4s), Li(2s)+Li(4p) and Li(2s)+ Li(4d) excited atomic asymptotes. These results are complement of our previous calculations for adiabatic potentials of Li_2 molecule [1]. We present comparisons between our results and other theoretical and experimental ones. To calculate with very high precision our long range adiabatic potentials of the Li_2 dimer, we use multiconfigurational self-consistent field/complete active space self-consistent field (MCSCF/CASSCF) method and multi-reference configuration interaction (MRCI) method. In this approach we do not include spin-orbit interaction. All calculations are performed by means of the MOLPRO program package [2].

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Time-dependent description of electronic predissociation in the LiH molecule

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Our attention is focused on the theoretical treatment of electronic predissociation processes in the lithium hydride molecule. We base our considerations on the NaI dimer, which is an interesting and well studied prototype molecule in femtochemistry [1-5]. We propose to investigate the LiH molecule which shows similar interesting behavior as NaI. Our project is divided into two parts: electronic structure calculations and nuclear wave packet dynamics induced by femtosecond laser pulses.

To calculate adiabatic potential energy curves of the LiH dimer we use multiconfigurational self-consistent field/complete active space self-consistent field (MCSCF/CASSCF) method and multi-reference configuration interaction (MRCI) method. In this approach we do not include spin-orbit interaction. All calculations are performed by means of the MOLPRO program package. In order to describe the two-channel electronic predissociation in the lithium hydride molecule, we have decided to consider five lowest laying adiabatic and diabatic potential energy curves for singlet sigma states, which correlate to the Li(2s)+H(1s) ground atomic asymptote and Li(2p)+H(1s), Li(3s)+H(1s), Li(3p)+H(1s), Li(3d)+H(1s) excited atomic asymptotes. Using adiabatic potentials and split diabatic representation method, we obtain diabatic potential energy curves. In order to present the nuclear wave packet dynamics induced by (ultraviolet) femtosecond laser pulses, we have to also calculate non-adiabatic couplings between considered states and transition dipole moments. These results are also performed by means of the MOLPRO program package [5] and overall agreement with other theoretical data is very reasonable. Calculated adiabatic and diabatic potentials, non-adiabatic couplings and transition dipole moments allow us to present and describe the two-channel electronic predissociation in lithium hydride molecule. We have decided to consider the transition from the $1^1\Sigma^+$ ground state, to $3^1\Sigma^+$ excited state. After transition we will investigate the propagation of the wave packet in the system of three crossings between the three lowest lying singlet sigma states of the LiH dimer.

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Theoretical study of the vibrational and electronic structure of the KLi dimer

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Alkali homo- and heteronuclear dimers have attracted attention of experimentalists and theoreticians for many years. Nowadays, cold molecular physics and chemistry are based mainly on these molecules. We report theoretical study of the vibrational and electronic structure of the KLi dimer. All calculated adiabatic potential energy curves are performed by means of the MOLPRO program package [1]. We present singlet and triplet, Σ, Π and Δ electronic states, which correlate to ground and several low-lying excited atomic asymptotes. Spectroscopic parameters for all states are also determined. We present comparisons between our results and other theoretical and experimental ones [2-4]. To calculate with very high precision our long range adiabatic potential energy curves of the KLi dimer, we use multiconfigurational self-consistent field/complete active space self-consistent field (MCSCF/CASSCF) method and multi-reference configuration interaction (MRCI) method.

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Angular distributions of atomic photoelectrons ejected by strong laser field

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We consider a charged particle, initially bound by an atomic potential, which is ejected from an atom by very short and strong laser pulses described in the dipole approximation by the electric field. When the external field is very strong the conventional time dependent perturbation theory cannot be used and no solution of the Time Dependent Schödinger Equation (TDSE) can be found in a closed form without some approximations. In this case, laser-atom interaction can be described by S-matrix formalism [1] and Strong Field Approximation (SFA) where the Coulomb potential is taken into account as a perturbation. We calculate direct ionization amplitude, when the electron does not experience the binding potential, and first correction to this approximation which corresponds to rescattering when the electron, after ionization, back to parent ion and scatters elastically. This calculation has been performed analytically and semi-analytically. We present angular distribution of ejected electron in the tunnelling regime. It can be observed that for the high photon energy the angular distributions show more complicated structure.

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XUV frequency comb spectroscopy

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Precision spectroscopy in the extreme ultraviolet on helium atoms and ions is very interesting as it could provide more stringent tests of quantum electrodynamics than currently possible with hydrogen. One problem is that spectroscopy in this region typically requires amplification and harmonic upconversion of visible light sources, which can introduce difficult to control systematic errors as a result of so-called frequency-chirping effects [1,2]. This issue can be overcome using a combination of amplification and harmonic upconversion of a frequency comb laser. With this technique a pair of phase-locked extreme ultraviolet pulses is generated and used to excite the $1s^2\ {}^1S_0{-}1s5p\ {}^1P_1$ transition in helium. Viewed in the frequency domain, the spectrum of the pulses in the XUV resembles again a frequency comb, but now in the form of a cosine-modulated spectrum. Viewed in the time-domain, excitation with phase-locked pulses is in fact a form of Ramsey excitation (see e.g. [3,4]).

The setup consists of a Ti:Sapphire frequency comb as a source of phase controlled pulses at 773 nm. A dedicated parametric amplifier is used to amplify two subsequent pulses from the comb laser to a few mJ per pulse. The 15th harmonic is used to excite the $1s^2 1s5p$ transition in atomic helium at 51.56 nm. The excited atoms are ionized with an infrared laser pulse at 1064 nm and detected in a time of flight spectrometer. By changing the delay between the pulses (i.e. the repetition rate of the frequency comb laser) in one-attosecond steps, we scan the cosine-shaped comb over the transition.

To achieve an accuracy in the MHz range, a careful analysis is required of phase shifts and wave front deformation in the amplification and the harmonic upconversion process, as it shifts the positions of the modes in the XUV. This is achieved with an interferometric measuring technique which has a single-laser shot accuracy of 10 mrad [5]. Many other systematic effects have been investigated in detail, which should allow an initial target accuracy of 10 MHz for the ground state of helium (which is 5 times the current best value [1,2])

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Density matrix description of ultra-short light pulses propagation and the multiple light storage effect in a double Λ configuration for cold atoms

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We investigate the influence of the Multiple Light Storage (MLS) [1] of the quantum information on the area of initially ultra-short light pulse. The propagation dynamics and its soliton-like behavior are investigated for the double Λ excitation within the hyperfine structure of the D1 line in cold sodium and rubidium atoms. The governing equations are the Maxwell's field equations for the radiation fields and the Liouville-von Neumann equations for the density matrix of the dressed atom. We have incorporated the atomic relaxations both radiation and collisional. The four color propagated pulses are assumed to be initially on resonance with their respective dipole-allowed transitions. Our numerical results show that the MLS is responsible for the production as well as the stabilization of the area for the propagating pulses. In addition we show that the presented optical soliton-like solution to the reduced Maxwell's field equations gives a good resemblance to the Manakov-like solitons [2-4] where in our case the MLS reveals the information transfer as well as the energy exchange among these solitons. It is to be emphasized that, in the present study, we have ignored the diffraction terms in the propagation of the coupled reduced-Maxwell's field equations. The present analysis is important for developing optical memory devices as well as optical switches.

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Collisions of ultracold polar molecules in microwave traps

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The collisions between linear polar molecules, trapped in a microwave field with a circular polarization, are theoretically analyzed. The microwave trap suggested by DeMille[1] seems to be rather advantageous in comparison with other traps. Here we have demonstrated that the microwave trap can provide the successful evaporative cooling for polar molecules not only in their absolute ground state but also in almost any strong-field seeking states and the collision losses should not be of much concern to them[2]. But the state in which molecules can be safely loaded and trapped depends on the frequency of the AC-field.

In this work we are studying the collisional dynamics of linear polar molecules in the $^1\Sigma$ and $^2\Pi$ states. For $^1\Sigma$ state molecules the collisional dynamics is mostly controlled by two ratios ν/B and $x = \mu_0 E_0/hB$ (ν is the microwave frequency, B is the molecular rotational constant, μ_0 is the dipole moment, and E_0 is the electric field strength). The AC- Stark splitting is characterized by $|J, M, n>$ states, where M is the projection of rotation spin J and n is the deviation of the photon number. We are mostly interested in the lowest energy strong-field-seeking state of the ground vibrational state, $|JM>=|00>$ and found rather large inelastic cross sections for molecules even in this state. But we found that the nature of this inelasticity is simply the "undressing" of molecules by one photon each and should not cause the loss of molecules from the trap. From the loading with molecules point of view we suggested that it is "safer" to load $|J = 0, M = 0>$ molecules at $\nu/B < 2$, $|J = 1, M = -1>$ at around $\nu/B = 3$, $|J = 2, M = -2>$ at around $\nu/B = 5$ and so on and it would be better to have the parameter $x < 1$ which makes the regions of strong mixing smaller. But x must not be too small in order to keep the depth of the trap practical. We are considering the collisional dynamics of $^2\Pi$ state like OH molecules[3] and discussing that now ratios ν/Δ and $x = \mu_0 E_0/\Delta$ (Δ is Λ-doubling splitting) play as controlling parameters.

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Anticrossing spectroscopy of He atoms excited by 10-30 keV He^+ and He impact

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The anticrossing spectroscopy has been used to determine the post-collisional states of He atoms excited by He^+ - ion impact for a wide energy range of projectiles [1]. It was shown, that for the intermediate energy, where the velocity of the projectiles is comparable with the Bohr velocity v_B, saddle dynamics [2] and electron promotion based on the atomic Paul trap mechanism [3] are suitable to describe this excitation process. The post-collisional He I states are coherent superpositions of spherical states with large electric dipole moments. These superpositions states vary from purely parabolic states for the projectile velocity vp $\approx$ 0.6 v_B (30 keV) to superpositions of $l \leq 2$ states for vp $\approx$ 1.7 v_B (300 keV).

In the present investigations we analyzed the excitation of He atoms by He^+ - ions and He-atoms impact for lower projectiles velocities 0.3 v_B – 0.6 v_B (10 – 30 keV). In this energy range single-electron excitation cross-sections of the 1s4l and 1s5l states change rapidly from near to minimum, to maximum at 35 keV. Therefore the anticrossing spectra of the spectral lines $\lambda(1s4l\text{-}1s2p\ ^3P)$=447 nm and $\lambda(1s5l\text{-}1s2p\ ^3P)$=402.6 nm have been measured for both He^+-ion and He - atom projectiles for several energies. In both cases the target and projectile atoms can be excited to the singlet states by direct excitation and to the triplet states by electron exchange. However, the evolution of He - He system with four equivalent electrons is more complex than the evolution of He^+ - He system, where one electron is promoted on two-centre potential of the He^+ - ions. In the measurements the interference filters with 2 nm half widths were used to fully separate the recorded spectral lines. It allows us to use the distributions of the amplitudes of the anticrossing peaks as well the shapes of the recorded anticrossing signal to determine post-collisional states of the target atoms.

Our measurements show, that these states possess electric dipole moments, that is, the charge distributions of the electronic clouds are asymmetric. This asymmetry is mainly due to coherent population of the $l \leq 2$ states.

Acknowledgment

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Precision spectroscopy of the 3s-3p fine-structure doublet in Mg^+

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Precision spectroscopy on single trapped ions has reached tremendous accuracies by probing narrow transitions in the resolved-sideband regime [1]. However, a variety of interesting transitions may not be studied in this regime, because their transition linewidths well exceed common (secular) trap frequencies. Accurate spectroscopy is then challenging, since an interrogating laser induces detuning-dependent heating and cooling which distorts the line profile. We present both theory and experimental demonstration of a spectroscopic method (Fig.1) which overcomes these limitations and allows to observe essentially unperturbed Voigt profiles with high signal-to-noise ratio (Fig.2) [2].

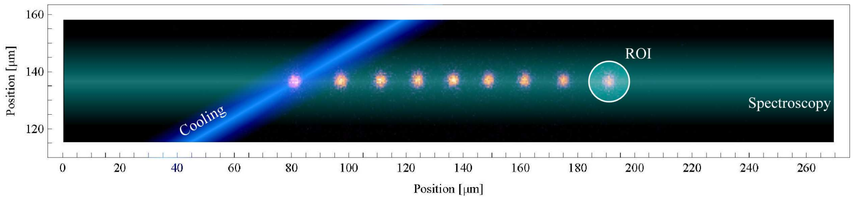

Figure 1: An ion chain is continuously laser cooled at one side only, a weak spectroscopy laser along the trap axis probes sympathetically cooled ions. This method allows for efficient sympathetic cooling, minimizes light shifts and background photons.

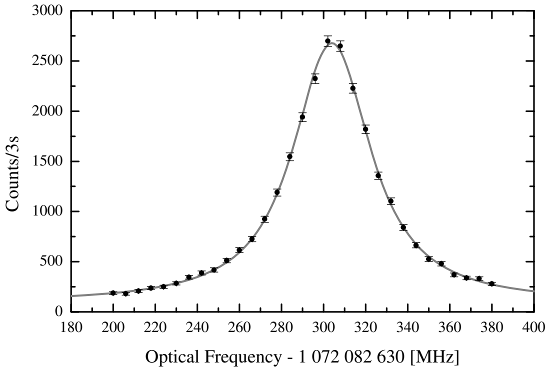

Figure 2: Typical line scan from a single trapped $^{24}Mg^+$ ion.

We deduce absolute frequency reference data for transition frequencies, isotope shifts and fine structure splittings that are in particular useful for comparison with quasar absorption spectra, to test possible space-time variations of the fine structure constant [3,4]. The measurement accuracy improves previous literature values, when existing, by more than two orders of magnitude.

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Ultracold polar molecules

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Polar molecules – molecules exhibiting a permanent electric dipole moment – have bright perspectives as systems with long-range and anisotropic interaction. These interactions have been the basis for numerous exciting theoretical proposals ranging from ultra-cold chemistry, precision measurements and quantum phase transitions to novel systems for quantum control with external magnetic and electric fields. I will present our recent work on the creation and characterization of a near-quantum degenerate gas of absolute ground-state polar ^{40}K^{87}Rb molecules.

Dipole-dipole interaction of several cold Rb Rydberg atoms

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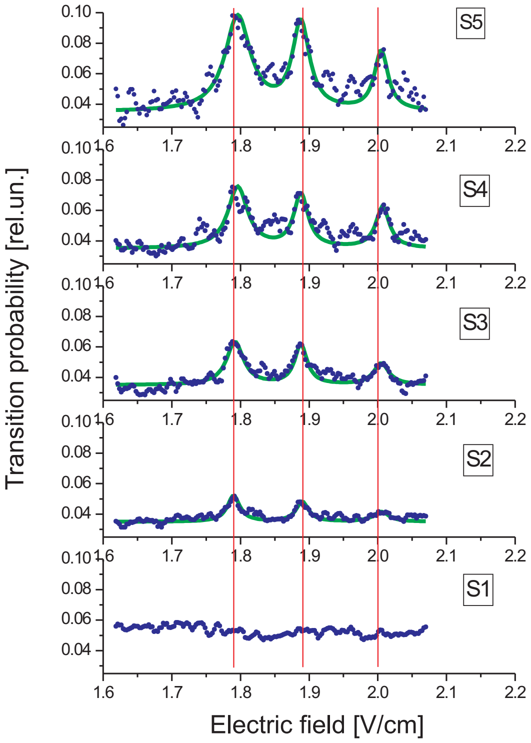

Figure 1: Spectra of the resonant dipole-dipole interaction.

Long-range interactions of Rydberg atoms can be used to implement quantum logic gates of a quantum computer based on neutral atoms. We studied the dipole-dipole interaction of a small definite number of cold rubidium Rydberg atoms trapped in a MOT [1].

The initial $37P$ Rydberg state was excited by two pulsed lasers in a crossed-beam geometry. The laser beams were focused inside of the cold atom cloud and intersected at right angles, providing a small excitation volume of 30 μm in size. Each laser pulse excited several Rydberg atoms, which were detected using the selective field ionization technique and a channeltron, which provided a single-atom resolution of up to 5 atoms.

We observed the Förster resonance transitions driven by dipole-dipole interaction:

$$\mathrm{Rb}(37P)+\mathrm{Rb}(37P) \rightarrow \mathrm{Rb}(37S)+\mathrm{Rb}(38S)$$

Exact resonance for this energy-exchange process was achieved by Stark tuning of the Rydberg energy levels. The atomic signals were sorted over the number of detected atoms. The spectra of the resonant dipole-dipole interaction for selectively detected 1 to 5 Rydberg atoms are shown in Fig. 1. The red lines indicate the calculated positions of the resonances. The dependences of the peak heights and widths on the number of Rydberg atoms are analyzed and compared with theory using a many-particle Monte-Carlo model for definite number of Rydberg atoms randomly positioned in the excitation volume.

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Quasiclassical calculations of BBR-induced depopulation rates and effective lifetimes of alkali-metal Rydberg atoms

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Rates of depopulation by blackbody radiation (BBR) and effective lifetimes of all alkali-metal nS, nP and nD Rydberg states have been numerically calculated for $n = 10 - 80$ at the ambient temperatures of 77, 300 and 600 K [1]. Quasiclassical formulas of Dyachkov and Pankratov [2] were used to calculate the radial matrix elements of the dipole transitions from Rydberg states. The advantage of the used quasiclassical model is its relative simplicity that nevertheless provides a good agreement with more sophisticated quantum-mechanical calculations.

We have also obtained a simple formula for estimates of BBR-induced depopulation rates that is valid for both low and high values of n (in atomic units):

$$\Gamma_{BBR} = \frac{4}{3n_{eff}^{5}c^{3}} \frac{1}{\exp\left[1/(n_{\mathit{eff}}^{3}T)\right] - 1} \tag{1}$$

Here n_{eff} is the effective quantum number and c is the speed of light. For practical use a modified Eq. (1) can be written in units of [s^{-1}] for temperature taken in Kelvins:

$$\Gamma_{BBR} = \frac{A}{n_{eff}^{D}} \frac{2.14 \times 10^{10}}{\exp\left[315780 \times B/(n_{\mathit{eff}}^{C}T)\right] - 1} \quad \left[\mathrm{s}^{-1}\right]. \tag{2}$$

The scaling coefficients A, B, C and D, obtained for all alkali-metal atoms [1], were introduced for better approximation of the numerical results. For high $n \sim 80$ the error of the approximation is less than 8%, while for $n \sim 50$ it is as low as 3.5%. Good agreement was observed with the recent experimental results [3] for Rb nS and nD states, while for nP states the theoretical curve goes below the experimental points. This points towards the need of new measurements in an extended n range.

Acknowledgment

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Speed dependence and dispersion-like asymmetry of the 326.1 nm ^{113}Cd line perturbed by Ar and Xe

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Precise measurements of line shapes of two hyperfine-structure components (F'=1/2→ F"=1/2 and F'=3/2→F"=1/2) of the intercombination 326.1 nm line corresponding to the 5^1S_0-5^3P_1 transition for the even-odd ^{113}Cd isotope perturbed by argon and xenon have been done. The laser-induced fluorescence experiment was performed using recently upgraded digital laser spectrometer [1], which allowed us to verify available data on the isotope structure of the line under investigation as well as to determine the value of the hyperfine splitting of the upper state 5^3P_1. The analysis was performed using the speed-dependent asymmetric Voigt profile (SDAVP). Functions describing the speed-dependence of the collisional broadening and shifting, incorporated in SDAVP, depend on assumed interaction potential for given emitter-perturber systems. Values of the broadening, shift and asymmetry coefficients for Cd–Ar and Cd–Xe determined in the course of a careful analysis are reported. The influence of the assumed interaction potential as well as the isotope and hyperfine structure on line shape parameters is discussed.

Effects due to the correlation between pressure and Doppler broadening of the 326.1 nm line were observed for both Cd-Ar and Cd-Xe systems (the emitter to perturber mass ratio for these systems equals to 0.35 and 1.15, respectively). Obtained values for the dispersion-like asymmetry confirm the presence of the effect associated with the finite time of the collision. No evidence has been found, however, for the existence of the line-mixing asymmetry in given systems.

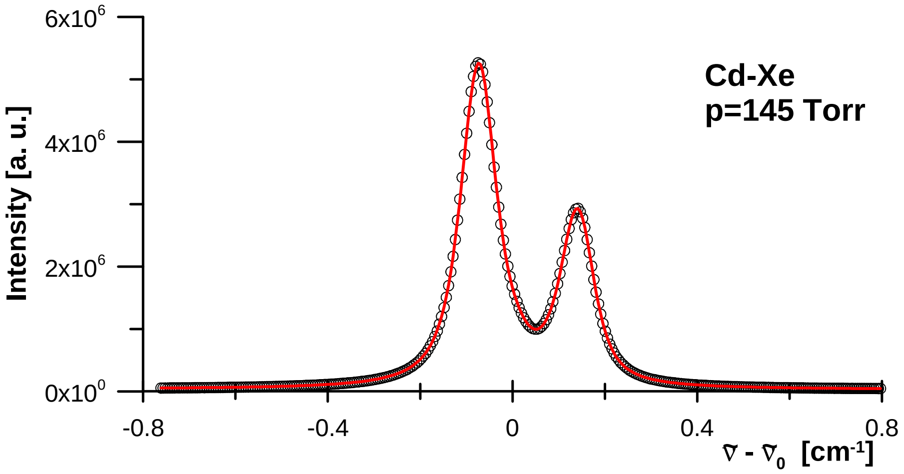

Figure 1: Line shape of 326.1 nm ^{113}Cd line perturbed by Xe at pressure 145 Torr: circles - experimental profile, solid line - fitted SDAVP

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Experimental and theoretical radiative decay rates for highly excited ruthenium atomic levels and the solar abundance of ruthenium

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Ruthenium plays an important role in stellar nucleosynthesis. When the stars are in the AGB phase, they experience thermal pulses, generating a rich nucleosynthesis by the *s*-process. The convective envelope of the star may penetrate the region where s-process elements have been produced, and may bring them to the stellar surface, where they become observable. A few s-process elements are particularly interesting in that respect because they provide information on the time scales involved in the process. Ruthenium is among these elements.

In the sun, nine Ru I lines were used to derive the solar content of this element [1] on the basis of the Holweger & Müller model [2]. This analysis, however, suffered from the lack of accurate branching fractions (BF), the only values available at that time being those of Corliss & Bozman [3]. In addition, this work represented a standard stellar abundance analysis based on a time-independent one-dimensional (1D) model atmosphere in hydrodynamic equilibrium. Since that time, there has been progress concerning our knowledge of the atmosphere of the sun with the advent of new three-dimensional (3D), time-dependent, hydrodynamical models (see e.g. [4-5]). As a consequence, a new determination of the solar abundance of ruthenium is now needed.

In the present work, the solar photospheric abundance of ruthenium is revised on the basis of a new set of oscillator strengths derived for Ru I transitions with wavelengths in the spectral range 225.0 to 471.0 nm. The new abundance value (in the usual logarithmic scale), $A_{Ru} = 1.72 \pm 0.10$, is in agreement with the most recent meteoritic result, $A_{Ru} = 1.76 \pm 0.03$. The accuracy of the transition probabilities, obtained using a relativistic Hartree-Fock model including core-polarization effects, has been assessed by comparing the theoretical lifetimes with previous experimental results. A comparison is also made with new measurements performed in the present work by the time-resolved laser-induced fluorescence spectroscopy for 10 highly excited odd-parity levels of Ru I.

The present results will be published in MNRAS.

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Lifetime measurements in singly ionized ruthenium. Oscillator strength and Landé factor calculations in singly and doubly ionized ruthenium.

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Determination of the Ru abundance in the atmospheres of stars of different spectral classes is important for understanding nucleosynthesis processes in the late stages of stellar evolution. Robust identifications of this element however are rare in upper main sequence CP stars. Cowley et al. (2008) suggested that Ru II was present in the unusual star HD 65969, based on wavelength coincidence statistics. In Przybylski's star (HD 101065), some Ru II identifications were also made by Cowley and Bidelman. For more details, see [1]. Also in the star HR 465, a number of identifications have been attributed to Ru I and Ru II transitions (see [2]).

A new set of theoretical f-values is reported for 138 Ru II transitions of astrophysical interest involving energy levels below 58022 cm^{-1}. The theoretical model, i.e. the relativistic Hartree-Fock (HFR) approximation including core-polarization effects [3,7], has been tested by comparing theoretical lifetimes with new measurements performed by time-resolved laser-induced fluorescence spectroscopy (TR-LIF) [5,6] for 23 4d^6(^{5}D)5p odd levels of Ru II and also by comparing theoretical and experimental Landé g-factors.

As an extension of these results, the first set of transition probabilities is proposed for 25 strong lines depopulating the 4d^{5}5p ^{6,7}P° terms of Ru III.

The present results are expected to help the astrophysicists for more quantitative investigation of the chemical composition of these CP stars based on robust line identifications. The analysis of some stellar spectra on the basis of the new f-values obtained in the present work is indeed in progress but the details will be reported elsewhere.

The present results will be published in A & A.

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Transition probabilities of astrophysical interest in Niobium ions (Nb II and Nb III)

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About half of the stable nuclei heavier than iron are believed to be synthesized through a slow *s*-process in the late stages of the evolution of stars with masses in the approximate range 0.8 - 8 M_{Sun}. This process occurs when the star is in the AGB phase of its life. A few *s*-process elements are particularly interesting because, along with giving a clue for the mere operation of the *s*-process, they provide information on the time scales involved. These elements are technetium, niobium and ruthenium.

In the present work, we have obtained a new set of accurate transition probabilities in niobium ions (Nb^+ and Nb^{2+}) for selected transitions of astrophysical interest.

To our knowledge, no transition probabilities or radiative lifetimes at all are available so far for Nb^{2+}. Experimental or theoretical transition probabilities in the spectrum of Nb II are very scarce. The most recent experimental work in Nb II is due to Nilsson & Ivarsson [1] who were able to measure branching fractions (BF) of 145 lines in the wavelength interval 260 - 460 nm and to deduce hyperfine splitting constants for 28 even and 24 odd levels.

In the present work, 17 lifetimes of Nb^+ have been measured with the time-resolved laser-induced fluorescence technique [2] and the results compared to HFR calculations including core-polarization effects [3,4]. New BFs have been also obtained with high-resolution Fourier transform spectroscopy.

A particularly good agreement is observed between theory and experiment and this agreement gives considerable weight to the new set of oscillator strengths obtained for 109 transitions of Nb II in the range 259-392 nm. Transition probabilities are also proposed, for the first time, for 76 Nb III transitions with wavelengths in the range 143 - 315 nm.

Application of the new results to the determination of the chemical composition of the sun and some r-process-rich very metal-poor stars will be discussed.

The present results will be published in A & A.

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Pulsed photodetachment microscopy and the electron affinity of Iodine

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A new position sensitive electron detector is used to carry out photodetachment microscopy in a pulsed-laser excitation scheme. In a more indirect detection scheme than with the first photodetachment microscope [1], every MCP-amplified photoelectron bunch is first sent onto a phosphor screen. The accumulated image of multiple electron impacts is then recorded every two laser pulses by a digital camera. Software analysis reduces the information to the barycentre of every electron impact, so as to recover the best possible spatial resolution. Histogramming these individual photoelectron events makes it possible to reconstruct the electron interferogram produced by photodetachment in an electric field with a resolution similar to CW-laser photodetachment microscopy [2].

The possibility of producing photoelectron interferograms in a pulsed regime makes a greater variety of laser sources available for photodetachment microscopy and opens the way to new experiments. Pulsed laser sources can be e.g. easily frequency doubled. This was the way we used to produce 405 nm radiation [3] suitable for the detachment of I^- negative ions. The standard double-pass technique was used to eliminate the unknown Doppler shift [4] and produce a Doppler-free measurement of the photoelectron kinetic energy, the variations of which were, as usual, checked against the variation of the laser wavenumber. The electron affinity of Iodine that can be deduced from this study [5], ${}^{e}\!A({}^{127}\mathrm{I})=2\,467\,287.4(29)\ \mathrm{m}^{-1}$, or 3.059 046 3(38) eV, improves the accuracy on ${}^{e}\!A({}^{127}\mathrm{I})$ by more than a factor of two with respect to the former measurement [6].

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Cold atoms gravimeter

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In the frame of the watt balance project led by Laboratoire National de Metrologie et d′Essais (LNE) and aiming at a new definition of the mass unit (the kilogram), SYRTE develops an absolute gravimeter. It will enable to obtain an extremely precise measurement of the gravity acceleration g. The principle of operation of this apparatus is based on techniques of atomic interferometry using cooled atoms. In a first step, about hundred millions atoms are captured in a magneto-optical trap. The atoms are cooled down to a temperature close to 2.5 micro Kelvin, before being released. During their free fall, they are submitted to a sequence of three laser pulses which split and recombine the atomic wave packets. Finally, the phase shift between the two arms of the interferometer, proportional to g, is deduced from the atomic state measurement at the output of the interferometer. The instrument sensitivity is currently 2 10-8g for a 1s measurement time, at the same level as the current State of the Art in classical absolute gravimeters. The evaluation of systematic effects is in progress and should enable to reach a relative accuracy of $10 - 9$.

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Line shapes of optical Feshbach resonances near the intercombination transition of bosonic Ytterbium

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The properties of bosonic Ytterbium photoassociation spectra near the intercombination transition $^1S_0$–$^3P_1$ are studied theoretically at ultra low temperatures. We demonstrate how the shapes and intensities of rotational components of optical Feshbach resonances are affected by mass tuning of the scattering properties of the two colliding ground state atoms. Particular attention is given to the relationship between the magnitude of the scattering length and the occurrence of shape resonances in higher partial waves of the van der Waals system. We develop a mass scaled model of the excited state potential that represents the experimental data for different isotopes. The shape of the rotational photoassociation spectrum for various bosonic Yb isotopes can be qualitatively different.

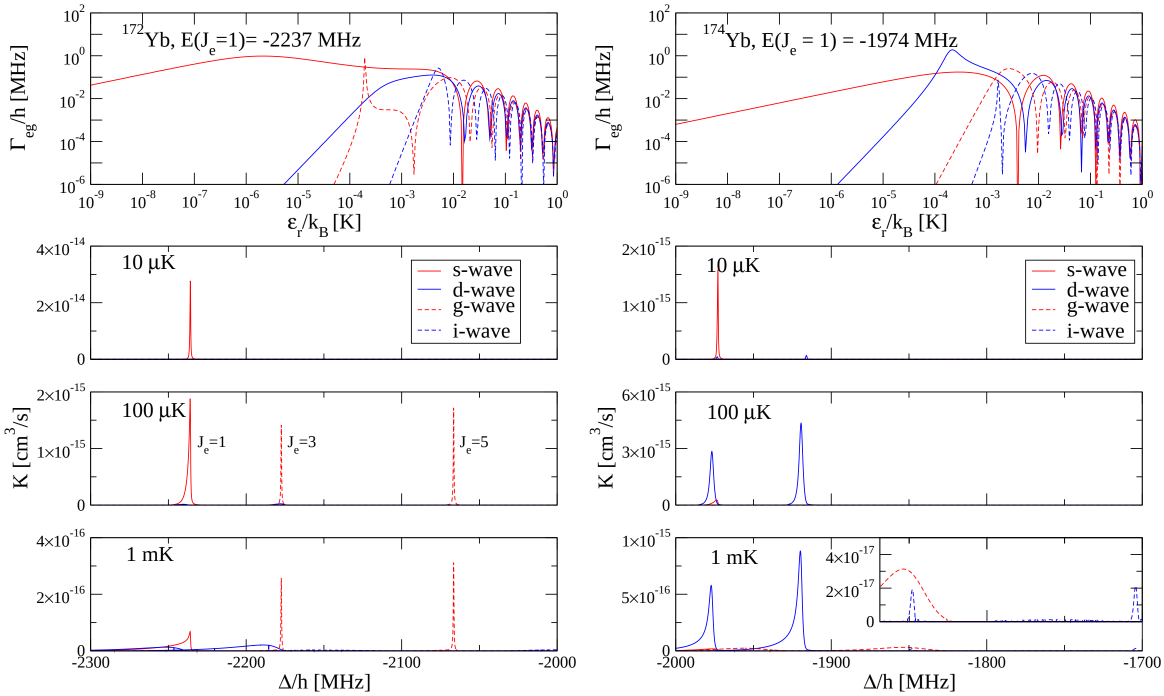

Figure 1: For the two isotopes: ^{172}Yb and ^{174}Yb the light induced width Γ_{eg} is shown as a function of the collision energy ε_r for a few lowest partial waves. The two-body loss rate coefficient K is also presented on the plot as a function of the laser detuning Δ, at different temperatures of the ultra cold gas. Results obtained at 100 μK clearly demonstrate the impact of shape resonances (g-wave in the case of ^{172}Yb and d-wave in the case of ^{174}Yb) on the simulated spectra.

Discrete soliton collisions in two-species Bose-Einstein condensates confined to a one-dimensional optical lattice

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We generalize the tight-binding approximation [1] to model a two-species Bose-Einstein condensate (BEC) in a one-dimensional optical lattice. We obtain a set of two coupled-channel discrete nonlinear Schrödinger equations, which we use to model interactions in two systems – the anticipated mixtures of two Ytterbium isotopes and a mixture of ^{87}Rb and ^{41}K recently reported by Thalhammer *et al.* [2]. We study collisions between solitons composed of different species. We observe that these collisions tend to be inelastic when the interspecies scattering length is positive and lead to destruction of the two solitons and creation of mutually-trapped states, while when the interspecies scattering length is negative the collision is – counterintuitively – elastic over a wide range of parameters.

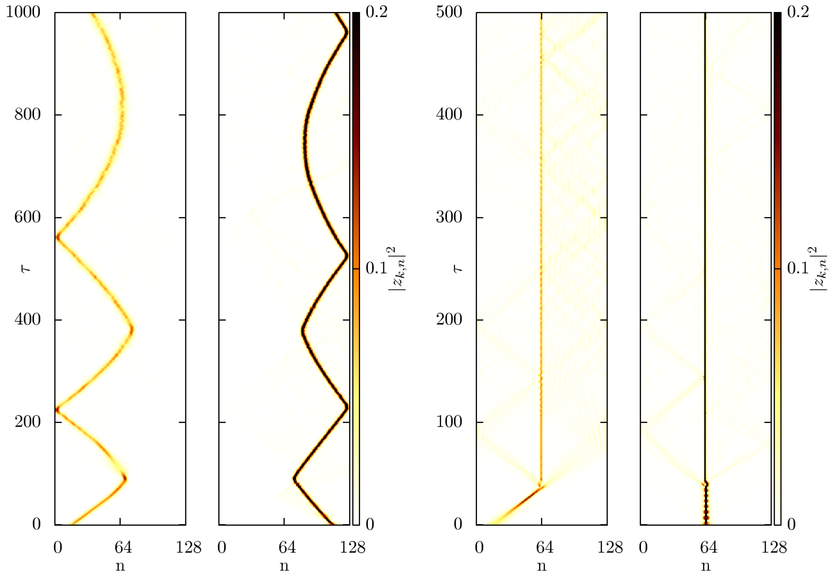

Figure 1: Left: collision of two travelling breathers in the case where the interaction between the two species is attractive (ie. described by a negative scattering length [3]), as it is in the case of ^{170}Yb and ^{174}Yb. The two solitons collide elastically. Right: a collision of a travelling breather (^{170}Yb) and a self-trapped state (^{168}Yb) with the interspecies interaction repulsive. The travelling breather is destroyed and becomes part of a two-species self-trapped state.

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Fourier-transform spectroscopy studies of the $(4)^1\Sigma^+$ state of KCs

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The KCs molecule is expected to be a promising candidate to produce the ultracold gas of polar molecules; in particular, due to the proximity of K($4p$) and Rb($5p$) atomic asymptotes, the energy structure of KCs is the closest to the RbCs molecule which was successfully produced in $(v = 0)X^1\Sigma^+$ state at temperature 10^{-4} K [1]. The empirical potential energy curves of KCs ground $X^1\Sigma^+$ and $a^3\Sigma^+$ states have been recently obtained [2]. As was revealed in [2], the excited $(4)^1\Sigma^+$ state of KCs is connected to both $X^1\Sigma^+$ and $a^3\Sigma^+$ states by optical transitions. Thus, the information on the $(4)^1\Sigma^+$ state properties could facilitate the selection of optical paths for efficient transformation of the respective ultracold atoms into the absolute rovibrational ground state $(v = 0, J = 0)X^1\Sigma^+$ of KCs; till now the $B(1)^1\Pi$ state and the $A(2)^1\Sigma^+ - b(1)^3\Pi$ system were considered for such purpose.

This contribution presents first study of the $(4)^1\Sigma^+$ state of KCs which has been performed by Fourier-transform spectroscopy of laser induced fluorescence (LIF) using a Bruker IFS125HR spectrometer with 0.03 cm^{-1} resolution. The KCs molecules were produced at 280 °C either in a sealed cylindrical glass cell or in a heat-pipe containing K (natural isotope mixture) and Cs metals. A single mode ring dye laser Coherent 699-21 with Rhodamine 6G dye was used as a light source; excitation frequencies varied between 16800 cm^{-1} and 17300 cm^{-1}. Term values of the $(4)^1\Sigma^+$ state have been obtained by adding transition frequencies to the respective ground state $(v_X, J_X)X^1\Sigma^+$ energies calculated from [2]. The dependencies of the $(4)^1\Sigma^+$ state term values on the factor $J(J+1)$ have been plotted spanning energy range from ca. 17000 cm^{-1} to 18000 cm^{-1} and J range from 10 to 170. The experimental dependencies have been compared with their theoretical counterparts based on calculations [3]; a preliminary vibrational identification for the obtained $(4)^1\Sigma^+$ state term values was suggested. Since both $(4)^1\Sigma^+ \to X^1\Sigma^+$ and $(4)^1\Sigma^+ \to a^3\Sigma^+$ transitions have been observed in LIF spectra, the perturbation of the $(4)^1\Sigma^+$ state by a triplet state is expected. According to theoretical term schematics [3], the $(3)^3\Sigma^+$ and $(2)^3\Pi$ could be the perturbing states. The work on vibrational assignment and potential energy curve construction of the $(4)^1\Sigma^+$ state of KCs is currently in progress.

Acknowledgment

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Atom interferometry measurement of the atom–surface interaction

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Atom interferometers are a well established tool to measure the phase shift induced by weak perturbations on the propagation of atomic de Broglie waves. Our Mach-Zehnder atom interferometer operates with lithium at thermal energy and Bragg diffraction by near-resonant laser standing waves is used to split, reflect and recombine the atomic beams. The distance between the two coherent atomic beams is about 100 μm, sufficient to apply a perturbation to one beam only and to observe the resulting phase shift and attenuation of the atomic wave on the interferometer signal. We have thus measured very accurately the electric polarisabiliy of ^7Li [1] and the index of refraction of rare gases for lithium matter waves [2].

To measure the van der Waals lithium-surface interaction, we introduce a 100 nm period nanograting on one atomic beam in our interferometer, thus following an experiment done by Perreault and Cronin with sodium [3]. The nanograting diffracts the atomic beam and only the zero-order beam interferes with the reference beam. The interference signals give access to the zero-order diffraction amplitude. The phase of this amplitude is solely due to the atom-surface Van der Waals interaction. We have carefully measured this phase as a function of the atom velocity from 700 to 3300 m/s (see figure 1) and we have obtained an uncertainty of the order of 3 milliradians, thus reducing the uncertainty of the previous experiment [3] by a factor 33! The velocity dependence of this phase is a test of the potential dependence with the atom-surface distance r and, if we assume a C_p/r^p potential, our data proves that $p = 2.9 \pm 0.2$, as predicted by theory. Our data can also be used to set new limits on non-Newtonian gravity in the $1 - 10$ nm range. Finally the phase gives a direct measurement of the lithium SiN$_x$ van der Waals coefficient $C_3 = 3.25 \pm 0.2$ meV/nm^3 in good agreement with theory.

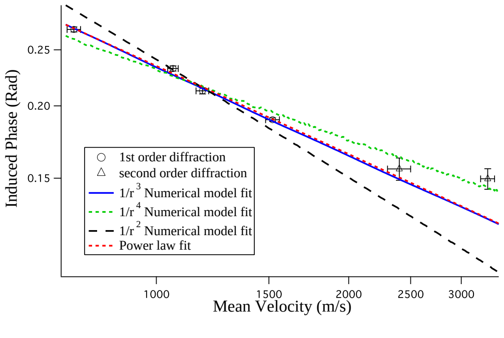

Figure 1: Measured phase of the diffraction amplitude as a function of atom velocity.

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Phase dynamics of atoms in micro-traps

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Controlling the phase of a single quantum system with high fidelity while not compromising fast time scales is one of the goals in developing quantum information devices. This usually requires excellent time-dependent control over several experimental parameters, making it technically challenging. For not-completely time-critical applications, however, adiabatic techniques can be used that allow to transfer time-dependent control into fixed system parameters.

Here we investigate techniques for state preparation of single, ultracold atoms in systems of spatially separated micro-traps. For such systems coherent transport can be achieved by tunneling and it was recently shown that an analogue to the celebrated three-level STIRAP technique in optics can be constructed [1]. However, spatial atom-optical systems posess various additional degrees of freedom as compared to optical systems (e.g. multiple spatial dimensions, particle interactions, quantum statistics, etc.). They therefore hold a large promise for developing new and exciting techniques based on dark states.

In this work we consider the influence of dynamical as well as geometrical phases on atoms in dark states for different experimental geometries. We first investigate the stability of angular momentum carrying states in the standard STIRAP process and show that it can be used for controlled phase engineering. In a second example we consider a four trap diamond arrangement in two dimensions and show that an atom trapped initially in a single trap can be transferred into an arbitrary, but well defined, spatial superposition state. This is due to the accumulation of a Berry phase and the process requires only control over individual trapping frequencies and the ability to carry out a STIRAP type positioning sequence of the traps. We show that this process does not only allow for large fidelities when carried out perfectly, but is also robust against many experimental uncertainties.

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Femtotesla atomic sensitivity with paraffin-coated Cs cells

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We present the latest results from our systematic study of more than 250 nominally identical alkali atom vapor cells produced by us. The room-temperature cells confine Cs vapor in evacuated, 28 mm inner diameter paraffin-coated Pyrex bulbs. We have developed an automated testing facility [1] for characterizing the cell performance. Each cell is mounted in a standard M_x magnetometer configuration [2] based on optically detected magnetic resonance with circularly polarized D_1 pumping on the $F{=}4 \rightarrow F{=}3$ transition. Signal amplitude and linewidths are inferred from in-phase and quadrature magnetic resonance signals. For each cell, we determine the intrinsic (i.e., extrapolated to zero light and zero rf power) longitudinal, Γ_{01}, and transverse, Γ_{02}, relaxation rates, as well as the power dependence of the widths and amplitudes. Our best cell shows $\Gamma_{01}/2\pi \approx 0.5$ Hz, and $\Gamma_{02}/2\pi \approx 2$ Hz. We find a linear correlation between both relaxation rates which we explain in terms of reservoir and spin exchange relaxation. For each cell we have determined the optimal combination of rf and laser powers which yield the highest sensitivity to magnetic field changes. Out of all produced cells, 94% are found to have magnetometric sensitivities in the range of 9 to 30 fT/$\sqrt{\text{Hz}}$ (in the shot-noise limit). We currently use those cells in a 25-sensor magnetometer array to register dynamic magnetic field maps of the human heart (see poster by M. Kasprzak *et al.*).

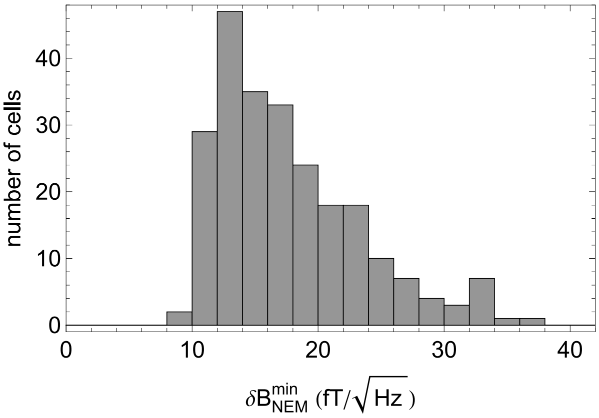

Figure 1: Histogram of the intrinsic magnetometric sensitivities of 241 cells.

Acknowledgment
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Frequency-stabilized cavity ring-down spectrometer for line shapes and line intensities measurements of oxygen B-band

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The frequency-stabilized cavity ring-down spectrometer (FS-CRDS) built in the Institute of Physics, Nicolaus Copernicus University uses a single-mode, continuous-wave cavity ring-down technique with the ring-down cell locked to the reference frequency of the HeNe laser stabilized to about 1 MHz. Such configuration allows us to obtain spectra which are insensitive to the probe laser power and frequency fluctuations. Moreover, the possibility of the HeNe laser frequency tuning by the AOM results in high spectral resolution of the spectrometer, limited by stability of the HeNe laser. The FS-CRDS spectrometer was used to investigate line intensities and line shapes of several transitions of the oxygen B-band ($\lambda = 689$ nm). Obtained signal-to-noise ratio of measured spectra exceeds 1000:1.

In this study spectra of six transitions of oxygen B-band were measured at pressures up to 30 Torr of O_2. The line intensities were determined with relative standard uncertainties lower than 0.6 % in most cases and collisional self-broadening coefficients were determined with relative uncertainties of order of a few percent. It was found that the collisional shift is smaller than our experimental errors in the case investigated here. The influence of the choice of the line shape model used for data analysis on resulting intensities and line-shape coefficients is discussed. Our experimental data are compared with data available in the literature.

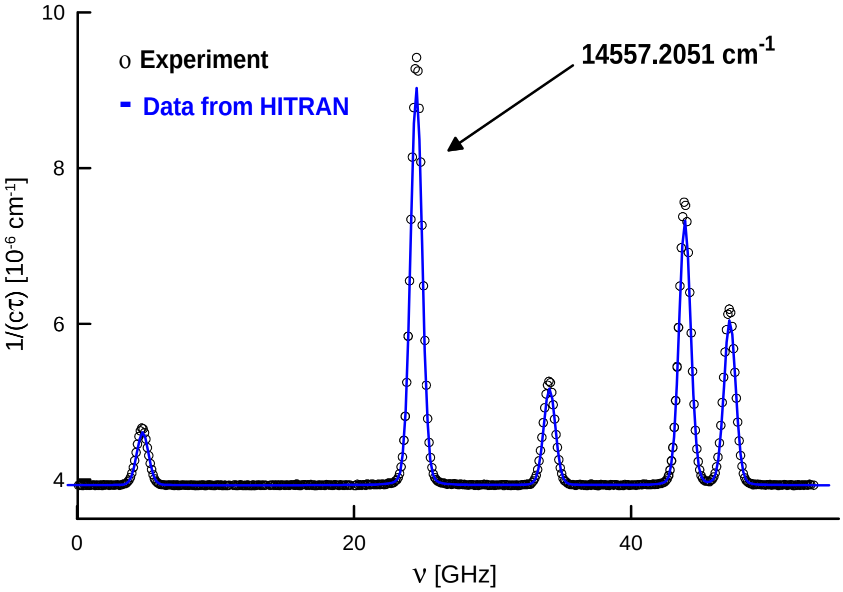

Figure 1: Comparison of experimental and simulated spectrum of five self-broadened O_2 B-band lines at pressure equal to 25 Torr.

Acknowledgment

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Structure of satellites and hypersatellites of $L\alpha_{1,2}$ and $L\beta_1$ lines in mid-Z atoms excited by oxygen ions

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The L-shell satellites and hypersatellites of $L\alpha_{1,2}$ ($L_3 \rightarrow M_{4,5}$) and satellites of $L\beta_1$ ($L_2 \rightarrow M_4$) x-rays transitions in zirconium, molybdenum and palladium excited by oxygen ions were measured. The measurements were performed in the Paul Scherrer Institute (PSI) in Villigen, Switzerland. The experiment was performed using the ion beam from the ECR ion source. The oxygen ions with energy 278.6 MeV were accelerated by the Philips cyclotron and transported to the crystal von Hamos spectrometer [1]. The von Hamos spectrometer is a high-resolution diffraction spectrometer having an instrumental energy resolution of about 0.3 ÷ 0.6 eV for studied x-rays. The absolute energy calibration of the spectrometer was about 0.3 eV [2]. In order to interpret the observed satellites and hypersatellites structures the relativistic MCDF calculations [3] were performed for multi-vacancy configurations expected to be excited in collisions with oxygen ions. In the presented work we report the experimentally determined hypersatellite to satellite ratio R for $L-$shell and the ionization probability p_M for the $M-$shell. These results are compared with the theoretical predictions of the SCA approximation using the relativistic, hydrogenic-like wave functions (HYD) and the relativistic, selfconsistent Dirac-Hartree-Fock wave functions (DHF).

To our knowledge, this is the first experimental observation of a direct excitation of the L-shell hypersatellites in ion-atom collisions, which is, additionally, clearly interpreted by a complex MCDF calculations revealing their internal structure corresponding to the multi-vacancy ($L^{-2}N^{-n}M^{-m}$) configurations. Analysis clearly demonstrates the satellite ($L^{-1}M^{-m}N^{-n}$) and hypersatellite ($L^{-2}M^{-m}N^{-n}$) transitions correspond to the excited multi-vacancy initial configurations. The relative intensities of x-ray satellites indicate the importance of the relativistic, self-consistent description of electrons in the L-, and M-shells.

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Dynamic electron screening in nuclear reactions and radioactive alpha decays

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Strongly enhanced electron screening of the Coulomb barrier between reacting nuclei has been recently observed in low-energy reactions preceding in metallic environments being a model for dense astrophysical plasmas. The theoretical calculations of the screening energy based on the self-consistent dielectric function theory including polarisation of both free and bound electrons fail by a factor of two compared to the experimental results. Since the alpha decay probabilities depend on the penetration through the Coulomb barrier analogously to nuclear reactions, one might expect a dependence of decay half-lives on the electron density of the medium. On the other hand, it is argued that the screening of the Coulomb barrier can be cancelled due to an internal screening effect increasing the binding energy of a decaying nucleus. Here, we show that the strength of both effects is different because of the velocity dependence of the electron screening and thus a residual, rather weak influence of medium on radioactive decays should be experimentally observed. As motivation for future experimental studies, theoretical calculations comparing half-lives of alpha and beta decays in insulating and metallic environments will be presented.

Influence of target surface contamination on experimental UHV screening energies

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The enhanced screening of the nuclear Coulomb potential due to the atomic electrons has lead been confirmed in many laboratory experiments. The electron screening effect in astrophysical plasmas can enhance nuclear reaction rates in the interior of stars by many orders of magnitude.

However, a reliable comparison between experimental data and theoretical predictions is still ambiguous because of some systematic errors in experiments. The measurements on deuterium inside metals are heavily affected by the formation of surface contamination layers under beam irradiation even in ultra-high vacuum (UHV) system.

Here, we present our recent experimental results obtained for deuteron fusion reactions taking place in the metallic Zr environment and give some rigorous calculations of the influence of surface contamination layers on UHV experimental data. We thoroughly analyzed the ion induced chemical surface reaction mechanisms and their influence on the obtained screening energies. Our investigations show that this process has crucial impact on the interpretation of the raw experimental data.

Manipulation of ion bunches with time-dependent field

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At present, the smallest spot size which can be achieved with state-of-art focused ion beam (FIB) technology is mainly limited by the chromatic aberration associated with the energy spread of the liquid-metal ion (LMI) source. We have already shown [1] that a new concept, the ultra-cold ion source, which is based on near-threshold ionization of laser cooled atoms, can provide lower energy spread than LMI sources [2].

In our experiment, rubidium atoms are confined in a magneto optical trap (MOT) built directly inside an accelerator structure [3]. A spherical portion of the cloud is ionized at the intersection of two laser beams and then accelerated by a pulsed electric field. The ultra low temperature of the source permits collimated bunches to be created at low energy, which allows using time dependent fields. These can be used to study space charge effects and also to lower the energy spread. The duration of the electric field pulse is tuned in order to cancel the negative lens effect due to the geometry of the accelerator structure. Even more, with the same principle, one can reverse the effect and create a focusing lens.

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The Born-Oppenheimer approximation breakdown in lithium dimer

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The lithium dimer is one of the most well studied dimers of alkali metals. New results of the direct potential fit of the ground $X^1\Sigma_g^+$ and $A^1\Sigma_u^+$ state potentials were reported recently [1]. In this study the Born-Oppenheimer approximation breakdown was studied by including in the fit adiabatic and nonadiabatic corrections for both electronic states simultaneously. Here we report a new approach to this analysis by studuing the Born-Oppenheimer approximation breakdown separately for the $X^1\Sigma_g^+$ and the $A^1\Sigma_u^+$ electronic states. This will reduce the possible correlations between the parameters used for description of the adiabatic and nonadiabatic corrections. New experimental data were collected in order to support the present analysis.

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A new design for a high-resolution gas phase electron spectrometer

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In this work, a new design for an electron spectrometer is presented that is characterized by high electron energy resolution and collection efficiency for gas phase electron spectroscopy. The setup consists of a homemade electron gun, a gas inlet system, a scattering chamber, hemispherical deflector analyzers (HDAs), electron detectors, a vacuum-pumping system and a data-acquisition system [9]. Based on our previous simulation results [2,3], we designed the new hemispherical deflector analyzer with a variable input lens position, and optimized the energy resolution over a broad energy band by biasing the electrostatic potential along the optic axis, while maintaining total transmission. This arrangement has been referred to as a “biased paracentric entry” HDA [4]. The combination of high energy resolution ability with high transmission and simple design makes this instrument very promising for a wide range of scientific and technological applications. Computer simulation based on the boundary element method is also used to give a physical interpretation of the fringing field effects and propose a method for a numerical evaluation of the first- and second-order aberrations arising in the fringing field regions of HDAs with a biased paracentric entry. The analyzer is implemented to measure the energies of electrons generated by electron–atom collisions. Our results demonstrate the wide range of applicability and usefulness of the new entry concept for other electron spectroscopic techniques.

Acknowledgment
This work is supported by TUBITAK in Turkey, through grant 106T722.

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Fluorimetric measurements in vivo of surface seawater around the Svalbard Islands

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The Nordic Seas have been for many years the subject of the research of ocean circulation conducted by the Institute of Oceanology PAS [1], especially the inflow of Atlantic water and the intensive turbulent mixing of these waters with Arctic and shelf waters. Ocean currents affect various biological processes, and affects the supply of organic matter and oxygen which constitute the base for the unique flora and fauna of Svalbard islands as well as changes occurring in this area are limiting.

Fluorimetric examinations of surface waters, with the Fluorimeter M32B produced by LDI Ltd [1], were carried out repeatedly during Arctic cruises on board of r/v Oceania. Results presented herein come from AREX campaigns 2003 and 2006.

The in vivo fluorescence excitation spectra of phytoplancton species in seawater were measured at one emission wavelength. The spectral range (excitation 400 to 660 nm, emission 680 nm) was aimed to reveal fluorescence of chlorophyll a induced via accessory pigments.

On the basis of the analysis of recorded spectra, it is possible to notice the rise in the abundance of the phytoplankton and changes of the spatial distribution of the phytoplankton species characteristic for Atlantic, Arctic and shelf waters. Comparisons of spatial patterns of the phytoplankton pigments abundance and the physical characteristics of water masses were conducted.

It is possible to conclude that the observed changes of the abundance and spatial distribution of the phytoplankton species are controlled by water mass properties being found in a given year, that is by the inflow of Atlantic waters into the area of Svalbard islands. In order to establish credible knowledge about the trends of phytoplankton changes a longer time-series is needed. Therefore the fluorimetric studies are being continued in order to determine the interannual variability and longer-term changes in the marine ecosystem of the archipelago [3].

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Formation of dark states in hyperfine level systems of Na via the Autler-Townes effect

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The Autler-Townes (AT) effect [1] has been extensively studied in atoms, while high-resolution molecular data is still scarce and is used in obtaining the transition dipole moment matrix elements [2, 3] or lifetimes and branching ratios of highly excited molecular states [4]. The AT effect and its dependence on the molecular magnetic quantum number M_J has been shown as an all-optical method for aligning non-polar molecules for chemical reactions [3]. In our latest work [5] we have studied the AT effect in more complex atomic and molecular systems, where hyperfine structure is present.

Here we consider different three-level ladder excitation schemes in Na coupled by two laser fields, where the intermediate level can be the $3P_{1/2}$ or the $3P_{3/2}$ state and the final level can be the $5S_{1/2}$ or the $4D_{3/2}$ state. The strong field is in the second step and the weak field is in the first step, probing the dressed states created by the coupling laser. The AT spectrum obtained is different for the two cases - when the number of hyperfine levels of the two strongly coupled states is the same or different. To understand this effect, we have developed a simple method for treating the laser-atom system based on solving the Schrödinger's equation to obtain the time evolution of the probability amplitudes in the atomic wavefunction. We show that application of a sufficiently strong coupling field between the intermediate and the final states leads to a full resolution of the M_F Zeeman sublevels if the number of hyperfine levels in the two strongly coupled states is equal (e.g. in the excitation scheme $3S_{1/2} \rightarrow 3P_{1/2} \rightarrow 5S_{1/2}$). However, if the number of hyperfine levels is different (e.g. in the scheme $3S_{1/5} \rightarrow 3P_{3/2} \rightarrow 5S_{1/2}$), the increase of the coupling field Rabi frequency above the separation between the hyperfine components leads to a rapid decrease (and eventually vanishing) of the intensity of all AT peaks besides the two side ones. We explain the latter result with the creation of multiple dark states [6] in a multilevel system coupled by a strong field.

For comparison, we have also performed simulations based on a theoretical model of solving the optical Bloch equations (OBE's) [7]. The OBE's method shows the same energy positions of the M_F Zeeman sublevels under the action of a strong laser field but different widths and intensities of the AT peaks, since no cascading due to spontaneous emission is included in Schrödinger's equation.

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Cross sections of Penning ionization for Rydberg atoms

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Collisions of two Rydberg atoms can lead to ionization via two mechanisms: associative and Penning ionization. Associative ionization is a short-range process, which requires close encounters enabling overlap of Rydberg atom wave functions. In contrast, Penning ionization is a long-range process, which occurs while atoms are well separated in space at antinuclear distances $r \gg n^{*2}$ (where n^* is the effective quantum number, atomic units are used) due to the long-range dipole-dipole interaction.

We study the formation of atomic ions in an Auger-type scheme: one of the Rydberg atoms undergoes a dipole transition from the initial state $n_1 l_1$ to a lower state $n'l'$, while the other one is excited from the initial state $n_2 l_2$ to the ionization continuum. Such ionization can take place if $(n'^*)^{-2} > (n_1^*)^{-2} + (n_2^*)^{-2}$. Perturbation theory [1] allows one to express the Penning ionization cross section σ_{PE} for alkali atom pairs as

$$\sigma_{PE} = \frac{\widetilde{\Gamma}^{2.5}}{v^{2.5}}\,; \quad \widetilde{\Gamma} = \sum_{n'} \frac{c\sigma_{ph}}{\pi\omega_{n_1n'}} |D_{n_1n'}|^2, \tag{1}$$

where $\sigma_{ph}(\omega_{n_1n'})$ is the photoionization cross section for the atom in the $n_2 l_2$ state, and $D_{n_1n'}$ is the reduced dipole matrix element for the $n_1 \to n'$ transition at frequency $\omega_{n_1n'}$.

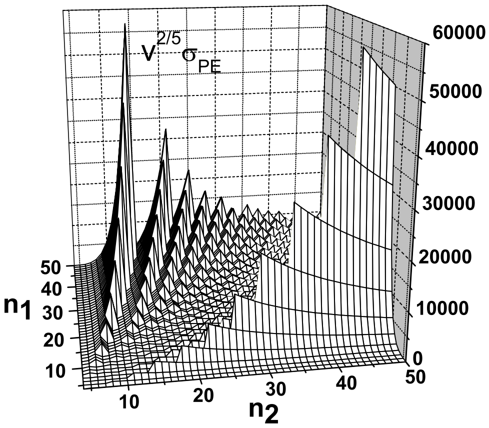

Figure 1: The reduced cross section $v^{2.5}\sigma_{PE}$ for two Na atoms with $l_1 = l_2 = 0$.

We have evaluated the Penning ionization cross sections using the semiclassical analytical formulae for photoionization cross sections and dipole matrix elements derived in [1] for Rb and Na atoms. The resulting σ_{PE} is an oscillating function of the principal quantum numbers n_1, n_2 (see Fig. 1). The nature of the oscillation is discussed in [2].

Acknowledgment

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Nonlinear spectroscopy of cold Cs atom beam

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A cesium beam is produced out of a modified pyramidal Magneto-Optical Trap (p-MOT [1]) used as an atom funnel. Briefly, trapping and repumping radiation are sent onto an arrangement of prisms and mirrors shaped in the form of a hollow pyramid realizing the beam configuration of a standard MOT; a hole (area ~ 2 mm^2) is drilled at the pyramid apex, hence no laser radiation is retroreflected along the pyramid axis. A continuous beam of atoms is then leaving the hole, forming the beam which is used for atomic nanofabrication purposes. Right after the hole, the beam is collimated by a 2-D transverse optical molasses. The residual divergence is in the mrad range for a flux up to 10^9 atoms/s in a transverse area $\sim 2 \times 10^{-1}$ cm^2. Due to atom funnel operation, longitudinal velocity of the atoms is around 10 m/s. The beam is probed by a strong narrow resonant laser of power P_l and the integral fluorescence I_{fl} is collected at right angles by CCD. The fluorescence intensity I_{fl} grows with increasing P_l (Fig. 1) far beyond the saturation limit (a few mW).

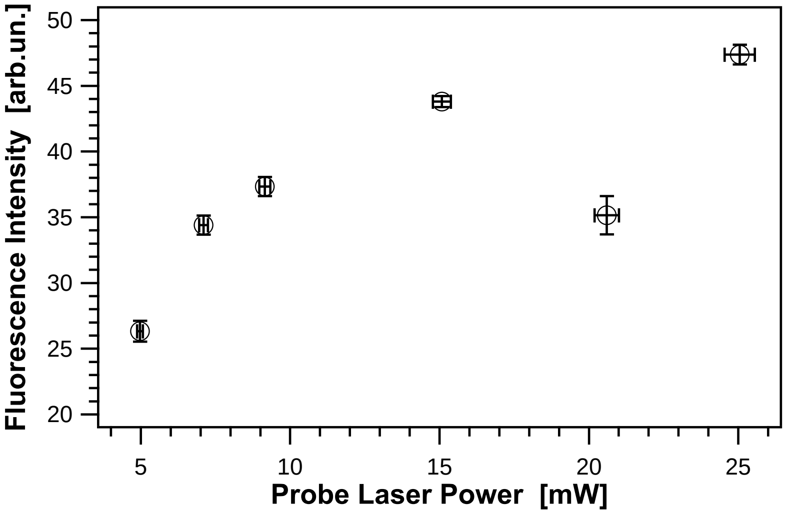

Figure 1: Fluoresence intensity from the laser cooled Cs beam as a function of the probe laser power P_l.

We attribute this experimental finding to the absorption of the escaping radiation. The probe laser dresses the atomic states and forms Mollow triplet in the fluorescence spectrum, whose side peaks are shifted from the absorption line center, resulting in bleaching the beam volume for the resonant frequencies. The shape of the curve $I_{fl}(P_l)$ appears to be sensitive to the beam density, thus allowing for a sensitive density diagnostics.

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Support by the Russian Foundation for Basic Research and by the E.I.N.S.T.E.I.N. consortium is acknowledged.

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Autler-Townes effect: linshape analysis and determination of excited state lifetimes

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A detailed theoretical analysis of the formation of Autler-Townes doublets [1] in the excitation spectra of molecules is presented. It assesses the validity and accuracy of our recently proposed technique for the determination of lifetimes of excited molecular states based on the measurement of peak ratios of Autler-Townes doublets [2]. Influence of various factors, like inhomogeneous line broadening and limited interaction time of molecules with the laser fields is analyzed. A ladder of three rovibronic levels (1, 2, and 3) of different electronic states is considered. Levels 2 and 3 are coupled by a strong dressing laser field, while a weak probe laser field is scanned across the 1-2 transition. Coupled density matrix equations have been solved numerically and by using the split propagation technique [3]. The peak ratio in the excitation spectrum of level 3 is found to be directly related to the lifetime ratio of levels 2 and 3, but this ratio is altered if the interaction time of molecules with the laser fields is comparable to lifetimes of the excited levels. Comparison of the calculations with the experimental spectra for the ladders $X^1\Sigma_g^+(0,7) \rightarrow A^1\Sigma_u^+(10,8) \rightarrow 5^1\Sigma_g^+(10,9)$ and $X^1\Sigma_g^+(0,7) \rightarrow A^1\Sigma_u^+(11,8) \rightarrow 6^1\Sigma_g^+(10,9)$ in Na_2 show that the lifetimes of the $5^1\Sigma_g^+$ and $6^1\Sigma_g^+$ (see Fig. 1) states are 35 and 40 ns, respectively. These should be compared to the corresponding theoretical values of 42 and 42 ns obtained form the molecular potential calculations.

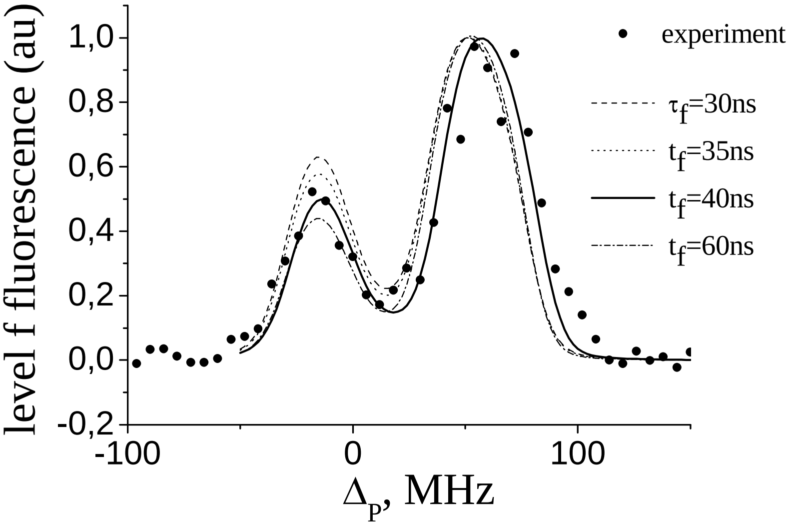

Figure 1: Fluorescence from the $6^1\Sigma_g^+(10,9)$ state as a function of probe laser detuning and comparisson with the theoterical curves.

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Optimization of Doppler profile in supersonic beams

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Doppler profile $P(\Delta\nu)$ in the laser excitation spectra of atoms and molecules in collimated beams is conventionally described by the Gaussian function [1]. However, a recent study [2] showed that the residual Doppler profile $P_\perp(\Delta\nu)$ upon excitation and observation at right angles to the particle beam axis resulting form nonzero scatter of transverse velocities v_r has the form $P_c(\Delta\nu) = \sqrt{1-\Delta\nu^2/\Delta\nu_D}$, which is clearly non-Gaussian. The effective Doppler width $\Delta\nu_D = (v_f/\lambda)R/L$ is determined by the flow velocity v_f of particles in the beam, the diameter of the beam nozzle d, the distance between the nozzle and the excitation zone L, and the radius R of the (collimating) entrance aperture of the excitation chamber. The function P_c was obtained assuming $d \ll R \ll L$. It describes the most essential core part of the profile $P_\perp$, wile the wings result from the (narrow) velocity distribution of particles around the flow velocity v_f.

Here, we present results for a general case of arbitrary d, when the core of the Doppler profile,

$$P_d(\Delta\nu) = \frac{2R}{d}\int\limits_{-d/2R}^{d/2R} d\widetilde{x}\sqrt{d^2/(4R^2)-\widetilde{x}^2}\int\limits_{-1}^{1} dx\sqrt{1-x^2}\sigma(\Delta\nu/\Delta\nu_D - x - \widetilde{x}), \qquad (1)$$

can be expressed via double integration over the nozzle opening plane (the variable $\widetilde{x}$) and the aperture plane (x). The function P_d exhibits a nonmonotonic variation of the residual Doppler width $\Delta\nu_d$ (HWHM) with increasing nozzle diameter. There exists an optimal value $d = R/2$ of the nozzle size which ensures the narrowest possible excitation profile and and highest density of particles in the excitation zone.

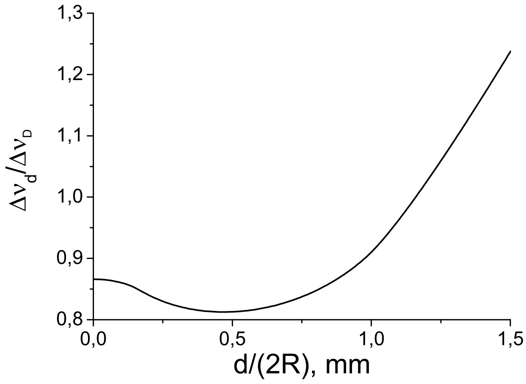

Figure 1: The residual Doppler width $\Delta\nu_d/\Delta\nu_D$ via the reduced nozzle radius $d/(2R)$.

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Corrections to transit time broadening

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We reconsider the effect of transit time on line broadening in dilute gases in the weak excitation limit, when the effects of reabsorption, saturation, and collisions are negligible. Two-photon excitation of excited molecular levels by counter-propagating laser fields is used in order to eliminate the Doppler broadening. Both laser fields have Gaussian profiles and are focused onto the supersonic beam of Na_2 molecules such that transit time is shorter than natural lifetime of the excited state. In experiment, the field 2 in the 2nd excitation step is detuned by 1GHz off from one-photon resonance between the intermediate rovibrational level in the $A^1\Sigma_u^+$ state and the final level $5^1\Sigma_g^+$ (v=10,J=9). The excitation spectrum of the final level is then recorded by scanning the field 1 across the two-photon resonance.

Usually in such a situation one would describe the absorption profile by a Lorentz function with the natural width Γ_{sp} and transit time τ_{tr} [1]:

$$P(\Delta) = \pi\widetilde{\Gamma}/\left(\Delta^2 + \widetilde{\Gamma}^2\right); \quad \Delta\omega = \frac{\widetilde{\Gamma}}{2} = \frac{1}{2}(\Gamma_{sp} + 1/\tau_{tr}), \tag{1}$$

where Δ is the detuning of field 1 from the two-photon resonance, and $\Delta\omega$ is the HWHM. Transit time $\tau_{tr} = L/v_f$ is determined by the flow velocity of molecules in the beam v_f and the spot size of the laser beams L. In our case the lifetime is τ_{sp}=42ns and the transit time is τ_{tr}=23ns.

Analytical solution for two-photon absorption shows that it is described by the Voight profile, which is in good agreement with the measured line profiles (see Fig. 1). The HWHM of this profile exceeds the value of $\Delta\omega$ given by Eq. (1) by a factor of 2.5.

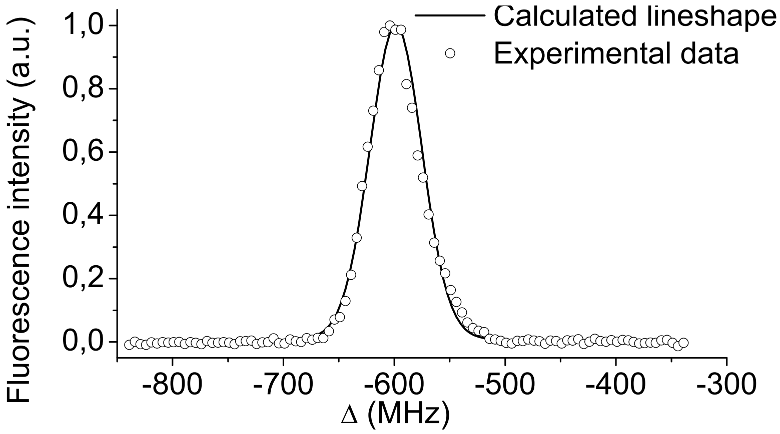

Figure 1: Doppler-free two-photon excitation spectrum of the $Na_2(5^1\Sigma_g^+$,v=10,J=9).

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Relativistic Jahn-Teller effects in the quartet states of K_3 and Rb_3: Experimental and theoretical investigations

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Spectroscopy of alkali-metal complexes on helium droplets (He_N, N = 1000 - 10000) provides the unique opportunity to observe high-spin species which exhibit prominent spin-orbit (SO) effects. In this work we present laser-induced-fluorescence and magnetic-circular-dichroism (MCD) spectra of the $2^4E'$ - $1^4A'_2$ band of Rb_3 and K_3 on He_N.

For Rb_3 we find a progression of four SO split bands, weakly perturbed by linear vibronic (Jahn-Teller) coupling. The K_3 transition was previously observed, and interpreted in terms of a linear and quadratic Jahn-Teller effect in the $2^4E'$ state [1]. The structure of the MCD spectrum, however, clearly reveals the importance of SO coupling also for the K_3 transition, and suggests a different assignment with weak linear- and no significant quadratic JT coupling [2]. The observed strong C-type MCD spectra arise from different populations of the ground-state Zeeman sublevels. Thus a quantitative analysis allows a determination of the spin temperature and since alkali metal complexes are situated on the surface of the helium droplet, this corresponds to a determination of the surface temperature. Our results from the trimer spectra are consistent with the value of 0.4 K which is found in the interior of a droplet.

In our theoretical calculations, we apply the Multireference Rayleigh Schrödinger Perturbation Theory of second order to obtain the adiabatic potential energy surfaces of the $1^4A'_2$ electronic ground state and the $2^4E'$ excited state of K_3 and Rb_3. As stated above, both trimers show a typical E×e Jahn-Teller distortion in their $2^4E'$ state, which is analyzed in terms of the relativistic Jahn-Teller effect theory. Linear, quadratic as well as spin-orbit coupling terms are extracted from the ab initio results and used to obtain theoretical spectra for a direct comparison with the laser-induced fluorescence and magnetic circular dichroism spectra.

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BBR-induced decay of Rydberg states in Na atoms

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The blackbody radiation (BBR) is an important factor affecting lifetimes of Rydberg states at room temperature. Thermal photons cause induced transitions from highly excited states into continuum (ionization process) and to other energy levels (excitation and decay). For rather high Rydberg states of atom and high ambient temperatures, the BBR-induced decay is the leading process among photostimulated depopulation channels. Its rate is comparable with the spontaneous decay at T=300K (for 45d $P^{dec} = 4524s^{-1}$ and $P^{sp} = 12416s^{-1}$).

We used Fues model potential with modification [1] for calculating the BBR-induced decay rates in Na nS-, nP- and nD-states with n=5–60. The calculated data were approximated with three-term formula similar to that for ionization [2]:

$$P_n^{dec} = \frac{a_0(1 + a_1 x + a_2 x^2)}{\tilde{\nu}^5\{\exp(0.3158x^3) - 1\}}, \quad \text{with} \quad x = \frac{1}{\tilde{\nu}T^{1/3}}, \quad \tilde{\nu} = \frac{\nu}{100}. \tag{1}$$

In this formula a_0 is constant for an l-series and corresponds to the high-n asymptotic behaviour of P_n^{dec}; a_1 and a_2 account for the position and magnitude of the maximum decay rate and slightly depend on temperature:

$$a_i = b_{i\,-1}T^{-1/6} + b_{i0} + b_{i1}T^{1/6}, \qquad i = 1, 2. \tag{2}$$

The two-step approximation provides rather accurate analytical representation of direct computation results at T=30–1000K and n>5 (see Fig. 1 as an example), which may be useful for simple estimates of the BBR-induced decay rates.

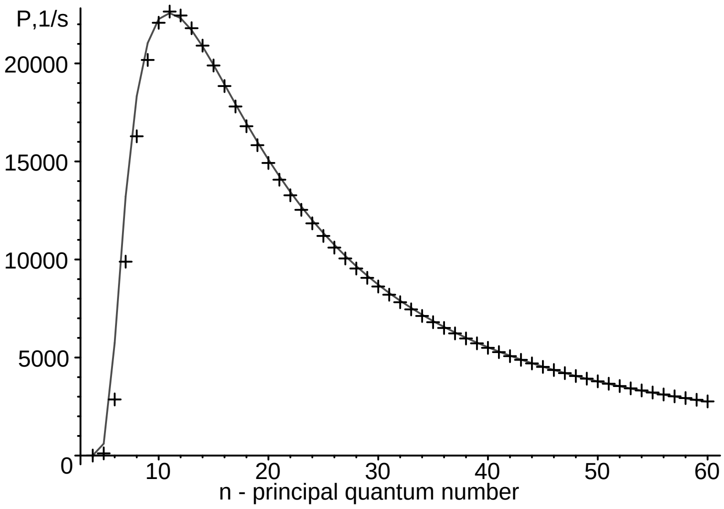

Figure 1: Approximate (solid line) and accurate (crosses) values of the photodecay rate of Na nD-states at T=300K.

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Atomic Fresnel biprism

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It is possible to take advantage of the transverse coherence of a standard supersonic atomic beam and a large longitudinal coherence length due to slow velocities, i.e. the atomic "de Broglie" wavelength gets into the nanometre range. Such a slowed atomic beam fills then the gap between the extremely well velocity – defined supersonic beam and the large atomic wavelength of the "cold atoms". A usual Zeeman slower configuration allows us to change the speed of the atoms from 560m/s to less than 10m/s [1]. Such an unusual atomic source is presently under study and will be used for atom – surface experiments, typically in the nanometres range.

The first new experiment that will be done is based on an efficient coupling between atomic Zeeman states (for atoms with internal angular momentum) allowed by the quadrupolar component of the surface-induced van der Waals (vdW) interaction [2]. This exo-energetic "vdW – Zeeman" transition provides a tuneable (magnetic field intensity dependent) beam splitter that we theoretically illustrate by the simplest possible interferometer: an atomic counterpart of the Fresnel biprism [3]. The velocity – adjustable atomic beam is here coming across two opposite surfaces (single slit of a nano-grating, see figure 1). For a large enough transverse coherent radius, the atom wave packet will be strongly inelastically diffracted by the two opposite surfaces at some distance from the slit to yield non localised interference fringes. The calculation has been done for Ar* metastable atoms with a grating of 100nm period and different velocities of the atoms (560 to 10 m/s). Via the interference pattern (Schlieren image), this device should give access to such novel information as the oscillating part of the complex vdW – interaction transition amplitude. This simplest configuration is not sensitive to inertial effect. As a next step, a loop – closing transmission grating will be added to realize a new type of compact closed interferometer.

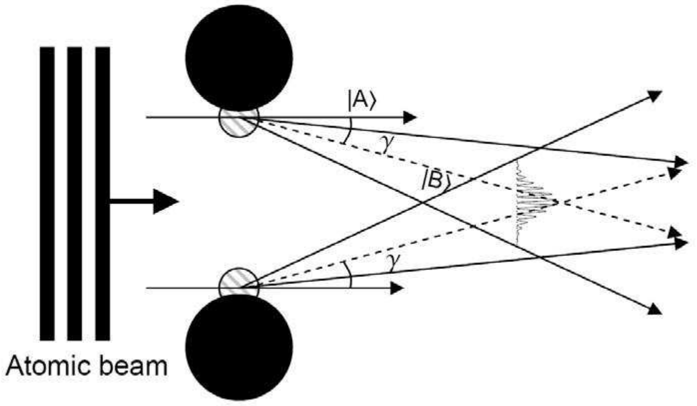

Figure 1: The atomic Fresnel biprism interferometer principle. γ is the angular deviation induced by the passage from the |A> to the |B> magnetic sub-level

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Negative refraction of matter-wave

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Similarities and differences between light and matter-wave optics originate in the properties of the associated particle. The extension of so-called "left-handed" optical meta-materials to negative-index media (NIM) for matter waves is a topic of particular importance [1]. Since the seminal paper of V.G. Veselago [2], many works have been devoted to optical NIM's and their properties (negative refraction, perfect focussing, reversed Doppler Effect, cloaking, etc.). Such artificial media are essentially characterised by a negative value of the optical index, i.e. the reversal of the wave vector $\vec{k}$ with respect to the Poynting vector $\vec{R}$. What should be the "de-Broglie optics" equivalent of those meta-materials [1]? To the energy flux corresponds the atomic probability flux, namely the current density of probability, or equivalently the group velocity v_g. Therefore, one has to reverse v_g with respect to $\vec{k}$, i.e. the phase velocity. However, contrarily to light optics where $\vec{R}$ remains directed outwards whereas $\vec{k}$ is directed towards the light source [3], for matter waves the direction of the phase velocity remains unchanged, whereas v_g is now directed towards the source [1]. Obviously, such an effect is necessarily transient. Our approach relies on both position- and time-dependent magnetic potentials [1]. We have shown that a novel class of potentials – "*comoving*" potentials [2] – provides us with a remarkably simple solution to devise negative-index media for matter waves [1]. These co-moving potentials are oscillating magnetic potentials which, by an adequate choice of the spatial period and oscillation frequency, can be made co-propagating with the atom wave [4]. The calculation of the induced matter-wave phase-shift demonstrates the possibility of producing transient negative group velocities for the atomic wave packet (see figure 1). With an adequate time-dependence of the co-moving field, we can devise cylindrical or spherical "*metalenses*". This extension of "meta-optics" down to the nanometer wavelength range opens novel applications in atom nano-lithography and interferometry.

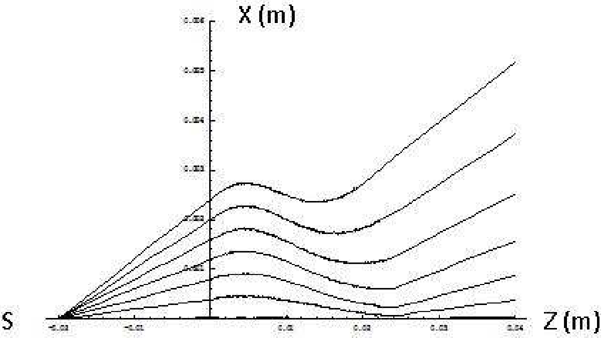

Figure 1: Trajectories of the wave packet center.

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Large linear magnetic dichroism in laser–excited K atoms

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Photoionization of polarized atoms opens up the possibility to study various phenomena related to electron emission in the presence of selectively populated magnetic substates, which under normal circumstances are degenerate [1]. These orientational features are all the more important when various correlation (i.e. many–electron) effects are studied, since these are often very sensitive to the symmetry properties of the electronic states.

Alkali atoms are especially suitable targets since they possess an s type electron outside a nobel gas –like closed shell structure. Laser pumping can be used to excite this valence electron into the corresponding p orbital, leading to orientation or alignment of the excited atoms. Orientation can be achieved by using circularly polarized laser radiation, which gives rise to uneven population of magnetic substates corresponding to $\pm|m|$. Linearly polarized laser radiation gives rise to alignment, where those magnetic substates are evenly populated.

In this work we discuss the observation of large linear magnetic dichroism (LMD) of the conjugated shakedown satellites in the $3p$ photoelectron spectrum of the $^2S_{1/2} \rightarrow ^2 P_{1/2}$ laser–excited potassium. The photoelectron spectra were recorded at the undulator beamline I411 of the storage ring MAX II in Lund. In a previous work [2] these satellite lines have been identified as originating from two–electron transitions $4p_{1/2} \rightarrow 4s$, $3p_{1/2,3/2} \rightarrow \epsilon p$ or $3p_{1/2,3/2} \rightarrow 4s$, $4p_{1/2} \rightarrow \epsilon p$. This leads to same final ionic states as in direct photoionization but with a shift in energy corresponding to the initial laser excitation energy.

The LMD amounts to using left– and right handed circularly polarized light in the laser excitation, and measuring the respective photoionization intensities, using linearly polarized synchrotron light. The difference of the two spectra yields the LMD.

Within the traditional picture the LMD for these satellite lines should be very close to zero, since it depends only on the difference of the phases of the continuum waves, which are only of the $p_{1/2}$ and $p_{3/2}$ type here, thus having a very small phase difference. A possible way to have nonzero LMD would involve large electron-electron interactions in the laser-excited states, thus enabling other continuum channel through configuration interaction effects. We therefore propose that the LMD gives an opportunity to study the degree of electron correlation in the ionic states.

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Photoassociation of LiCs in the rovibrational ground state

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Ultracold LiCs molecules are formed in the absolute ground state $X^1\Sigma^+$, $v''=0$, $J''=0$ via a single photoassociation step starting from laser-cooled atoms [1]. The selective production of $v''=0$, $J''=2$ molecules with a 50-fold higher rate is also demonstrated. The rotational and vibrational state of the ground state molecules is determined in a setup combining depletion spectroscopy with resonant- enhanced multi-photon ionization (REMPI) and time-of-flight spectroscopy. Using the determined production rate of up to 5×10^3 molecules/s, we describe a simple scheme which can provide large samples of externally and internally cold dipolar molecules.

The surprisingly large absolute rate constants for photoassociation at large detunings from the atomic asymptote are modeled using a full coupled-channel calculation for the continuum state, taking all relevant hyperfine states into account [2]. The enhancement of the photoassociation rate is found to be caused by an increased amplitude of the singlet scattering wave function at the inner turning point of the lowest triplet state $a^3\Sigma^+$. This perturbation can be ascribed to the existence of a Feshbach resonance. Our results elucidate the important role of couplings in the scattering wavefunction for the formation of deeply bound ground state molecules via photoassociation.

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Lineshapes of even Ar(np', nf', $J = 0, 1, 2$) autoionization spectra excited from selected low-lying odd excited $J = 1$ levels

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Recent laser photoionization studies yielded the first results for the lineshapes of the even Ne(np') autoionizing Rydberg states (ARS), as excited from the metastable Ne($3s\,^3P_2$, $3s'$ $^3P_0$) [1] and from the short-lived Ne($3s$, $^3P_1$, $3s'$, $^1P_1$) levels [2]. Configuration interaction Paul-Fock including core polarization (CIPF CP) calculations of the Ne(np') spectra yielded good overall agreement with the shapes, widths and energy positions of the measured resonances [1,2]. However, a proper theoretical description of the Ne($np'\,[1/2]_0$) resonances, especially the strong differences between the spectra, excited from the two $J = 1$ levels, turned out to be demanding [2]. These differences were found to be the result of the interference between the direct $\langle 3s|r|np\rangle$ and the intershell $\langle 3s|r|3p\rangle\langle 3p|V(2p\,2p)|np\rangle$ amplitudes which is constructive in the $3s' \rightarrow np'$ transition and destructive in the $3s \rightarrow np'$ transition. Calculations of the np' spectra of the heavier rare gas atoms exhibit trends which clearly reflect the influence of the rising spin-orbit splitting of the ion core [3].

A very recent two-color photoionization experiment on Ar by Lee *et al.* [4], combining excitation of ground state Ar atoms to several low-lying odd parity (ms, md) $J = 1$ levels (especially $7s'[1/2]_1$ and $8s[3/2]_1$) by monochromatized synchrotron radiation with subsequent laser excitation to Ar(np', nf') resonances raised questions on the validity of our theoretical predictions, especially for the different lineshapes of the Ar(np', $J = 0$) resonances. To shed further light on this problem, we carried out a new two-step excitation experiment, using the pulsed Zürich atomic beam setup. The three excited levels Ar($4s'[1/2]_1$, $3d[1/2]_1$, $5s[3/2]_1$) were prepared from the Ar ground state by a pulsed XUV laser source [5] (width 12 GHz) and further excited by Fourier-transform limited UV laser (width 100 MHz), perpendicular to the XUV beam. The UV laser was continuously tuned to record the Ar(np', nf') autoionization spectra of interest. The linear polarization vectors of both light beams could be chosen parallel or perpendicular to each other. An observation of particular interest, presenting a challenge to theory, is the near-absence of the np', $J = 1, 2$ resonances (n around 15) in the ARS spectra excited from the Ar($4s'[1/2]_1$) level.

At the conference we shall compare the experimental spectra from both the previous [4] and the Zürich experiments with our most advanced calculations.

Acknowledgment

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The coupled states $X^1\Sigma^+$ and $a^3\Sigma^+$ in KLi by high resolution Fourier transform spectroscopy

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We report a joint analysis of the $X^1\Sigma^+$ and $a^3\Sigma^+$ states of KLi molecule, correlated to the ground-state atomic asymptote of the atom pair K+Li. Molecular vapour, containing predominantly either $^{39}K^7Li$ or $^{39}K^6Li$ molecules, was produced in a heat-pipe oven and several $B^1\Pi(v', J') \leftarrow X^1\Sigma^+(v'', J'')$ transitions were excited with a single mode ring dye laser. Laser-induced fluorescence spectra of the $B^1\Pi$ – $X^1\Sigma^+$ and $B^1\Pi$ – $a^3\Sigma^+$ systems (the latter made observable due to perturbation of high vibrational levels in $B^1\Pi$ by the $b^3\Pi$ state) were recorded at high resolution by Fourier transform spectroscopy technique. Combination of the experimental data for both isotopologues enabled isotopically consistent description of the X and a states by their potential energy curves (reliable up to the dissociation limit) and also provided a measure of the adiabatic correction to the Born-Oppenheimer approximation for the $X^1\Sigma^+$ state. The resulting potentials form a solid basis for quantitative modelling of cold collisions for all combinations of K+Li isotope pairs.

Electron-impact double and triple ionization of tungsten atoms and ions at low ionization stages

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Due to a very low sputtering rate of tungsten it is used as the first wall material in large tokamaks, such as ASDEX Upgrade, and is planned to use in ITER. However, some its ions migrate to the central region of discharge and may be the reason of large radiation losses. Thus it is up-and-coming to investigate the role of the Auger decay of the states with a vacancy and the direct multiple ionization in the production of tungsten ions during their interactions with electrons.

The double and triple ionization of tungsten ions by electron impact at low ionization stages was measured and described by semiempirical formula [1], but no *ab initio* calculations were made. In this work the calculations of cross sections of these processes are performed taking into account the Auger decay of states with the vacancy in 4d, 4f, 5s, 5p and 5d shells as well as the direct double ionization considered using sudden perturbation model. The direct single ionization cross section is obtained in the relativistic distorted wave or binary-encounter-dipole approximations; the contribution from the indirect ionization by excitation-autoionization process is included too. The calculations are performed using Flexible Atomic Code [2]. It is shown that both processes – Auger decay and direct double ionization play an important role in the double ionization process. The calculated cross sections are compared with experimental data.

The contributions from the Auger transitions and from the sudden perturbation to the double ionization cross section are obtained of the same order, though the latter process plays a smaller role, especially for the higher ions. Most of the Auger transitions end in the configurations of the next ionization stage, thus the triple ionization cross section is more determined by the direct ionization.

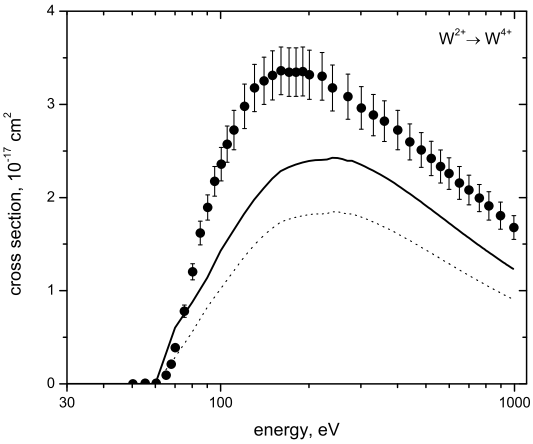

Figure 1: Electron-impact double ionization cross section of W^{2+} ions. Experiment [1], points with error bars. Results of calculation: dotted curve, single ionization following the Auger transitions; full curve, total double ionization.

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New even parity levels in neutral lanthanum

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Electronic levels system in lanthanum atom becomes very complicated at energies above 30000 cm^{-1}. In order to describe this levels system, a configurations basis including more than ten configurations has to be considered. Because of lack of experimental results concerning g_J factors and hyperfine structure constants for many electronic levels, their assignment to individual configurations is often doubtful and attempt of application of *ab initio* calculated radial integrals yields considerable discrepancies between the calculated and the experimental results.

In this situation the only solution seems to be measurement of hyperfine structure for a great number of known levels, as well as determination of energies, J quantum numbers and hyperfine structure constants for new, previously not observed electronic levels. In our recent works [1, 2] we published experimental results obtained for more than 100 levels with known energy values and 50 entirely new levels belonging to even configurations in La. In this work a few more electronic levels are presented. Classification of these levels is still a little doubtful, but they might prove very helpful in solving some problems in calculation of radial integrals with a semiempirical method.

Procedure of investigation of new levels (described in detail in [1]) begins with measurement of hyperfine structure of unclassified spectral lines of lanthanum with laser spectroscopy in a hollow cathode discharge with optogalvanic detection. Afterwards an initial identification of the lower and the upper levels involved follows. Finally the correctness of identification is verified by search for fluorescence channels from the lower (known) level.

Acknowledgment

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Rare low angular momenta energy levels in neutral praseodymium

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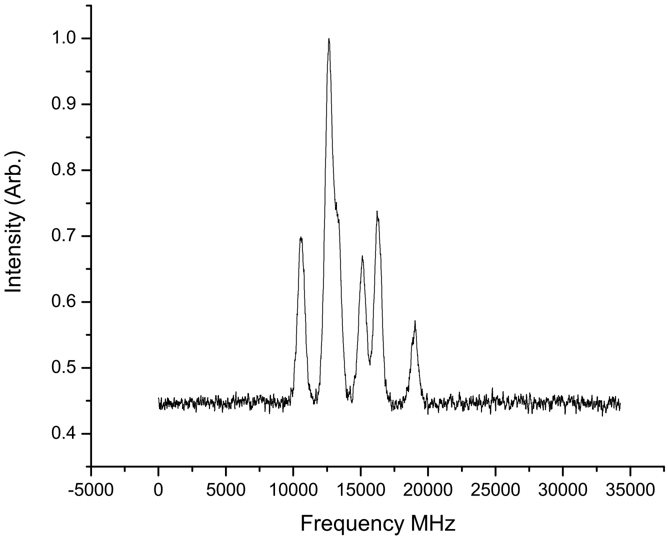
The interaction between electromagnetic multipole nuclear moments- magnetic moment, electric quadrupole moment etc. and electromagnetic field produced at the nucleus by electrons results in hyperfine splitting of fine levels. Nucleus has a compound structure comprising protons and neutrons each with 1/2 intrinsic spin, giving the nucleus net angular momentum with nuclear spin quantum number I. In analogy with LS coupling I and J quantum numbers couple together to produce total angular momentum quantum number F for the atom. For praseodymium the nuclear spin quantum number I is 2.5. The number of hyperfine components are determined by $2I + 1$ for $J > I$ and by $2J + 1$ for $J < I$.

In the investigation of neutral praseodymium atom in a hollow cathode discharge using laser spectroscopy, we have discovered large number of previously unknown energy levels with various angular momentum values. We present here energy levels with quite low angular momenta, namely 1/2, 3/2 and 5/2. Of special significance are energy levels with $J = 0.5$, since for these the resulting hyperfine splitting is due to the interaction between magnetic field produced by the intrinsic electron spin S with $L = 0$ and the nuclear magnetic moment. As an example we discuss the excitation of the line at 5756.49 Å. The S/N ratio for the recorded structure was quite reasonable and we were able to fit the structure as a transition $J = 1/2$ to 3/2 with quite good quality factor. From the determined magnetic interaction constants A, we were able to identify as lower level 13033.471 cm^{-1}, even parity, $J = 1.5$ and $A = 905(4)$ MHz. Using the centre of gravity excitation wavelength, the energy of the upper level was determined to be 30400.353 cm^{-1}, odd parity, $J = 0.5$ and $A = 1885(5)$ MHz. Following is the recorded structure for the line 5756.49 Å, observed at fluorescence line 5448 Å, the same structure is also observed at fluorescence line 5141 Å.



Discovery of new energy levels in praseodymium

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One most important incentive in searching for new energy levels is the high energy level density of an atom. Praseodymium is such a candidate. Our research group is extensively involved in the investigation of the fine structure of praseodymium using the hyperfine structure of the investigated transitions. Apart from some applications in other branches of Physics, the hyperfine structure studies and complete mapping of energy levels in praseodymium is of special significance for the theoretical understanding of the interactions inside the atom.

We have discovered more than 600 new energy levels both in even and odd configurations in last two years in a hollow cathode discharge using laser spectroscopy. Using high resolution Fourier Transform Spectra (FTS) [1], one can very precisely tune the laser wavelength to a hyperfine component to be investigated and then search for fluorescence from excited levels. The excitation source is a ring-dye laser system pumped by a solid state diode-pumped, frequency doubled Nd:Vanadate (Nd:YVO_4) Verdi V-18 laser system or by a Krypton ion laser. The spectral region covered during these investigations lie in the spectral range of Rhodamine 6G, Sulforhodamine B (Keton Red), DCM and Coumarine Dyes.

As an example we discuss here the excitation of the lines 6092.35 Å and 6048.79 Å in which we discovered a system of previously unknown lower and upper energy levels. The signal-to-noise ratio for both the recorded structures was quite good and we were able to fit both structures as transitions J = 15/2 to 15/2 and J = 17/2 to 15/2, respectively, with high quality factor. From the determined magnetic interaction constants A we were unable to indentify lower or upper levels in the data base of known levels. The fluorescence observed for both transitions were the same and are 6081 Å, 5555 Å, 5387 Å, 5316 Å, 5032 Å. After detailed investigations we concluded that we were exciting the same unknown upper level from two unknown lower levels. We then made an excitation of the line 6081.51 Å to the same unknown upper level as this line appeared as fluorescence line at the two first excitations. This time from the determined magnetic interaction constants A we were able to identify as lower level 17765.348 cm^{-1}, odd, 6.5 and 490(3) MHz. Using the center of gravity excitation wavelength, the energy of upper level was determined to be 34204.135 cm^{-1}. It has even parity, $J = 7.5$ and $A = 442(1)$ MHz. From the energy of upper level we determined the data for the two lower levels as 17794.23 cm^{-1}, odd parity, $J = 7.5$ and $A = 221(1)$ MHz and 17676.482, odd parity, $J = 8.5$ and $A = 857(1)$ MHz.

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Investigation of the hyperfine structure of Pr I lines in the region 5650 Å to 6200 Å

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Some unclassified spectral lines of the praseodymium (Pr) atom have been studied in the region from 5650Å to 6200Å. The hyperfine structure of these lines has been recorded by using the method of laser induced fluorescence in a hollow cathode discharge. During this investigation, eighteen new energy levels have been discovered, eight energy levels with odd parity and ten energy levels with even parity. The excitation sources are operated with R6G or Kiton red ring-dye laser pumped by a solid state diode-pumped, frequency doubled Nd:Vanadate Nd:YVO4 Verdi V-18 laser system. J-quantum numbers and magnetic dipole interaction constant A-values for upper and lower levels have been determined from the recorded hyperfine structure. The energies of new levels have been obtained by using these constants, excitation and fluorescence wavelengths. The excitation wavelengths have been taken from FT Spectra [1]. Levels confirmed by a second laser excitation are given in the following table.

			Involved new energy levels				
	Excitation Wavelength (λ_{air}) in Å	Signal/Noise in FT Spectra	Angular Momentum J	Magnetic Hyperfine Constants in MHz	Electric	Parity	Energy in cm^{-1}
1	5771.190	2	4.5	724(5)	0	e	29053.279
2	5665.975	9	5.5	689(5)	0	e	30465.398
3	5702.252	9	6.5	594(5)	54(13)	e	29278.391
4	5711.383	6	4.5	526(5)	16(6)	e	31506.346
5	5836.392	6	5.5	1138(5)	-21(4)	o	28313.518
6	5763.901	23	3.5	720(5)	0	o	28264.931
7	5660.990	6	6.5	729(5)	0	o	27334.913
8	5701.444	3	6.5	555(5)	0	o	32772.692
9	5824.037	4	6.5	596(5)	0	e	32512.894
10	5751.203	6	7.5	720(5)	0	o	30850.357
11	5797.194	4	4.5	509(5)	19(4)	o	31713.229
12	5798.548	6	7.5	460(5)	38(13)	e	30242.931
13	5683.636	9	6.5	581(5)	68(23)	e	29335.783
14	5992.673	12	3.5	679(5)	0	e	27336.533
15	5909.890	8	6.5	589(5)	33(6)	e	28238.556
16	5751.219	9	5.5	734(5)	0	o	26026.641
17	6144.727	21	5.5	556(5)	0	e	24519.756
18	6161.215	5	2.5	938(5)	0	o	26144.279

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New levels of Pr I discovered via far infrared spectral lines

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The Fourier transform (FT) spectrum of Praseodymium [1] shows hundreds of spectral lines in the infrared and far infrared region, many of them are unclassified. We found 15 levels of Pr during the classification of these lines [2]. The continuation of this work led us to the discovery of further new levels. The procedure of finding the new level was the same as we have used in our previous work [2]. Nine newly discovered levels are reported here.

The line 7039.935 Å is a known and unclassified line with relative intensity of 50. The hyperfine structure of the line has small components on left side of the main structure, this clearly tells it is a $\Delta J = 1$ transition. The best fit was obtained with $J_o = 4.5$ and $J_u = 3.5$ and allowed to determine the hyperfine constants A_o and A_u. By adding the wave number of the line to the wave number of the level 6535.53 cm^{-1}, identified via A_u, the new level 20736.29 cm^{-1} was introduced, which explains nine lines, five of them already known but unclassified, four of them new lines found in the FT spectra.

Table 1: Lines classified by new odd level 20736.29 cm^{-1}.

Wavelength	Upper level with odd parity			Lower level with even parity			Remarks
[Å]	J_o	Energy	A_o	J_u	Energy	A_u	
6299.531	4.5	20736.29	611	5.5	4866.53	867	Unclassified line
6703.542	4.5	20736.29	611	4.5	5822.89	861	Unclassified line
6931.411	4.5	20736.29	611	5.5	6313.25	756	Unclassified line
7039.935	4.5	20736.29	611	3.5	6535.53	979	Unclassified line
7221.674	4.5	20736.29	611	5.5	6892.95	551	Unclassified line
7620.522	4.5	20736.29	611	3.5	7617.44	868	New line
7857.527	4.5	20736.29	611	3.5	8013.14	165	New line
8395.930	4.5	20736.29	611	4.5	8029.28	797	New line
8717.872	4.5	20736.29	611	5.5	9268.75	977	New line

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Systematic analysis of the even configurations of Ta II

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We studied the complex atomic structure of the tantalum ion. This was done using a new package for semi-empirical calculations of the fine- and hyperfine structure [1], allowing up to four open sub-shells. We included the following 25 configurations :

$5d^4 + 5d^3n'g\ (n'=5\text{-}6) + 5d^36s + 5d^36d + 5d^26s^2 + 5d^26sn'g\ (n'=5\text{-}6) +$
$5d^26sn''d\ (n''=6\text{-}10) + 5d^26sn'''s\ (n'''=7\text{-}10) + 5d^25f6p + 5d^26p^2 +$
$5d6s^2n''d\ (n''=6\text{-}7) + 5d6s6p^2 + 5d5f6s6p + 5d5f6s7p + 5d6s6d7s.$

We also calculated eigenvectors and g_J-factors and improved the values of the parameters for the configuration interactions, most complicated in this spectrum. For all energy levels we obtained the exact spectroscopic description.

Acknowledgment

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Investigation of the hyperfine structure of Ta I-lines by laser-induced fluorescence

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Systematic investigations of the hyperfine structure of spectral lines of neutral tantalum have been performed by our international collaboration group since the beginning of 90's of the 20^{th} century[1].

In 1997, a theoretical analysis of the even tantalum energy levels in the configurations system $(5d+6s)^5$ [2] showed that the knowledge of the electronic structure of tantalum atom was far from being complete. But even after discovery of a large number of even energy levels [3,4], most of them filling gaps in the mentioned theoretical analysis, predicted levels remain which were never found.

That was the main reason to continue investigations of tantalum spectral lines by LIF (Laser-Induced Fluorescence) method in the spectral range covered by a coumarine 102 dye laser (4700 - 5100 Å), which had not been yet thoroughly studied. Previously only few lines were investigated and reported in this range [5-7].

In this work we report the discovery of 1 new energy level of even parity and 1 new energy level of odd parity. For new levels, beside their wave number, their total angular momentum quantum number J, their parity, as well as their magnetic dipole and electric quadrupole hyperfine interaction constants A and B were determined. All data for new levels are listed in table 1. We classified altogether 22 lines by means of laser spectroscopy in a hollow cathode discharge, 17 of them by laser excitation and 5 via fluorescence decay. These results are presented within this work.

Table 1: Parameters of the new Ta I levels.

Parity	J	Energy / cm^{-1}	A / MHz	B / MHz	λ_{ex}(air) / Å
even	9/2	54496.666(6)	210(8)	250(100)	4760.680
odd	1/2	47418.095(11)	-661(13)	0	4835.614, 4997.192

Acknowledgment
This work was performed within the framework of DS63-029/09.

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Investigation of fine and hyperfine structure of neutral La using highly resolved Fourier transform spectra

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Highly resolved Fourier transform spectra (resolution app. $0.03\,cm^{-1}$ in the spectral range 3800 to 8800 Å have been recorded using a see-through La hollow cathode lamp as light source, operated with Ar at 1 mbar and 60 mA dc current. The carefully done wavelength calibration has been checked using standard Ar lines.

With help of these spectra, an improvement in the knowledge of the electronic structure of the La atom (and also its first ion) can be reached:

- improvement of level energies
- classification of spectral lines by means of their characteristic hyperfine patterns
- determination of the hyperfine constants A and B, if unknown, of certain levels
- finding of new La spectral lines not implemented in commonly used spectral tables
- allowance for setting the excitation wavelength in laser spectroscopic investigations to the highest peaks of a hyperfine pattern

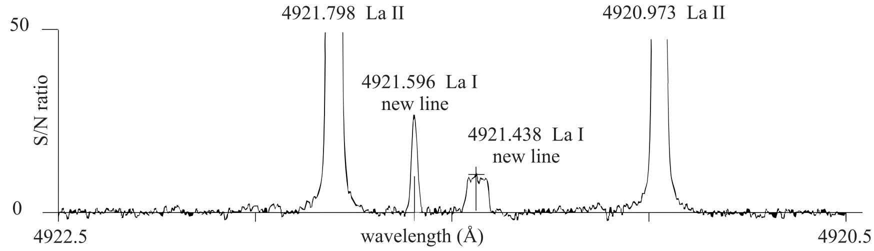

Figure 1: Small part of the Fourier transform spectrum with La II and La I lines.

The new line 4921.596 Å could be classified as transition 36851.32 cm^{-1}, J=5/2, even - 16538.39 cm^{-1}, J=7/2, odd. The new line at 4921.438 Å could be investigated by means of laser excitation and detection of laser-induced fluorescence. It is a blend between the transition 35117.70 cm^{-1}, J=5/2 even - 14804.08 cm^{-1}, J=5/2, odd and a second transition, in which a new, up to now unknown La I energy level is involved.

This new level could be located with help of the recorded hyperfine pattern and excitation and fluorescence wavelengths. Its data are 36556.76 cm^{-1}, J=9/2, even, A=472(5) MHz , and the line is interpreted as transition to 16243.17 cm^{-1}, J=9/2, odd. This new level explains also the new lines 4886.825 Å and 4994.019 Å with respect to wavelength and hyperfine structure.

A coupled dark state magnetometer

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Measuring magnetic fields by means of spectroscopic-optical methods has advantages in many respects. E.g. in best case the magnetic field sensor of an optical magnetometer can only be made of a (nonmagnetic) glass cell containing a tiny amount of an alkali metal non perturbing the external magnetic field. Moreover, the optical sensor is working near room temperature. Thus unlike to the (in common more sensitive) superconducting quantum interference device (SQUID) magnetometer an extensive cooling down to cryogenic temperatures can be avoided.

We consider a compact vertical surface emitting laser (VCSEL) based coupled dark state magnetometer (CDSM). In such kind of optical scalar magnetometer the zeeman split (magnetic sensitive) components of the coherent population trapping (CPT) resonance spectrum are coupled by a multi chromatic light field. The resulting CDSM-resonance is used to determine an external magnetic field. Thus, by applying the Breit-Rabi formula the scalar value of the external magnetic field can be derived directly from the frequency of the magnetic sensitive CDSM-resonance signal.

In our investigations the advantages and constraints of such a compact magnetometer type in terms of sensitivity, measurement bandwidth, noise and influence of magnetic field gradients are outlined.

Acknowledgment

The work is founded by the Fonds zur Förderung der wissenschaftlichen Forschung (FWF) (Project No.: L300-N02).

Homo- and hetero-nuclear inelastic cold collisions of ^{7}Li and ^{23}Na in a two species magneto-optical trap

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In a magneto-optical trap homo- and hetero-nuclear cold collision processes between alkali atoms have been investigated [1, 2]. Inelastic collisions can be divided into mainly three groups according to the change of internal state of colliding atoms, that is Radiative Escape (RE), Fine-structure Changing Collisions (FCC) and Hyperfine-structure Changing Collisions (HFCC). RE and FCC occur when one atom is in ground state and the other is in excited state while in HCC both atoms are in excited state. These exoergic collisions cause trap losses in the magneto-optical trap (MOT).

We have measured the trap loss coefficients for ^{7}Li-^{23}Na-collisions as a function of different laser intensities in a new vacuum chamber which consists of high grade demagnetised steel with 42 vacuum flanges of different size, compared to the old chamber with only 10 flanges. The new setup allows us to trap three species simultaneously.

At low intensities FCC are main causes of trap losses [3, 4]. We extract the homo- and hetero-nuclear trap loss coefficients $\beta_{^7\mathrm{Li}}^{^7\mathrm{Li}}$ and $\beta_{^7\mathrm{Li}}^{^{23}\mathrm{Na}}$ by measuring the decay curve of ^{7}Li with and without presence of cold ^{23}Na-atoms at different laser intensities.

For a cooling laser intensities of 107mWcm^{-2} we found $\beta_{^7\mathrm{Li}}^{^{23}\mathrm{Na}} \approx 2.5 \times 10^{-11}\mathrm{cm}^3\mathrm{s}^{-1}$, gradually increasing towards lower intensities. These results obtained by the new MOT-configuration are in good agreement with results in [3, 4] as shown in the following figure.

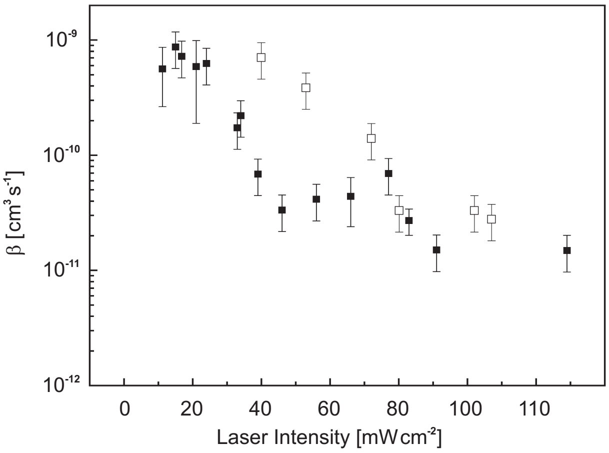

Figure 1: Lithium trap laser intensity dependence of $\beta_{^7\mathrm{Li}}^{^{23}\mathrm{Na}}$ for ^{7}Li in presence of ^{23}Na. The open and closed squares refer to the new results and those from [3, 4] respectively.

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Ultra-cold Rydberg atoms in magneto-optic and optical dipole traps

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In a Rydberg atom an electron is excited to a state with high principal quantum number n, very close to the ionisation threshold. Having so weakly bound electron, these atoms exhibit extreme sensitivity to external fields, including fields due to nearby Rydberg atoms. One excited atom can inhibit the excitation of its neighbours thus causing a "local blockade effect". This leads to the formation of spatial regions in which only a small fraction of the atoms can be excited. The dynamics of a dense sample of ultra-cold Rydberg gas, prepared by exciting laser-cooled alkali atoms, are dominated by these enhanced interactions to the extent that the atomic motion is unimportant. At the Open University, we are developing an experiment to study small numbers of atoms stored in micron sized optical dipole traps, in which the strong Rydberg-Rydberg interactions give rise to collective states of the entire sample.

In our experiment, ^{87}Rb atoms are trapped and cooled in a magneto-optic trap and then transferred to an optical dipole trap where they then undergo a two-photon laser excitation to a Rydberg state. Our objective is to study the collective states in a wide range of situations by controlling the density, Rydberg state or applied external fields. The current status of the experiment will be described.

Study of the 5P → 5D transition in Rb MOT

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Magneto-optical trap offers a convenient environment for subtle, Doppler-free, high resolution studies of cold atoms. We performed a spectral study of the nonlinear effects in the $5P_{3/2}(F') \rightarrow 5D_J(F'')$ hyperfine transitions in the ^{85}Rb MOT. A two-photon cascade excitation scheme $5S_{1/2}(F) \rightarrow 5P_{3/2}(F') \rightarrow 5D_J(F'')$ was used with a relatively strong pump beam in the first step and a weak probe beam in the second one. The transmission spectra of the probe influenced by the presence of the pump were observed for a number of detunings and intensities of the strong beam. The registered spectra reveal complex features (see the exemplary run in Fig. 1). Their discussion and an explanation within multi-level dressed atom approach will be presented.

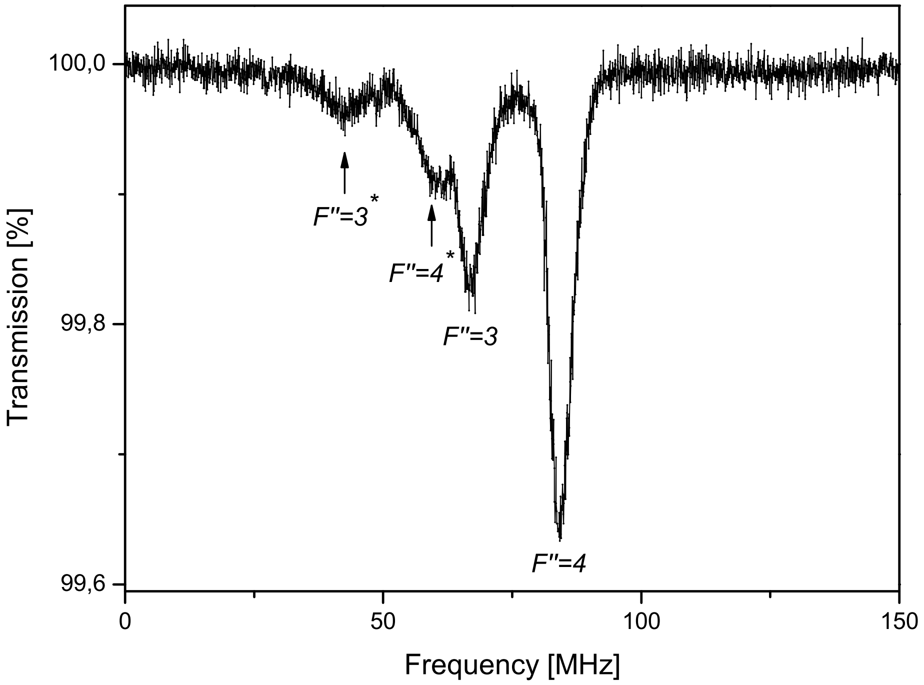

Figure 1: Transmission spectrum of the $5P_{3/2}(F' = 4) \rightarrow 5D_{3/2}(F'' = 3, 4)$ resonances in the cloud of cold ^{85}Rb atoms. The $5P_{3/2}(F' = 4)$ level was modified by the interaction with the strong beam detuned by few MHz from the resonance.

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Dynamics of rf trapped Ca^+ ions

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Radiofrequency (rf) trapped ions are an ideal test bed for a wide range of applications from frequency metrology to quantum computation. Our new experiment aims to trap a large ion cloud to study its dynamics, in particular phase transitions to the crystallized state as well as finite-size effects. The density of the charged ion cloud is limited by the Coulomb repulsion and depends on the electrodynamic potential which is applied for confinement. We intend to trap a cloud of 10^7 ions in a linear trap of 50 mm length, in order to achieve densities which allow to study crystallization dynamics and ordered structures of a large atomic ensemble. We will present the design of a double radiofrequency trap being composed of a quadrupole and a multipole part which allows to shuttle the ions from a parabolic potential well to a flatter potential and which will give insight on the influence of the potential form on the phase transition process.

The set-up of the experiment is accompanied by molecular dynamics simulations for the evaluation of the dynamics of ions in radiofrequency traps of different geometry, using the pseudo-potential approximation or the exact time oscillating description. Doppler laser cooling is taken into account by momentum kicks on absorption and emission of a photon by an ion.

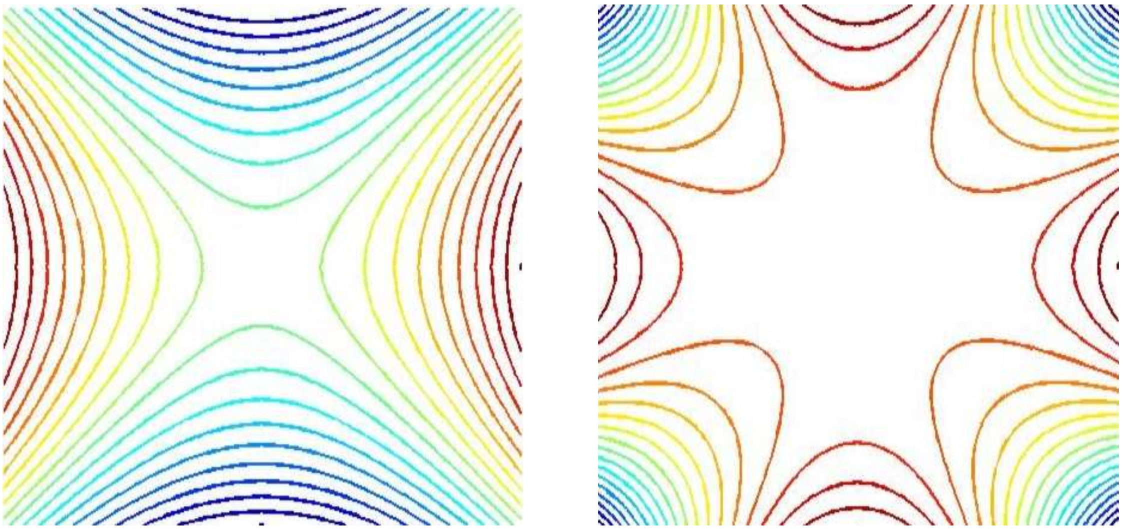

Figure 1: Isopotential lines of a quadrupole (*left*) and an octupole (*right*) trap.

Laser-driven Cs magnetometer arrays for cardiomagnetic field imaging

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Magnetocardiography is an innovative diagnostic method for cardiac diseases, based on the measurements of the weak magnetic fields (50–100 pT amplitude) produced by the electrical activity of a human heart. In current practice, magnetometers based on superconducting quantum interference devices (SQUIDs), which require cooling to 4 K, are the sensor of choice. However, due to the high capital investment and maintenance costs of such devices, there is a need and an interest in alternative methods of heart field detection. This issue has been investigated by the Fribourg Atomic Physics Group (FRAP) and resulted in the development of an optical Cs magnetometry system adapted to the heart measurement problem [1,2]. The magnetometer sensors record the Larmor precession frequency of Cs atoms in paraffin-coated vapor cells (28 mm diameter) via the optically detected magnetic resonance technique. A system of 25 Cs magnetometers, arranged as 19 second-order gradiometers with full digital control electronics has been built (Fig. 1). It is currently used for magnetic field imagining of healthy subjects and cardiac patients. This poster will give details on the sensors and their operation in the multichannel arrangement.

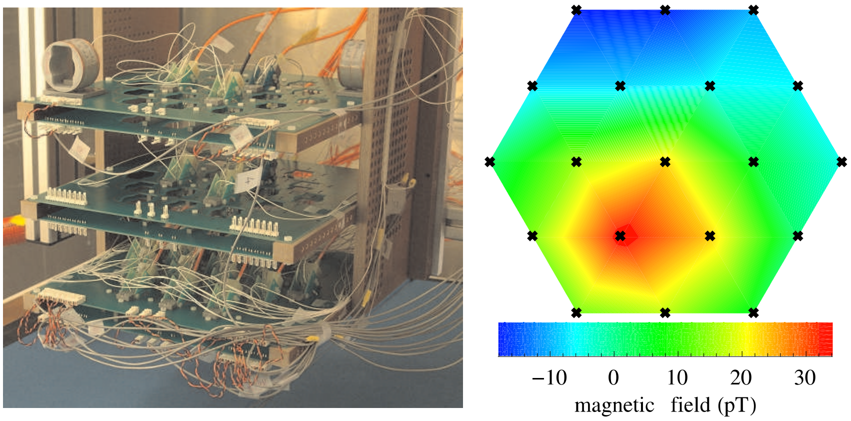

Figure 1: Left: The 19 channel second-order magnetic gradiometer system using 25 mounted sensors. The lowest plane contains 19 sensors, and the two upper planes contain each three sensors generating reference signals used to form the second-order gradiometer signal. Right: Magnetic field map of the artificial heart at the maximum of the R-peak.

Acknowledgment

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Laser-driven Cs magnetometer arrays for magnetic field control in an nEDM experiment

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In the search for a possible neutron electric dipole moment (nEDM), neutrons are simultaneously exposed to electric, $\vec{E}$, and magnetic, $\vec{B}$, fields. The neutron magnetic moment, and thus its spin, and any hypothetical EDM, will precess in the magnetic field. The signature of a nonzero nEDM is a linear dependence of the neutron Larmor precession frequency on the magnitude and orientation ($\hat{E} \cdot \hat{B}$) of the applied electric field. Any effect would be small, hence the temporal and spatial stability of the applied magnetic field throughout the volume used to confine the neutrons is of paramount importance. Magnetic field fluctuations contribute directly to the final sensitivity of the experiment, which relies on the Ramsey-resonance technique (100–200 s free precession time), so efforts must be made to stabilize both the temporal and spatial changes of the magnetic field.

We present a 'divide-and-conquer' approach to the problem using a three-dimensional array of laser-driven optically-pumped double-resonance atomic-cesium magnetometers (OPM). The sensor heads have a modest size (80 mm characteristic dimensions) and low production cost, while maintaining high magnetic sensitivity ($\sim 15\,\mathrm{fT}/\sqrt{\mathrm{Hz}}$) as well as vacuum and high-voltage compatibility. For the existing fully-operational multisensor magnetometry arrays, all-digital control using a dedicated FPGA system is being developed.

The sensors and their in-array operation will be detailed, and information given on future applications, such as the Paul Scherrer Institute nEDM experiment, a high stability current source, the ability of OPMs to read ^{3}He magnetometers, and real-time feedback techniques. More details on the magnetometers and in-array operation can be found in the contributions of Castagna, *et al.*, and Kasprzak, *et al.*

Electron-spin resonance and Rabi oscillations on Helium nanodroplets

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Superfluid helium nanodroplets provide a versatile substrate to cool atoms and molecules and, if desired, assemble weakly bound complexes. Electron-spin resonance (ESR) is a versatile probe of the electronic environment in radicals and, via spin tags, in ESR silent species. We demonstrate the first application of ESR to doped helium nanodroplets and exploit the scheme of optically-detected magnetic resonance (ODMR), since direct detection is not possible due to a lack of sensitivity. Laser light in combination with a magnetic dichroism scheme [1,2] is used to prepare the states of interest, and to detect them after manipulation with a microwave field. We measure sharp, hyperfine-resolved, ESR spectra of single K and Rb atoms isolated on He nanodroplets. The shift of the ESR lines with respect to free atoms directly reflects the distortion of the valence-electron wavefunction due to the He nanodroplet and denotes in an increase of the hyperfine constant consistent with an increase of the Fermi contact interaction. We are able to follow this change as a function of droplet size (see Fig. 1) attesting the sensitivity of the method for many foreseeable applications. The observation of Rabi oscillations (see Fig. 2) indicates a long decoherence time and proves our ability to perform coherent manipulation of the spin.

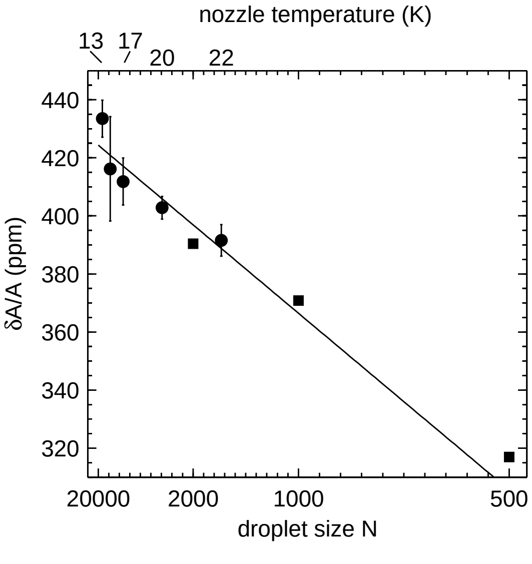

Figure 1: Influence of the droplet size, N, on the relative variation of the hyperfine constant, $\delta A/A$, for ^{85}Rb. Computed variations (squares) affirm a 1/N dependence of the experimental values (circles).

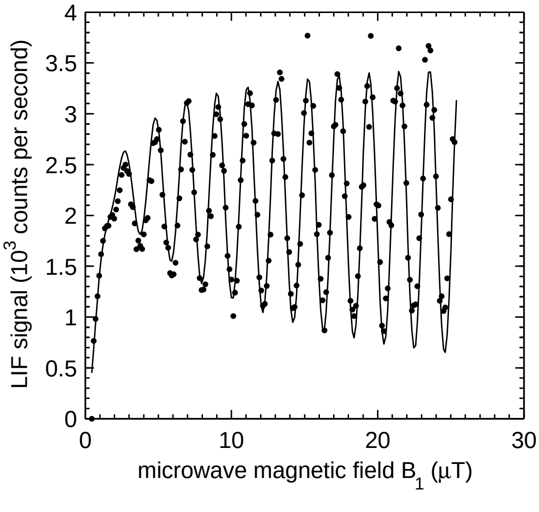

Figure 2: Increasing the microwave magnetic field amplitude results in coherent oscillations of the population (Rabi oscillations).

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Ultra-cold Rydberg atoms

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Rydberg atoms have a lot of interesting properties i.e. they have large sizes, very strong polarizability, they are sensitive to different kinds of electromagnetic field perturbations and they can interact strongly with other excited atoms. Applying laser cooling techniques makes it possible to investigate Rydberg atoms in the ultra-cold regime, where van der Waals and dipole-dipole interactions play dominant part in the dynamics of the system. These interactions can cause one excited atom to restrain the excitation of adjacent atoms, causing a local blockade effect.

At the Open University, we are finalizing an experimental setup where small numbers of Rubidium atoms will be confined in micron-sized dipole traps. This will allow us to achieve very high atomic densities and we will be able to fully exploit the local blockade effect so that only a little fraction of atoms in each dipole trap will be excited to Rydberg state. By selecting the Rydberg state and the atomic sample density, we will be able to control the number of excited atoms. Ultimately in our experiment there will be only one excited atom per a trap.

Laser excitation to Rydberg states is obtained via a two-photon process. To obtain a stable frequency of the excitation laser sources we apply a technique that involves electromagnetically induced transparency (EIT) in a cascade system, as an atomic reference to lock these lasers [1]. The EIT relies on cancellation of absorption of the coupled beam by the atoms of the sample in a presence of a weak probe beam tuned to another resonance of the sample.

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Interference effects in the resonant CO($1s^{-1}\pi^*, v$) excitation studied by the CO$^+$(A–X) fluorescence

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Resonant Auger decay is one of the most suitable prototype for studying quantum mechanical interferences. The strong interferences between different transition amplitudes of resonant photoionization and weak direct photoionization, known as electronic states interference (ESI), was recently found in the resonant Auger decay of the Kr $3d^9np$ states [1]. The interference between transition amplitudes via different vibrational levels of the same electronic state, known as lifetime vibrational interference (LVI), is another type of quantum mechanical, which can be studied by the inner-shell resonance excitation of molecules [2].

In the present work we report a joint theoretical and experimental study of the ESI and LVI in the $1s^{-1}\pi^*(v)$ resonant excitation and subsequent Auger decay in randomly oriented CO molecules. For this purpose, polarization analysis of the A $^2\Pi(v') \rightarrow$ X $^2\Sigma^+(v'')$ fluorescence in the CO$^+$ ion excited in the vicinity of the C*O and CO* resonances has been performed. The energy dependencies of the angular distribution parameters for the A $^2\Pi(v')$ photoelectrons and for the subsequent A $^2\Pi(v') \rightarrow$ X $^2\Sigma^+(v'')$ fluorescence in the vicinity of the C*O and CO* resonances are predicted theoretically. These energy dependencies are due to the electronic states interference and lifetime vibrational interference. The interference has a long energy range character and is important even in case of the C*O excitation.

The present theoretical results are verified at the U49/2 PGM1 beamline, BESSY II, Berlin, by means of the photon-induced fluorescence spectroscopy (PIFS) [3]. The resolution of the linearly polarized exciting synchrotron radiation was set to 75 meV at 289 eV for the C*O resonance and to 135 meV at 535 eV for the CO* resonance in order to be in the Raman regime for core excitations. Polarization analysis of the dispersed A $^2\Pi(v') \rightarrow$ X $^2\Sigma^+(v'')$ fluorescence has been performed in the visible spectral range from 378 nm to 578 nm with the resolution of about 0.5 nm using a Wollaston prism.

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Irregularities in highly excited electronic energy states of Cd_2: experiment versus *ab initio* calculations

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Vibrational and isotopic structures of highly excited $^31_u(6^3S_1)$ and $^10_u^+(6^1S_0)$ electronic energy states of Cd_2 were extensively investigated in a cold environment of supersonic free-jet expansion beam. Laser induced fluorescence excitation spectra were recorded in the ultraviolet region (206-218 nm *i.e.*, 48530-45860 cm^{-1}) using the $^31_u \leftarrow X^10_g^+$ and $^10_u^+ \leftarrow X^10_g^+$ bound←bound transitions. The measured spectra provide characteristics of the ^31_u and $^10_u^+$ - state potentials. At the present stage, it is concluded that the shape of the experimentally determined potential of the triplet excited state ($D_e'(^31_u)$=10959 cm^{-1}, $R_e'(^31_u)$=2.60 Å) is close to the result of *ab initio* calculations [1]. However, for the singlet excited state ($D_e'(^10_u^+)$=6569 cm^{-1}, $R_e'(^10_u^+)$=3.54 Å) the above statement is not true - the experiment gives result far from the *ab-initio* calculated one [1]. Beside the bound←bound transitions, a part of the excitation spectrum *i.e.*, region of 207-208 nm, incorporates features that may indicate a presence of free←bound transitions. To explain the recorded signal, we assumed proximity of a crossing of the $^10_u^+$ - state potential with that of ^11_u state that correlates with a Rydberg atomic asymptote lying above the 6^3S_1 and 6^1S_0 atomic levels, similarly as reported for the case of Hg_2 [2].

The reported experiment constitutes part of our ongoing activity focused on studies of interatomic potentials of ZnRg, CdRg (Rg=rare gas), Zn_2 and Cd_2 van der Waals complexes [3], aiming at determination of mechanisms of molecular internal vibrational cooling, as well as experimental verification of Bell's inequality for a pair of neutral atoms "born" in a controlled dissociation of diatomic molecule in an expansion beam [4].

Acknowledgment
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Cavity ring-down measurements of the line parameters of water rotation-vibration transitions near 1.39 μm

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Water vapor dominates the absorption of incoming (solar) and outgoing (thermal) radiation in the Earth's atmosphere, and its rotation-vibration spectrum is relevant to remote sensing techniques. In many applications, such as propulsion, combustion, ultra-high purity gases for semiconductor manufacturing, particle synthesis, human breath analysis, the measurement of water vapor amount via absorption spectroscopy provides essential information for system quantification, control, and optimization. Moreover commercially available and widely used optical hygrometers use water absorption transition near 1.39 μm.

In this study a low uncertainty line intensities and line shape parameters were measured for rotation-vibration transitions of water vapor near 1.39 μm. High-resolution absorption spectra of water vapor/nitrogen mixtures were acquired using the frequency-stabilized cavity ring-down spectrometer at the National Institute of Standards and Technology [1]. The NIST primary standard humidity generator [2] was used to produce a stable and accurately known amount of water vapor in a nitrogen carrier gas stream. Line intensities and line shape parameters were determined for 15 water transitions perturbed by nitrogen. A combination of semiclassical line shape models, which take into account collisional broadening and shifting, as well as the collisional narrowing and the speed-dependence of collisional effects, with a multi-spectrum fits of spectra measured for different gas pressures allowed us to determine a set of line shape parameters which are linear with pressure. The relative combined standards uncertainties of reported line intensities are smaller than 0.4% in most cases. We also discuss the influence of the choice of line shape model on fitted line intensities and line shape parameters. Our experimental results are compared to experimental and theoretical data available in the literature. Agreement between our experimental intensity measurements and those derived by recent *ab initio* calculations of the dipole moment surface of water vapor is within 1.5% [3].

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Feshbach resonances and cold collisions between two alkali atoms

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Feshbach resonances [1], named after Herman Feshbach, have become very important in ultracold atomic and molecular physics the last ten years. Feshbach resonances are an important ingredient in the ongoing exploration of these systems and in the tremendous progress made after the first successful creation of a Fermi gas [2].

The attractive properties of these systems stems from the possibility of tuning the interatomic interaction by varying the magnetic field around a Feshbach resonance. The scattering length is the important parameter which characterizes the atom-atom interaction in ultracold gases [3] (together with the Pauli principle). The scattering length behaves in a peculiar way as one pass through a Feshbach resonance - it diverges and changes sign (see e.g. figure 1). This makes it possible for the experimentalists to attain full control of the interactions by varying the magnetic field strength. Many systems have Feshbach resonances that are accessible through relatively low magnetic field strengths.

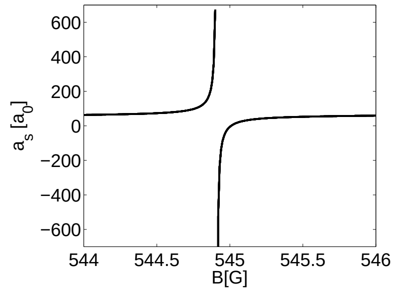

Figure 1: Scattering length a_s vs. magnetic field showing a narrow Feshbach resonance.

We present a model applicable to cold diatomic collisions and solve the close-coupled equations for the particular ^{6}Li$_2$ and K$_2$ systems. The calculations are performed ab initio with the matrix elements for the relevant interactions written in the molecular Hund's case (a) basis. The *s*-wave scattering length is reported for magnetic field strengths between 0-1000 G for a range of different hyperfine states in both systems. Several Feshbach resonances, of different widths and characters, are found in both ^{6}Li$_2$ and K$_2$. The calculated resonance positions agree very well with the observed resonance positions for ^{6}Li$_2$ [4] and K$_2$ [5].

In addition, the short range hyperfine interaction has been included in the calculations, and its effect on the scattering length investigated. Molecular hyperfine parameters were obtained from separate *ab initio* calculations.

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Aggregation of metal atoms on quantized vortices in superfluid ^{4}He and nanowire formation

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Quantized vortex lines in superfluid ^{4}He are known to bind electrons, atoms, and ions. One therefore expects the growth of nanoscopic (possible monoatomic) quasi one-dimen-sional filaments by the coalescence of atoms and nano-clusters along vortex lines. The formation of filament-like structures by impurity particles in superfluid helium has indeed been reported by several authors, whereas in normal fluid only spherical clusters were observed [1]. All previous observations were only visual, and could thus only set a lower limit of a few microns for the filament thickness. Here we report the first direct experimental evidence that the filaments formed by the coalescence of impurity atoms and/or clusters in superfluid He indeed have transverse dimensions in the nanometer range.

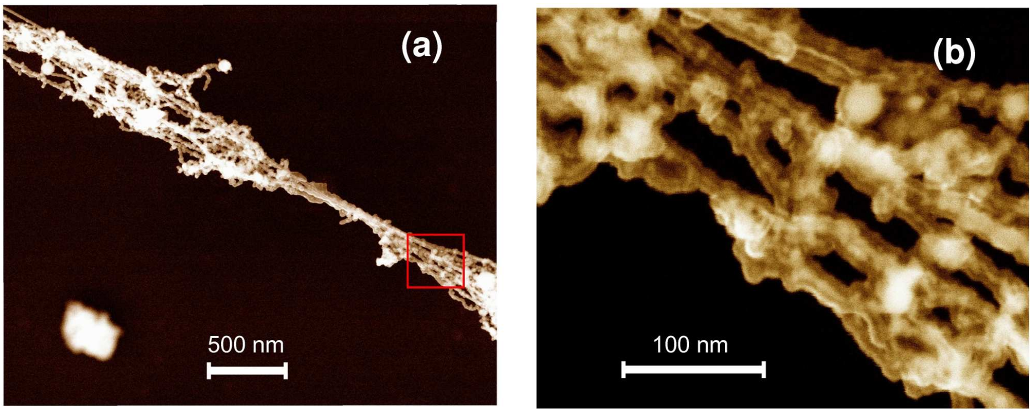

Figure 1: SEM images of gold nanowires produced by laser ablation in superfluid ^{4}He.

Gold atoms were introduced into superfluid ^{4}He (T = 1.5 K) by pulsed laser ablation from a gold target [2]. The gold filaments – collected after warming up the cryostat – were analyzed by a scanning electron (SEM) microscope, which reveals a very dense "spider web" structure (Fig. 1.a) made from a large number of thin fibers with diameters of 2-20 nm (Fig. 1.b). These nanowires are twisted together and form thicker "ropes" that are visible to the naked eye. The characteristic length of an individual nanowire is larger than 3μm, whereas the "ropes" have lengths comparable to the cryostat cell dimensions ($\simeq$6 cm). It is thus conceivable that the length of a nanowire could reach several centimeters when produced under better controlled conditions.

Acknowledgment

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Probing cold atoms using tapered optical fibres

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In this paper, we discuss the coupling of light emitted by cold rubidium atoms into the guided mode of a tapered optical fibre [1,2]. Tapered fibres are promising tools for manipulating and trapping cold atoms via the evanescent light field [3,4]. In order to fully understand the processes present when a cold atom is close to the surface of an optical fibre, the spontaneous emission rate of atoms near the fibre's surface must be studied. Fibres used in our work typically have diameters of ∼600 nm, with a transmission at 780 nm of ∼60% prior to installation into the vacuum chamber. A schematic of the setup is shown in Fig. 1. Light coupled into the fibre is monitored using a single photon counting module connected to one end. Using this technique, we have measured the profile of the atom cloud by moving the cloud across the narrowest region of the tapered fibre and recording the photon count rate. We have used a similar technique to measure the lifetime and decay time of the atom cloud. Our results are compared to those obtained by imaging the cloud directly onto a photodiode.

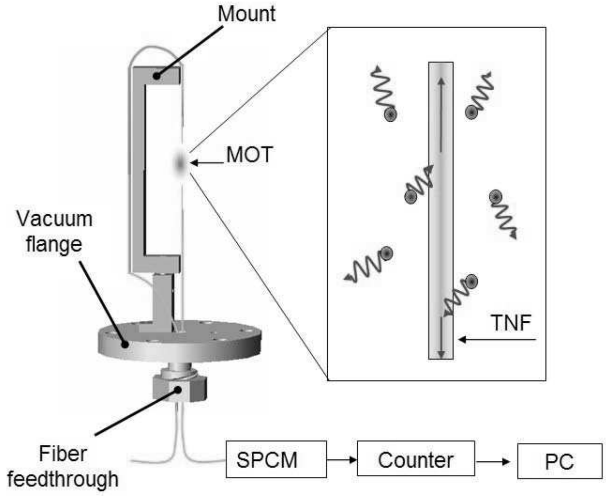

Figure 1: Schematic of the experimental setup

It is worth noting that the tapered fibre proves to be a more sensitive tool for few atoms, giving an increased decay time of the cloud, thereby providing a method of analysing density distributions in MOTs with a high degree of precision.

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K-X-ray spectra structures for various valence electronic configurations of 3d and 4d transition metals

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We caried out (using extensive multiconfiguration Dirac-Fock (MCDF) calculations with the inclusion of the transverse (Breit) interaction and QED corrections [1]) investigation of changes influence in the valence electronic configuration (types $(N-1)d^{q-r}Ns^{r}$ (r=2,1,0) and other types created by ionization of valence shell) on parameters and structure of $K\alpha_{1,2}$, $K\beta_{1,3}$ and $K\beta_2$ X-ray spectra for various $3d$ and $4d$ transition metals. In the present work, the structures of the K-X-ray spectra for various valence electronic configurations have been presented and analyzed with regards to their parameters like shapes, $K\beta/K\alpha$ intensity ratios and energy shifts.

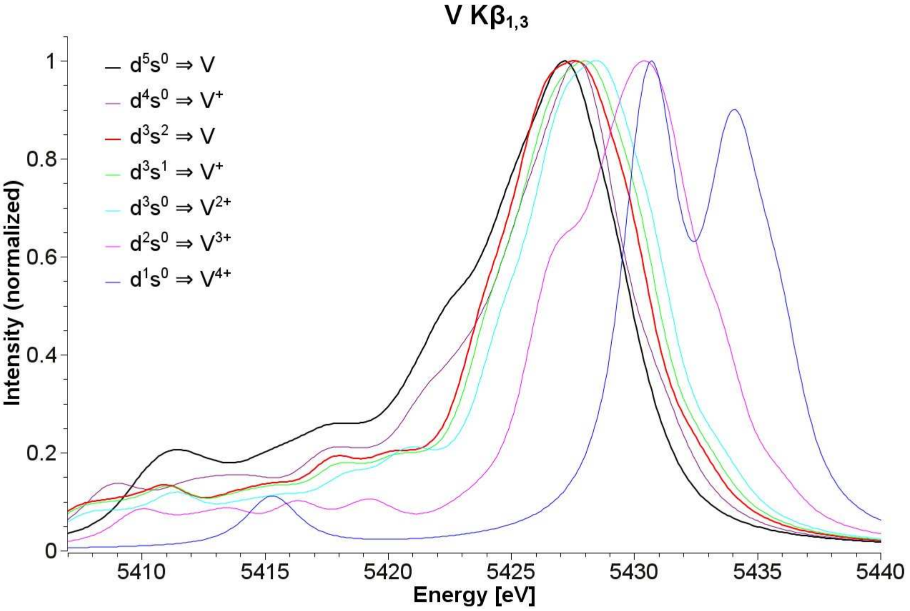

Figure 1: Vanadium $K\beta_{1,3}$ x-ray line shapes for variuos valence configurations.

It has been found that the changes of line positions of the $K\alpha_{1,2}$, $K\beta_{1,3}$ and $K\beta_2$ X-ray lines for different valence configurations are small but discernible and it is possible to detect this effect experimentally. Also the $K\beta/K\alpha$ intensity ratios and line shapes (see Fig. 1) have been changed for various valence electronic configuration. The observation of the K-X-ray spectra shapes and other parameters seems to be very good method to investigate electronic valence structure, especially for the study of the changes in the valence configuration caused by the chemical environment [2, 3].

Acknowledgment

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Structures of L-X-ray spectra for various valence electronic configurations of 4d transition metals

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In order to explain the influence of the changes in the valence electronic configuration on structure of $L\alpha_{1,2}$ and $L\beta_1$ X-ray lines for $4d$ transition metals the extensive multiconfiguration Dirac-Fock calculations with the inclusion of the transverse (Breit) interaction and QED corrections [1] have been carried out on zirconium, palladium and silver.

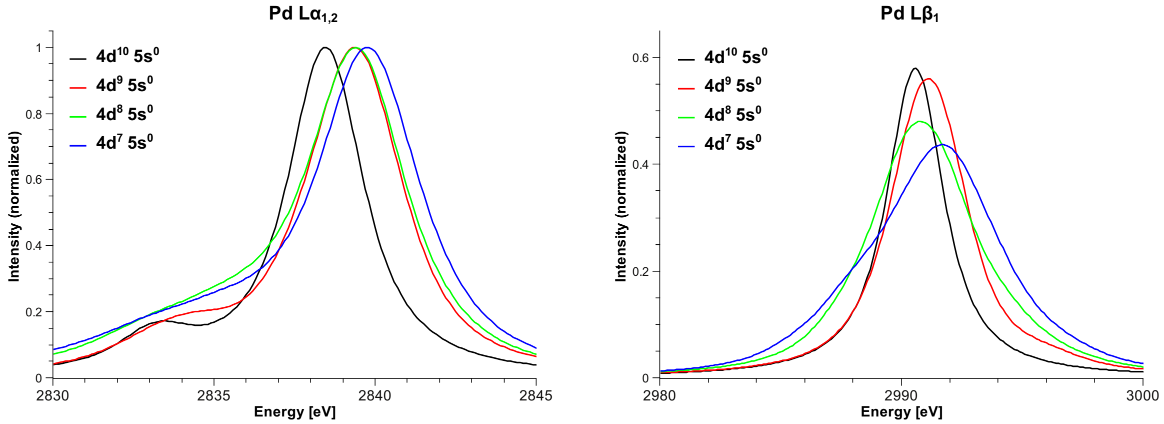

Figure 1: Influence of the changes in the valence electronic configuration on the structure of $L\alpha_{1,2}$ and $L\beta_1$ X-ray lines of palladium.

Table 1: $L\alpha_{1,2}$ and $L\beta_1$ x-ray line positions and $L\beta/L\alpha$ intensity ratio for various valence configurations of zirconium and palladium.

Valence configuration	Number of transitions	$L\alpha_{1,2}$ [eV]	$L\beta_1$ [eV]	$L\beta/L\alpha$ ratio
Zr: $4d^0\ 5s^2$	3	2042.44	2124.99	0.518
Zr: $4d^2\ 5s^2$	1576	2041.98	2124.54	0.469
Zr: $4d^4\ 5s^0$	22266	2041.80	2124.48	0.497
Pd: $4d^{10}\ 5s^0$	3	2837.93	2990.58	0.525
Pd: $4d^7\ 5s^0$	8522	2838.60	2991.31	0.535

It has been found (see Fig. 1 and Tab. 1) that the L-X-ray line structures (shapes and positions) and $L\beta/L\alpha$ ratios depend noticeably on electronic valence configuration. Therefore the observation of the shapes and parameters of L-X-ray lines seems to be very good method to investigate electronic valence structure, especially in the study of the influence of the chemical environment on the changes in the valence configuration [2].

Acknowledgment

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K-X-ray hypersatellite intensity ratios and lifetimes of the doubly K-shell ionized states

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In the last decades the $K^h\alpha_{1,2}$ hypersatellite lines in the X-ray spectra were measured by using different experimental techniques. High-resolution measurements of such spectra [1, 2, 3] give direct access to the studies of the K-shell hollow (i.e. doubly K-shell ionized) atoms. The present work provides the interpretation of the spectra for the K-shell hollow atoms based on the advanced theoretical analysis of the $K^h\alpha_{1,2}$ hypersatellite lines. The de-excitation of the doubly K-shell ionized state via the $K^h\alpha_1$ transition is forbidden in the pure LS coupling scheme (the spin flip $^1S_0 \rightarrow {}^3P_1$) but allowed in the j-j coupling scheme (see Fig. 1).

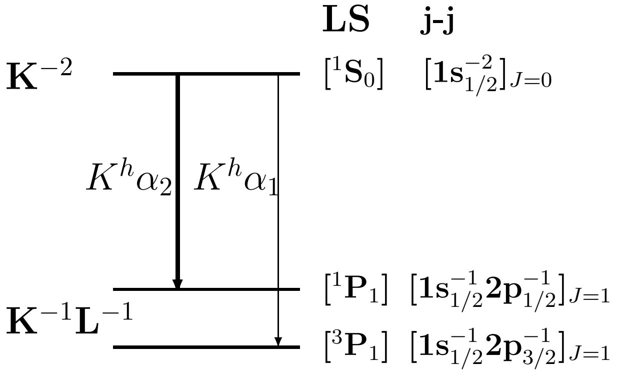

Figure 1: $K^h\alpha_{1,2}$ hypersatellite X-ray transitions.

As a result, the $I(K^h\alpha_1)/I(K^h\alpha_2)$ intensity ratio changes with the atomic number from small values (for the LS coupling limit at low Z) to large values (for the j-j coupling limit at high Z). It has been found that although the intensity ratios of the corresponding lines demonstrate strong hindrance of the $K^h\alpha_1$ transitions for low Z, the lifetimes of doubly K-shell ionized states do not lengthen in any case (i.e. they are always two times shorter than for single K-shell ionized states). The effect is explained as a result of significant mixing of the $^3P_1$ and $^1P_1$ states (in the LS coupling). The obtained theoretical results are in agreement with experimentally observed data.

Acknowledgment

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Study of the satellite and hypersatellite M-X-ray line structures for uranium

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In order to explain the structure of various satellite (additional vacancies in N and/or O shells) and hypersatellite (additional vacancies in M or M and N shells) $M\alpha_{1,2}$ and $M\beta_1$ lines in the X-ray spectra of heavy atoms the extensive multiconfiguration Dirac-Fock calculations [1] have been carried out on uranium. For every calculated type of $M\alpha_{1,2}$ and $M\beta_1$ lines the theoretical stick spectra (line positions with their relative intensities) have been presented. Moreover, for each type of lines two theoretical spectra have been predicted: one being a sum of the Lorentzian natural line shapes and the other one being a convolution of the Lorentzian natural line shapes sum with the Gaussian instrumental response (see Fig. 1).

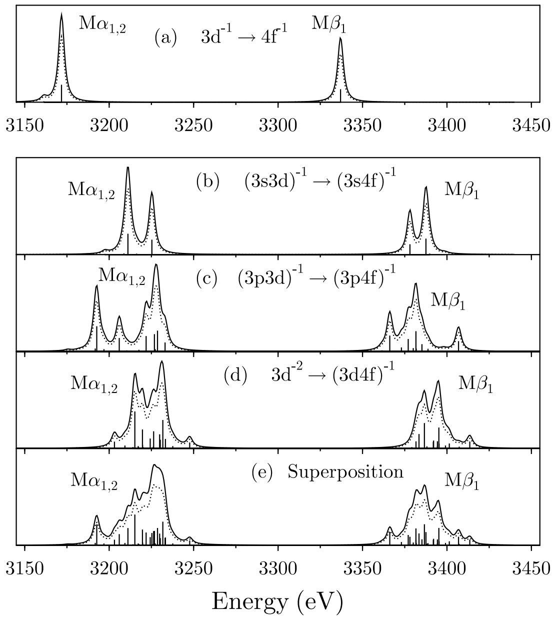

Figure 1: Calculated stick and predicted spectra for the $M\alpha_{1,2}$ and $M\beta_1$ diagram and M-shell hypersatellite transitions [(b)-(e)] for uranium. Spectrum (e) is the summary spectrum [(b)+(c)+(d)].

The obtained results will be helpful in reliable quantitative interpretation of a very complex origin structure of $M\alpha_{1,2}$ and $M\beta_1$ lines in various high-resolution X-ray spectra of heavy atoms induced by different light and heavy projectiles. Moreover, the absolute intensities of the U M-X-ray lines can be helpful in application of X-ray measurements from UO_2 as a reference material (virtual standard) for wavelength-dispersive electron probe microanalysis (WDS-EPMA) [2]. This technique provides non-destructive method of probe surface analysis and can be contribution to further research.

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Nitrogen K-shell photoabsorption

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We have computed atomic data for the spectral modeling of the nitrogen K lines which leads to useful astrophysical diagnostics; for instance, the estimate of the nitrogen abundance in the ejecta of η Carinae [1] and the characterization of the warm absorber of the MR 2251-178 quasar [2]. This work is part of a wider project to compute atomic data in the X-ray regime to be included in the database of the popular XSTAR modeling code [3].

The atomic data sets comprise valence and K-vacancy energy levels, wavelengths, A-values, radiative and Auger widths and K-edge photoionization cross sections. An important issue is the lack of measurements which are usually employed to fine-tune calculations to attain spectroscopic accuracy; for this reason, two atomic structure codes, namely AUTOSTRUCTURE [4, 5] and HFR [6], are used to estimate data quality. In the calculation of the photoabsorption in the K region with the Breit–Pauli R-matrix method [7, 8, 9, 10], both radiation and Auger dampings, which cause to the smearing of the edge, are taken into account.

Extensive comparisons with previous computations have been carried out, and the opacities obtained from XSTAR for different ionization parameters and nitrogen abundances will be fitted to astronomical observations.

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Evolution of $2p_{3/2}^{-1}4x^{-1} - 4x^{-1}4d^{-1}$ X-Ray satellites spectra in the $L\beta_2$ region

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The X-ray satellite spectra arising due to $2p_{3/2}^{-1}4x^{-1} - 4x^{-1}4d^{-1}$ (x ≡ s, p, d) transition array, in elements with $Z = 40$ to 92, have been calculated. The energies of various transitions of the array have been determined by using available Hartree-Fock-Slater data on $1s^{-1} - 2p^{-1}4x^{-1}$ and $2p_{3/2}^{-1} - 4x^{-1}, 4x'^{-1}$ Auger transition energies, their relative intensities have been estimated by considering cross sections of singly ionized $2x^{-1}$ (x ≡ s, p) states and then of subsequent Coster-Kronig and shake off processes. The calculated spectra have been compared with the measured satellite energies in $L\beta_2$ spectra. Their intense peaks have been identified as the observed satellite lines. It has been established that various $2p_{3/2}^{-1}4d^{-1} - 4d^{-2}$ transitions combine to give rise to a high-energy satellite near the $L\beta_2$ line. The most intense transition $^3F_4$—$^3F_4$ one, and seven others of this array is the main source of the emission of the satellite $\beta_2^{(a)}$, reported in the spectra of elements with $Z < 60$. In the range $Z > 70$, the second most intense transition, namely the $^1D_2$—$^1D_2$, and a comparatively weaker transition, namely the $^3D_3$—$^3P_2$ one, deviate from this group. Unfortunately, no experimental data are available on the intensities of these satellites. This suggests a need of detailed investigation, both theoretical and experimental, of these spectra.

Hartree-Fock-Slater (HFS) transition energies and relative intensities of $L\beta_2$ X-Ray satellites spectra in the 5d transition elements

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The X-ray satellite spectra arising due to $2p_{3/2}^{-1}3x^{-1} - 3x^{-1}4d^{-1}$ (x$\equiv$s, p, d) transition array, in elements with Z = 42 to 90, have been calculated. While the energies of various transitions of the array have been determined by using available Hartree-Fock-Slater data on $1s^{-1} - 2p^{-1}4x^{-1}$ and $2p_{3/2}^{-1} - 4x^{-1}, 4x'^{-1}$ Auger transition energies, their relative intensities have been estimated by considering cross sections of singly ionized $2x^{-1}$ (x$\equiv$s, p) states and then of subsequent Coster-Kronig and shake off processes. The calculated spectra have been compared with the measured satellite energies in $L\beta_2$ spectra. Their intense peaks have been identified as the observed satellite lines. The one to one correspondence between the peaks in calculated spectra and the satellites in measured spectra has been established on the basis of the agreement between the separations in the peak energies and those in the measured satellite energies. It has been established that four satellites observed in the $L\beta_2$ region of the X-ray spectra of various elements and named β_2^I, β_2^b, β_2^{II} and β_2^c in order of increasing energy are mainly emitted by $2p_{3/2}^{-1}4d^{-1} - 4d^{-2}$ transitions. In the present study, we report the transition assignments to the satellites β_2^I, β_2^b, β_2^{II} and β_2^c reported in the spectra of elements with Z = 42 to 52 and the satellites named β_2^I and β_2^{II} in the L – emission spectra of the elements of $_{74}$W to $_{90}$Th. It is observed that out of these four satellites, β_2^b can be assigned to superposition of $^3F_4$–$^3G_5$ and $^3F_4$–$^3D_3$ transitions and that this must be the most intense of all these satellites in the elements $Z = 42 - 50$. In the range of elements Z = 52 to 77, the satellite β_2^I is emitted by these transitions. The same transitions have been proved to be the main origin of the satellite β_2^{II}, reported in the elements $_{79}$Pt to $_{90}$Th. It has been well established that the transitions $^1F_3$–$^1G_4$ and $^3D_3$–$^3D_3$ is the main source of the emission of the satellite β_2^{II} in the elements $_{42}$Mo to $_{77}$Ir. Coming to the other two satellites in this region of the spectra, the line β_2^c, observed in the spectra $_{42}$Mo to $_{50}$Sn, is mainly assigned to the transition $^3P_1$–$^3D_2$. Lastly, the line β_2^I, observed in the spectra of elements Z = 42 to 46, is assigned to the transitions $^3D_3$–$^3F_4$ and $^1D_2$–$^1F_3$, while in the range of elements with Z = 78 to 90, β_2^I has been assigned to these transitions. In the elements $_{48}$Cd and $_{50}$Sn, the line β_2^I has been associated with transition $^3F_4$–$^3F_4$. Unfortunately, no experimental data are available on the intensities of these satellites. This suggests a need of detailed investigation, both theoretical and experimental, of these spectra.

$L_2M_x - M_xM_{4,5}$, $L_3M_x - M_xM_{4,5}$ and $L_3M_x - M_xN_{4,5}$ Coster-Kronig, Shake off probabilities and Gaussian curves of L X-Ray satellites spectra

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The X-ray satellite spectra arising due to $L_2M_x - M_xM_{4,5}$, $L_3M_x - M_xM_{4,5}$ and $L_3M_x - M_xN_{4,5}$ ($x \equiv 1-5$) transition array, in elements with $Z = 29$ to 99, have been calculated, using available Hartree-Fock-Slater (HFS) data on $K - L_3M_x$ and $L_3 - M_xM_{4,5}$ Auger transition energies. The relative intensities of all the possible transitions have been estimated by considering cross - sections for the Auger transitions simultaneous to a hole creation and then distributing statistically the total cross sections for initial two hole states L_3M_x amongst various allowed transitions from these initial states to $M_xM_{4,5}$ final states by Coster-Kronig (CK) and shake off processes. In both these processes, initial single hole creation is the prime phenomenon and electron bombardment has been the primary source of energy. Each transition has been assumed to give rise to a Gaussian line and the overall spectrum has been computed as the sum of these Gaussian curves. The calculated spectra have been compared with the measured satellite energies in $L\alpha_1$ $L\beta_1$ and $L\beta_2$ spectra. The one to one correspondence between the peaks in calculated spectra and the satellites in measured spectra has been established on the basis of the agreement between the separations in the peak energies and those in the measured satellite energies. Their intense peaks have been identified as the observed satellite lines. The peaks in the theoretical satellite spectra were identified as the experimentally reported satellites $L\alpha_3$, $L\alpha_4$, $L\alpha_5$, $L\alpha'$, $L\alpha^{ix}$, $L\alpha^{x}$, $L\beta_1^{I}$, $L\beta_1^{II}$, $L\beta_1^{III}$, $L\beta_1^{IV}$ $L\beta_2^{I}$, $L\beta_2^{(b)}$, $L\beta_2^{II}$ and $L\beta_2^{(c)}$ which lie on the high-energy side of the $L\alpha_1$, $L\beta_1$, $L\beta_2$ dipole line. Each of the remaining satellites is found to have different origin in different elements. The possible contributions of suitable transitions to all these lines have also been discussed.

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Interaction of $4p^5 4d^{N+1}$ and $4p^6 4d^{N-1} 4f$ configurations in the isoelectronic and isonuclear sequences of ions and its influence on the photoexcitation and emission spectra

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The interaction of $4p^5 4d^{N+1}$ and $4p^6 4d^{N-1} 4f$ configurations strongly influences the photoexcitation and emission spectra corresponding to the transitions from or to $4p^6 4d^N$ configuration. The main effect is the quenching of many lines and the formation of a narrow group of intensive ones [1–3]. Such emission is considered as a promising source of EUV radiation for lithography; on the other hand, it causes large radiation losses from highly charged tungsten ions in the tokamak plasma.

The aim of this work was the theoretical investigation of such interaction in the isoelectronic sequences from the ionization degree $q = 5$ till $q = 27–37$ as well as for the isonuclear sequences of Sn^{q+} and W^{q+}. The calculations have been performed in the quasirelativistic approximation [4] or in the relativistic Dirac-Fock-Slater approximation [5]. We have considered the photoexcitation (or excitation by electron impact in the plane wave Born approximation) from the ground level of $4p^6 4d^N$ configuration and the subsequent emission after such excitation. It corresponds to the conditions in the plasma of low density.

The formation of the main group of lines in photoexcitation and emission spectra is determined by the mixing of both excited configurations; the influence of the other configurations manifests only by the general shift of the position of all group. The concentration of lines in a small interval of wavelengths is typical for all isoelectronic sequences at various numbers of 4d electrons. This effect is most expressed at $N = 4$, 6–9, except small ionization degrees, as well as for $N = 5$ in the whole isoelectronic sequence and for $N = 2, 3$ at medium ionization degrees. The reason of the concentration of lines is the tight relations among the expressions for the dipole transition amplitude and matrix elements of Coulomb exchange and configuration interaction.

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Quantitative spectroscopy of atoms in a strong magnetic field based on an atomic vapor cell with $L = \lambda$

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Sub-Doppler nature of optical resonances forming in atomic spectra in alkali metal vapor cells of nanometric thickness L [1] allows one to study peculiarities of magneto-optical processes occurring in magnetic field for the case when L is of the order of (λ is a laser resonant wavelength). A "$L = \lambda$ Zeeman technique" (λ–ZT) method has been developed and implemented for investigation of the individual transitions between the Zeeman sublevels of the hf structure of alkali atoms in a wide range of a B–field [2]. The λ–ZT employs a nanometric cell with $L = \lambda$ thickness and a cw diode laser radiation resonant with $D_{1,2}$ lines of atomic ^{85}Rb, ^{87}Rb (λ = 794, 780 nm). At the laser intensity of a few mW/cm^2, narrow (~10 MHz) velocity selective optical pumping/saturation (VSOP) resonances appear in the transmission spectrum localized exactly at the atomic transitions. The VSOP peaks are split into separate components in a B–field; the amplitudes (which are proportional to transition probabilities) and frequency positions of the components depend on the B–field. The preliminary studies have proved that λ–ZT is a very efficient and convenient tool for determination of uniform and strongly non-uniform B–field strength in the range of 0.1 mT $\div$ 0.24 T. Among the advantages of λ–ZT is the possibility to apply very strong magnetic fields using conventional strong permanent ring magnets (PRM). In [2] the strong B–field was produced by two 30 mm PRMs, with $d = 2$ mm holes to allow radiation to pass, placed on opposite sides of the nanocell oven and separated by a distance varied between 35 and 50 mm. In spite of strong inhomogeneity of the B–field (in our case it can reach ~20 mT/mm), the variation of B inside the atomic vapor column is a few μT, i.e., by several orders less than the applied B value because of small thickness of the nanocell (~800 nm).

Recently we have modified the nanocell oven design (typical operation temperature is ~100^{o}C), which allowed us reducing the distance between the PRMs down to 20 mm, and thus increasing B up to ~0.5 T. We prove that λ–ZT method is still perfectly valid even for this high B value. In particular, a huge ~7.5 GHz frequency shift of the VSOP resonance formed at $F_g = 1 \rightarrow F_e = 2$ transition of ^{87}Rb D_1 line from the $B = 0$ position in the case of circular polarized excitation (σ^+) is observed when $B \sim 0.5$ T, meanwhile for σ^- excitation the VSOP resonances amplitude strongly reduces with B. The comparison of the experimental results with detailed calculations shows a good coincidence. Possible applications of λ–ZT for diagnostics and mapping of large magnetic gradients and for compact widely tunable frequency references will be addressed too.

Acknowledgment

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Reorientation, alignment and coherence effects in Ca-RG collisions

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The main purpose of the present work is to perform a detailed analysis of the alignment, orientation and coherence effects in Ca($4s4p,^3P_j$) colliding with rare gas (RG) atoms. The calculations are based on the standard close-coupling formalism (used for example in [1,2]) with application the relevant pseudopotential curves of Czuchaj, Krośnicki, Stoll [3].

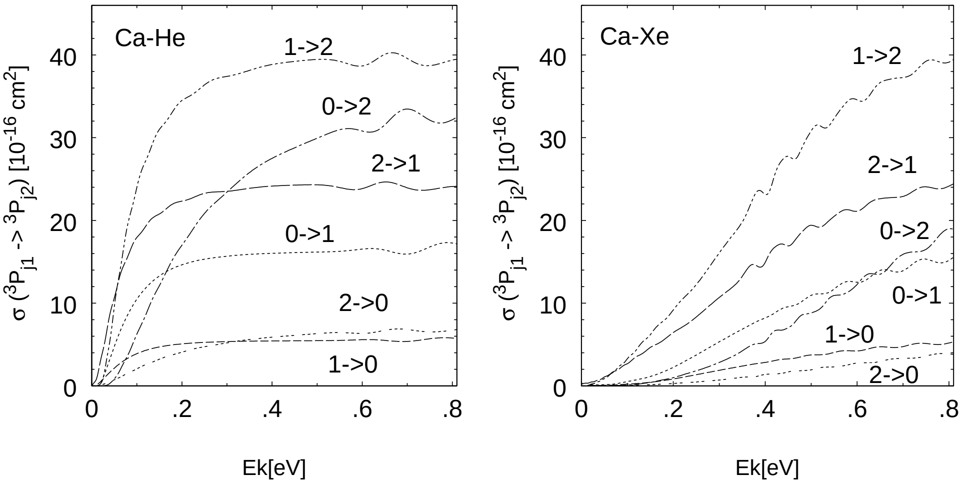

Figure 1: Total integral cross-section for the Ca($4s4p,^3\mathrm{P}_{j_1}->^3\mathrm{P}_{j_2}$) spin changing transitions induced by He and Xe as a function of translational energy.

The reorientation effect and angular distribution of scattered calcium atoms associated with the inelastic transition $j_1m_1 \to j_2m_2$ are discussed *via* multi-structure differential cross-sections

$$\frac{\mathrm{d}\sigma_{m_1\to m_2}(j_1 \to j_2; \mathbf{k}_{j_1}, \mathbf{R}))}{\mathrm{d}\Omega} = \frac{k_{j_2}}{k_{j_1}} \mid f_{j_1m_1\to j_2m_2}(\mathbf{k}_{j_1}, \mathbf{R}) \mid^2, \tag{1}$$

where $f_{j_1m_1\to j_2m_2}$ is the scattering amplitude and the vectors $\mathbf{k}_{j_1}$ and $\mathbf{R}$ define the incident velocity and the scattering directions, respectively. The alignment effects are described by means of the conventional and coherence cross-sections

$$\sigma_{m_1m_1'\to m_2m_2'}(j_1 \to j_2; \mathbf{k}_{j_1}) = \frac{k_{j_2}}{k_{j_1}} \int d\hat{\mathbf{R}} f_{j_1m_1\to j_2m_2}(\mathbf{k}_{j_1}, \mathbf{R}) \cdot f^*_{j_1m_1'\to j_2m_2'}(\mathbf{k}_{j_1}, \mathbf{R}). \tag{2}$$

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Spatial light modulators for cold atom manipulation: guiding into a Laguerre-Gaussian mode

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Spatial Light Modulators (SLM's) are programmable optical elements that can act as dynamical holograms. They provide a flexible method to create by holography any distribution of laser intensity. It only requires a good determination of the phase-hologram to apply to the laser beam.

Such a method allows one to generate a large variety of optical potentials and to foresee applications for cold atom manipulation. In this context, with helical phase-holograms we have first generated almost-pure Laguerre-Gaussian laser modes of k order (LG_0^k). Then we have applied the obtained beam to a cold – 10 micro-Kelvin – sample of rubidium atoms. Using a blue-detuned laser light we have confined the atoms inside the dark region of the LG mode.

We present a quantitative study of the guidance efficiency versus the laser detuning, the order of the Laguerre-Gaussian beam and the beam dimension. We propose a two-dimensional capture model to interpret the results. We discuss also future possible development of this work.

Vibrational quantum defect for the analysis of weakly bound molecules. Application to Rb_2 and Cs_2 0_u^+ data.

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In the context of cold molecule physics, the spectroscopic data and their analysis play an important role. The photoassociation spectroscopy of alkali dimmers, performed by laser excitation of cold atoms, is one of the methods providing high-resolution data about the vibrational levels lying close to the dissociation limit.

Such weakly bound molecules are described by the dipole-dipole interaction, i.e. $-1/R^3$ where R is the inter-nuclear distance and their eigen energies are close to the Le Roy-Bernstein formula. The discrepancies to the formula law are due to the short-range interactions of the potential and to couplings between potentials. We have expressed the discrepancies via a parameter – the vibrational quantum defect (VQD) – defined similar to the atomic quantum defect The VQD deduced from the data and plotted versus the energy allows us to emphasize the couplings. Furthermore, a fit of the graph using a 2-channel model provides the value of the coupling and a characterization of the 2 potentials.

We have applied the method to Rb_2 [1] and Cs_2 [2] data of the 0_u^+ series. The coupling due to spin-orbit interaction has been deduced, the perturbing levels identified and the wavefunction mixing deduced.

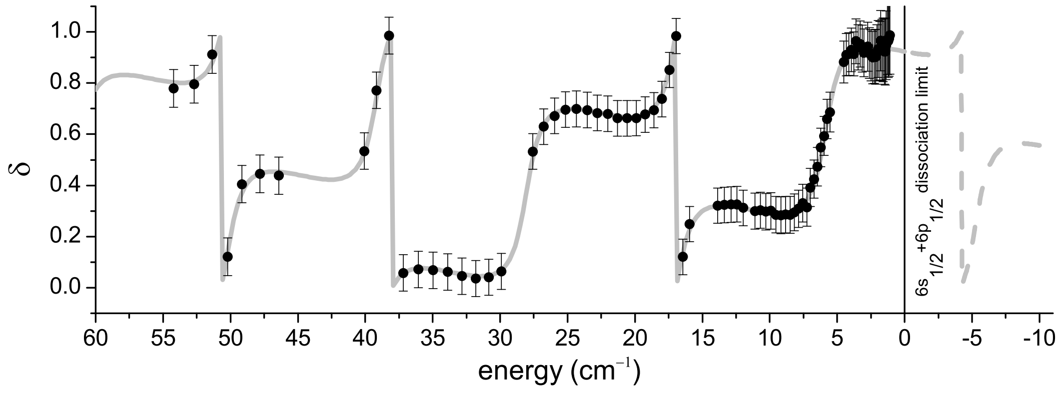

Figure 1: VQD versus energy for the $Cs_2 0_u^+$ series analysed using a 2-channel model.

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Ultracold Rydberg atoms in optical lattices

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In recent years, Rydberg atoms have been the subject of intense study and have become a valuable tool for exploring quantum systems with long-range interactions. Generally, interactions between neutral atoms are weak, but atoms excited to the Rydberg states exhibit electric dipole moments that lead to long-range dipole-dipole interactions. One interesting application of Rydberg atoms is the dipole blockade, which offers exciting possibilities to manipulate quantum bits stored in a single collective excitation in mesoscopic ensembles [1], as well as to realize scalable quantum logic gates [2]. To excite rubidium atoms into Rydberg states and to control the interactions between them we use a two-photon excitation scheme 5s1/2→6p3/2→ns or nd. We achieve the first step using blue laser light at 420 nm (obtained by frequency-doubling a 840 nm MOPA laser), and the second step using a laser at around 1000 nm that is frequency-locked to the blue laser. After the excitation to the Rydberg state we apply a pulse of electric field to ionize the Rydberg atoms. The ions produced are then detected using a channeltron an ion detector. The dipole blockade effect has so far been demonstrated by a number of research groups. The recent results with only two atoms trapped independently show the possibility of creating an entangled state [3, 4]. In order to extend these results to a larger number of atoms we use Bose Einstein condensates in optical lattices.

In this poster I will present our first results on the Rydberg excitation of ultra cold atoms in optical lattices.

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Low energy-spread ion bunches from a laser-cooled gas

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Pulsed and continuous ion beams are used in applications such as focused ion beams. The smallest achievable spot size in focused ion beam technology is limited by the monochromaticity of the ion source. Here we present energy spread measurements on a new concept, the ultra-cold ion source, which is based on near-threshold ionization of laser cooled atoms [1]. The low energy spread is important for focused ion beam technology because it enables milling and ion-beam-induced deposition at sub-nm length scales with many ionic species, both light and heavy.

In the experiment, Rubidium atoms are captured in a magneto optical trap (MOT) inside an accelerator structure where they are ionized by a pulsed laser in a DC electric field. Time-of-flight measurements show two orders of magnitude lower energy spread than in the current industry standard reached with Gallium liquid-metal ion sources. Bunches with energy of only 5 eV can be produced with a root-mean-square energy spread as low as 0.02 eV. We show that the slowly moving, low-energy-spread ion bunches are ideal for studying intricate space charge effects in pulsed beams, i.e., the transition from space charge dominated dynamics to ballistic motion. [2]

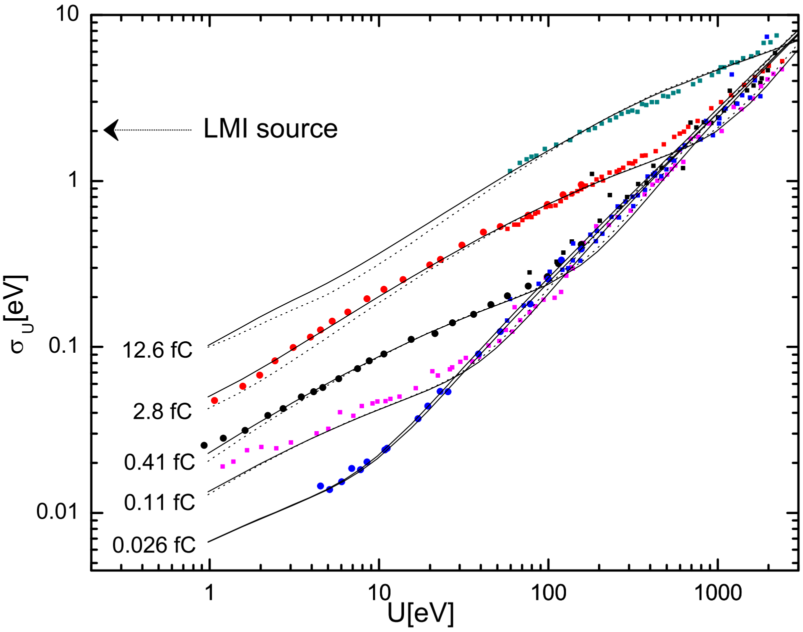

Figure 1: Measured energy spread σU as function of the beam energy U for various bunch charges (scatter plots), together with particle tracking simulations (dotted and solid curves).

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Stark shift of the Cs clock transition frequency: A CPT-pump-probe approach

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The Stark effect describes the shift of atomic energy levels by an external electric field. In Cs atomic clocks, the AC Stark shift, caused by the blackbody radiation, is an important source of systematic frequency shifts. Past measurements of the AC and DC Stark shift of the clock transition are not consistent with each other. We propose a new method to clarify this situation by use of a fully optical Ramsey pump-probe experiment on a thermal Cs atomic beam.

The polarizability, α, that describes the energy shift of a level via

$$\Delta E(n, L_J, F, M_F) = -\frac{1}{2}\alpha\mathcal{E}^2 \tag{1}$$

is traditionally expanded in a perturbation series whose lowest order terms are

$$\alpha = \alpha_0^{(2)}(n, L_J) + \alpha_0^{(3)}(n, L_J, F) + \alpha_2^{(3)}(n, L_J, F)\frac{3M_F^2 - F(F+1)}{I(2I+1)}. \tag{2}$$

Our main objective is to measure the third-order scalar term $\alpha_0^{(3)}$ which dominates the blackbody shift.

The principle of the experimental method is very similar to that of Cs atomic beam clocks except that the microwave cavities are replaced by a coherent population trapping preparation and interrogation. The interference signal obtained in this configuration produces a Ramsey fringe pattern. Any energy shift induced in the atoms of the beam in the 30 cm free evolution zone between the two CPT interaction zones will result in specific fringe shifts. Measuring the shift of the central Ramsey fringe as induced by an applied static electric field will allow us to measure the DC Stark shift of each Zeeman component of the Cs ground hyperfine states. Moreover, we will measure the M_F^2 dependence of the tensor polarizability term, $\alpha_2^{(3)}$, which is roughly two orders of magnitude smaller than $\alpha_0^{(3)}$ [1]. We will show measurements of the Ramsey signal already obtained and discuss the technical challenge in the calibration of the $\mathcal{E}$ field as well as expected accuracy.

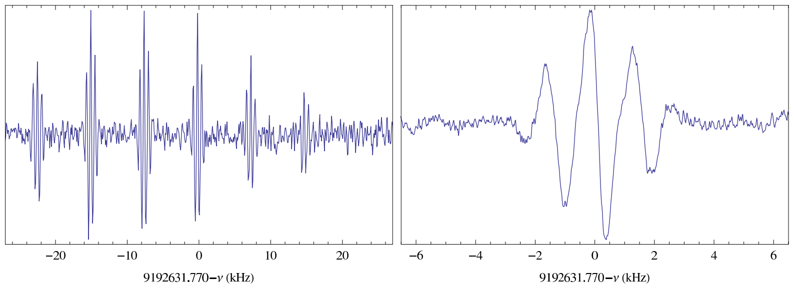

Figure 1: Left: the seven possible Ramsey interferences induced by CPT on the ground states of Cs using σ^- polarization. Right: a dispersive shape Ramsey fringe pattern for the Cs clock (M_3=0 → M_4= 0) transition.

Acknowledgment

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Towards a *g*-factor determination of the electron bound in highly charged, medium-heavy ions

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Bound-state quantum electrodynamic (BS-QED) calculations can be tested by high-precision measurements of the magnetic moment of the electron bound in hydrogen-like and lithium-like ions. In the past, g-factor measurements were done on hydrogen-like carbon (Z=6) and oxygen (Z=8) [1]. A relative experimental uncertainty as low as $5\cdot 10^{-10}$ has been achieved.

Since the influence of the BS-QED increases with the nuclear charge, experiments with medium-heavy ions are of particular interest. In the current experiment [2] we plan to measure the g-factor of lithium-like and hydrogen-like silicon (Z=14) and calcium (Z=20) ions, respectively. The aim is to reach a relative uncertainty $\delta g/g$ in the order of 10^{-9}. The g-factor measurement on a single ion will be performed in a double Penning-trap setup via the precise measurement of its cyclotron and spin precession frequency. The first one is obtained by measuring all three eigenfrequencies of the ion in the so-called precision trap and using the invariance theorem [3]. The axial frequency can be measured directly using a tank circuit. In contrast the magnetron and the cyclotron frequency are measured by sideband coupling [4]. The spin precession frequency can be determined by measuring the spin flip probability [4] for different excitation frequencies. Therefore, the trapped ion is irradiated with microwaves at a frequency close to the Larmor frequency and the spin state before and after irradiation is observed. To this end, in the analysis trap an inhomogeneous magnetic field is used to generate a small difference in the axial frequency for the two spin directions. To reach the precision aimed for, the experiment is operated in a closed system at 4.2 K to reduce the electronic noise of the newly developed low-noise detection electronics and to reach storage times of several weeks of the highly charged ions created in-trap by a mini-electron beam ion source [5]. Commissioning experiments on single ions will be presented.

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Millimetre wave spectroscopy of high Rydberg states of xenon: hyperfine structure and Stark effect

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In the range 0–45 cm^{-1} below the ionisation limit, the separation between adjacent electronic states (Rydberg states with principal quantum number $n > 50$) of atoms and molecules is smaller than 2 cm^{-1}. In order to resolve the fine or hyperfine structure of these states, it is necessary to combine high-resolution vacuum ultraviolet (VUV) laser radiation, which is required to access the Rydberg states from the ground state, with millimetre wave radiation [1]. Such double-resonance experiments have been used to study the hyperfine structure of high Rydberg states of ^{83}Kr [2], H_2 [3], and D_2 [4].

Millimetre wave transitions (240–350 GHz) between $n\ell$ ($52 \leq n \leq 64, \ell \leq 3$) Rydberg states of different xenon isotopes were detected by pulsed field ionisation followed by mass-selective detection of the cations. Because of the high polarisability of high-n Rydberg states ($\propto n^7$, $\sim 10^4$ $\text{MHz}\,\text{cm}^2\,\text{V}^{-2}$ for $n \approx 50$), it is necessary to reduce the electric stray fields to values of the order of 1 mV/cm (or less) to minimise the (quadratic) Stark shift of the millimetre wave transitions. Several p and d Rydberg states of Xe are nearly degenerate and efficiently mixed by small stray fields, making it possible to observe transitions forbidden by the $\Delta\ell = \pm 1$ selection rule and transitions exhibiting the linear Stark effect characteristic of degenerate high-ℓ Rydberg states.

Multichannel quantum defect theory (MQDT) was used to analyse the millimetre wave data and to determine the hyperfine structure of the $^2P_{3/2}$ ground electronic state of $^{129}\text{Xe}^+$ and $^{131}\text{Xe}^+$.

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High-resolution spectroscopy of np Rydberg states of He$_2$: ionisation energy of the metastable He$_2^*$ and rotational autoionisation dynamics

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A supersonic beam of metastable He$_2^*$ a $^3\Sigma_u^+$ molecules was generated using a pulsed discharge at the exit of a pulsed valve prior to the gas expansion into vacuum [1]. Transitions to high np Rydberg states were recorded using photoionisation and Rydberg-state-resolved threshold ionisation spectroscopy [2]. Overview scans at moderate resolution (0.3 cm^{-1}) have been obtained with ionisation fields from 1.3 to 133 V/cm, lowering the ionisation thresholds by 5.5 and 55 cm^{-1}, respectively. Using a solid-state UV laser system [3] with a 20 MHz bandwidth, high-resolution spectra of Rydberg series with n up to 150 and with resolved fine structure of the initial He$_2^*$ a $^3\Sigma_u^+$ (N'') state were recorded. The assignment of the observed Rydberg states is based on multichannel quantum defect theory (MQDT) calculations from a recent study of pulsed-field-ionisation zero-kinetic-energy (PFI-ZEKE) photoelectron and photoionisation spectra of He$_2$ [1]. The extrapolation of the observed Rydberg series to their limits enabled the determination of the ionisation energy of the a $^3\Sigma_u^+$ state and the rotational structure of the He$_2^+$ ion with a precision of better than 20 MHz.

Many of the observed Rydberg states associated with rotationally excited levels of the ion core (rotational quantum number N^+) are embedded in the ionisation continua associated with the N^+-2 and N^+-4 ionisation channels. The rotational autoionisation dynamics is complex and is strongly influenced by the application of weak electric fields. Several series are immune to ionisation and the corresponding states are metastable. An interpretation of the effects of the electric fields on the autoionisation dynamics is proposed.

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Adiabatically and nonadiabatically corrected potential for H_2

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Due to its simplicity, H_2 is an ideal specimen for testing *ab initio* and other theoretical methods. Thus, a good-quality Born-Oppenheimer potential (BOP) is available for the ground state of H_2, its adiabatic, relativistic and radiative corrections also being accurately determined [1]. Unfortunately, an adequate theory for nonadiabatic corrections is still lacking, and one can only rely on various semi-empirical approaches to include these corrections and make a direct comparison with the experimental data.

In this report, a new method will be demonstrated, which enables to ascertain all corrections to the initial BOP simultaneously. To this end, an inverse perturbational approach was used, based on repeated very accurate solution of the Schrödinger equation. The problem was solved step-by-step, building a parametrized auxiliary potential and trying to fit its discrete energy spectrum with the experimental data. Exact match with the most acknowledged rotationless spectrum for H_2 [2] was achieved with only 4 cycles of computations. By constructing such a pseudo-potential, one artificially removes the dependence of nonadiabatic corrections on level energies (E_{vJ}) replacing them with an effective mean value (E). However, the mentioned state-dependence is a higher-order effect, which can be taken into account by slightly shifting the centrifugal energy (if $J \neq 0$). Simple analytic formulas for the shift have been derived, which can be used for a wide range of vibrational and rotational quantum numbers. Good agreement with the available astrophysical data was achieved.

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Rydberg atoms as a source of cold electrons

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We recently demonstrated a new type of pulsed electron source [1] based on ultracold plasmas (UCPs), which are formed by photo-ionization of laser cooled atoms just above the ionization threshold. Here we employ similar concepts by extracting electrons from a gas of frozen nS- and nD-Rydberg atoms.

The experimental setup consists of a vapor-cell magneto-optical trap (MOT) for rubidium built inside a dedicated accelerator structure [2], followed by a detector consisting of a micro-channel plate with phosphor screen. A narrow cylinder of the atoms is irradiated by a pulsed dye laser tuned to high Rydberg states, which are then field-ionized using a fast electric field pulse. The free electrons are accelerated towards the detector, and images of the electron bunch are then used to derive the source temperature using a model of the beam transport system.

For S-states with n = 26..35, an electron temperature of 9±4 K is obtained, while for D-states T=36±5 K [3]. We conclude that field ionization of Rydberg atoms is an alternative way to reach source temperatures in the 10 K regime.

The Rydberg states used so far correspond to beam energies up to 1.4 keV. To reach higher energies, states with lower n can be used. The setup is currently being modified in order to control the beam also at these conditions. The aim is to determine the source temperature with 14 keV electrons using Rydberg states down to n = 15.

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Gravity measurements with cold atom interferometry

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We will present some experiments on gravity using atom interferometry. We use a Raman ligth-pulse interferometry scheme on a rubidium atomic fountain to determine the gravitational constant G. We also working to test the Newtonian gravitational law at micrometric distances using an ultracold strontium sample trapped in an optical lattice. Other experiments in progress, planned or being considered using ultracold atom devices for applications in gravity monitoring and in space will be also discribed.

Very accurate quantum calculations of vibrational transition energies in diatomic systems

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Very accurate variational calculations of the pure vibrational transitions of some two- and three-electron diatomic molecules have been performed within the framework that does not assume the Born-Oppenheimer (BO) approximation. The non-BO wave functions expanded in terms of one-center explicitly correlated Gaussian functions multiplied by even powers of the internuclear distance are used to calculate the leading relativistic corrections. Up to 10000 Gaussians are used for each state. We show that such calculations reproduce the experimental vibrational transitions with the accuracy better than 0.1 cm^{-1}. For three-electron systems this is the first time such an accuracy is reached in calculations based on first principles.

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Polarization analysis of nonlinear magneto-optical resonances in 87Rb fluorescence

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In the present report we discuss new results obtained using differential scheme of registration of Coherent Population Trapping [1,2] (CPT) in Hanle configuration in two orthogonal polarizations [3,4]. This is a nonlinear modification of ground state Hanle effect [3] observed in the spontaneous emission from the upper level. The ground state coherency is transmitted from the laser field and as a result higher rank (k) polarization moments (PM) are created, e.g. octupoles ($k = 3$) and hexadecapoles ($k = 4$). The moments with rank higher than 2 are not directly observable in the spontaneous emission and/or in transmission. Nevertheless, the laser field conjugates the different components in the equation evolution and makes the higher rank moments observable. The experimental results are compared with our theoretical predictions. The theoretical description of the atomic polarization moment evolution is based on the density matrix formalism specified for transition transition ($F_e = 1 \rightarrow F_g = 2$) of the Rb D1 line, and the experimental geometry. Comparing the obtained results it is possible to follow easily the influence of the different parameters on the observable components and the mutual conversion between high-rang polarisation moments and quadruple moments.

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Interferometric study of collision-time asymmetry and speed-dependent effects on the 748.8 nm selfbroadened neon line

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Using an interferometric method, detailed analysis of profiles of the selfbroadened 748.8 nm Ne line emitted from the glow discharge in neon was performed which revealed departures from ordinary Voigt profile. These departures are shown to be consistent with fits of speed-dependent asymmetric Voigt profile to experimental profiles. It was shown that the neglect of the correlation between Doppler and collsional broadening may cause errors in the values in determined line shape parameters. Coefficients of the pressure broadening, shift and collision-time asymmetry are determined and compared with those calculated in the adiabatic approximation for the van der Waals and Lennard-Jones potentials.

Thermodynamic parameters Mg^{2+}, Ni^{2+} and Cd^{2+} ion binding with polynucleotides being in different conformations

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Interest in studies on the dependence of polynucleotide conformational states on metal (Mt) ion concentrations and temperature is generated with ecological problems and with a possibility of polynucleotide metal complexes use in therapy (as therapeutic agents). Binding constants (K) and stoichiometry (n) of the complexes are main thermodynamic parameters conditioning the concentration range of stabilities of Mt ion-nucleic acids complexes.

By phase diagrams of polyU·polyA·polyU (A2U) complexes with Mg^{2+} [1], Ni^{2+} [2] and Cd^{2+} [3] ions and by the clip theory [1], K and n values were calculated for three-, double- and single-stranded polynucleotides consisting of adenine and uracile, with these ions. The data obtained permitted to ascertain the physical nature of different effects of the above ions on temperature of 2(polyA·polyU) (AU)→A2U+polyA transition (2→3 transition) $(Tm)_{23}$, observed in phase diagrams of these ion complexes with AU. It is shown that widening of the AU existence region in the presence of large Ni^{2+} concentrations is caused with the fact that the difference between association constants of these ions with AU and polyA is larger than that one between association constants of these ions with A2U and AU. As a result, opposite relations of differences in binding constants of Mg^{2+} ions and these polynucleotides lead to $(Tm)_{23}$ lowering. As Mg^{2+} ions, Cd^{2+} lower $(Tm)_{23}$. But, unlike the case with magnesium, such a decrease is conditioned with the strong interaction of Cd^{2+} ions with single-stranded polyA bases.

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M1-E2 interference in the Zeeman spectra of 6s^{2}6p^n ($n = 1, 2, 3$) ground configurations of Pb II, Pb I and Bi I

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The measurement of the ratio $D{=}A^{E2}/(A^{E2} + A^{M1})$ of the electric-quadrupole (E2) and magnetic-dipol (M1) transition probabilities in mixed forbidden lines can provide stringent test of theoretical wave-function calculations. In addition accurate knowledge of this quantity is essential for existing and future measurements of parity nonconserving optical rotation.

According to [1], the spontaneous transition probability for a single photon emission in the presence of the magnetic field can be expressed as:

$$a_{ab} = (1 - D)a_{ab}^{M1} + Da_{ab}^{E2} \pm 2\sqrt{D(1 - D)}a_{ab}^{M1-E2}, \qquad (1)$$

where D is percentage admixture of E2 radiation, a_{ab}^{M1} and a_{ab}^{E2} are pure magnetic-dipol and electric-quadrupole components, respectively and the cross term a_{ab}^{M1+E2} describes the interference effect. The sign of the interference term in (1) can be predicted if the wave functions of the electronic states involved in the transition are known.

Our experimental results are presented in Table 1.

Table 1: Values of the electric quadrupole admixtures and phase signs in mixed type transitions in lead and bismuth.

Configuration	Transition	E2 admixture	Phase sign ϕ
$6s^26p$ Pb II	(^{2}P$_{3/2}$ - ^{2}P$_{1/2}$) 710.2nm	4.25 ± 0.18 % [2]	negative
$6s^26p^2$ Pb I	(^{1}D$_2$ - ^{3}P$_1$) 733.2nm	4.12 ± 0.07 % [2]	positive
$6s^26p^3$ Bi I	(^{2}D$_{3/2}$ - ^{4}S$_{3/2}$) 875.5nm	0.70 ± 0.11 % [3]	negative
	(^{2}D$_{5/2}$ - ^{4}S$_{3/2}$) 647.6nm	17.5 ± 0.4 % [3]	positive
	(^{2}P$_{1/2}$ - ^{4}S$_{3/2}$) 461.5nm	7.84 ± 0.14 % [3]	positive
	(^{2}P$_{3/2}$ - ^{2}D$_{3/2}$) 459.7nm	3.49 ± 0.35 % [4]	positive
	(^{2}P$_{3/2}$ - ^{2}D$_{5/2}$) 564.0nm	37.1 ± 1.8 % [4]	negative

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Perturbation in the $A^1\Pi$ $(v = 1, J = 5)$ state of AlH

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The high-resolution emission spectrum of the $A^1\Pi - X^1\Sigma^+$ transition of AlH was observed in the 18000 - 25000 cm^{-1} spectral region using a conventional spectroscopic technique. The AlH molecules were excited in an Al hollow-cathode lamp filled with a mixture of Ne carried gas and a trace amount of NH_3. The emission from the discharge was observed with plane grating spectrograph and recorded by a photomultiplier tube. In total 163 transitions wavenumbers belonging to six bands $(0-0, 1$ and $1-0, 1, 2, 3)$ were precisely measured and rotationally analyzed. The four off-diagonal $(0-1, 1-0, 1-2, 1-3)$ bands have been recorded for the first time since 1954 [1].

So far not pointed out [2] a very slight rotational perturbation has been discovered in the $v = 1$ $(J = 5)$ vibrational level of the excited $A^1\Pi$ state. This perturbation affects all branches of the $1 - v''$ progression bands: $R(4)$, $Q(5)$, and $P(6)$ respectively. It confirms that both e and f components of the $A^1\Pi$ state have been perturbed (see Figure 1) and indicates that the perturbing state is not $X^1\Sigma^+$. Shift of the f components: $\Delta E_{F1f} = 0.0228$ cm^{-1} is about four times bigger than e one: $\Delta E_{F1e} = -0.0051$ cm^{-1}. Also, the fact that the perturbation appeared to be sharp, suggests that the perturbing state has rotational constants quite different from those of the perturbed $A^1\Pi$ state. On basis of above mentioned conclusions, we suggest that the $a^3\Pi$ state ($B_e = 6.704$ cm^{-1}), which lies about 9000 cm^{-1} lower is responsible for perturbation in the $A^1\Pi(v = 1)$ state. The exact assignment of the perturbing vibrational level was impossible, due to the lack of information about vibrational constants of the $a^3\Pi$ state (only uncertain $\omega_e = 1688$ cm^{-1} value is known [3]). In order to get more precise estimation of the perturbation value, we calculated true (perturbed) values of the rotational terms for the $A^1\Pi(v = 1)$ state, by means of the method introduced by Curl and Dane [4] and Watson [5]. The obtained terms values have been compared with those derived from molecular constants for upper $(v' = 1)$ and lower $(v'' = 0 - 3)$ vibrational levels obtained by using traditional hamiltonian method. The terms differences are plotted in Figure 1.

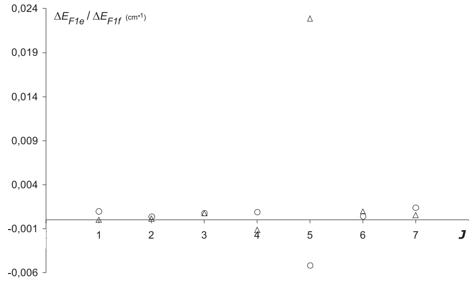

Figure 1: Calculated terms energy shifts of $A^1\Pi, v = 1$ (△ for f component, ○ for e component). The perturbation at $J = 5$ is clearly shown.

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Reanalysis of the $A^1\Pi$–$X^1\Sigma^+$ bands system of the $^{13}CD^+$ ion radical

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In the $^{13}CD^+$ isotopic ion radical spectra of the $A^1\Pi$–$X^1\Sigma^+$ bands system have been obtained. Emission spectra of the bands were observed in the 22800–25100 cm^{-1} spectral region using a conventional spectroscopic technique. The $^{13}CD^+$ molecules were produced by an electric discharge in an aluminum water-cooled hollow-cathode lamp, operated at 400 V and $180 \div 200$ mA DC. Nonflowing mixture of 3 Torr of He carried gas and 1 Torr of $^{13}C_2D_2$ was found as optimal for production of strong $A^1\Pi$–$X^1\Sigma^+$ emission. The spectra were observed in the 6th order with the 2-m Ebert plane grating PGS-2 spectrograph equipped with 651-grooves/mm grating with a total number of grooves of 45 600, blazed at 1.0 μm. The reciprocal dispersion was in the range 0.066–0.075 nm/mm and theoretical resolving power was about 270 000. The spectrum of $^{13}CD^+$ was recorded by translating on a linear stage an exit slit and photomultiplier tube (HAMAMATSU R943-02) along the focal curve of the spectrograph. The entrance and exit slit widths were 0.035 mm. The line intensities were measured by a single photon counting (HAMAMATSU C3866 photon counting unit and M8784 photon counting board) with a counter gate time of 50-500 ms (no dead time between the gates) depending on spectrum intensity. Positions of the exit slit were measured using He-Ne laser interferometer synchronized with the photon counting board (during the counter gate time the position is measured 64 times and a mean value with the counts number are transmitted to PC as a measurement point). The total number of the measurement points was about 73 000 for one scan with the sample step of 3 μm (sample step it is the translation of the exit slit during the counter gate time). Simultaneously recorded some thorium atomic lines [1] obtained from several overlapped orders of the spectrum from a water-cooled hollow-cathode tube were used for absolute wavenumber calibration. For the wavenumber calculations seventh-order interpolation polynomials were used. The typical standard deviation of the least-squares fit for the 70-80 calibration lines was about 0.0012–0.0016 cm^{-1}. The calibration procedure was tested (with two Th lamps simultaneously – one as an examination light source and the second one to provide the reference spectrum) to be ± 0.0015 cm^{-1}. Comparison of the wavenumbers of the 0–0 band obtained in this study with those of [2] shows differences (about 0.015–0.020 cm^{-1}) of both wavenumber values. Finally we improved molecular constants for both electronic states: $A^1\Pi$ as well as $X^1\Sigma^+$ by means of the direct fit. Till nowadays only one experimental publication discussing $^{13}CD^+$ ion molecule appeared [2].

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Opto-electrical cooling of polar molecules

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Opto-electrical cooling [1] offers exciting prospects for obtaining ensembles of polar molecules at sub-mK temperatures for a broad range of molecules. As exemplified in Fig. 1, the varying stark shift in DC electric fields of different internal molecular states can be used to implement a Sisyphus-type laser-cooling scheme. Due to the strong electric field - dipole interaction, up to 1 K of kinetic energy can be removed from the molecules per spontaneously emitted photon. Loading the molecules into an electric trap with the required step-shaped offset electric field for the cooling process would allow for the approximately 10 s required to cool molecules from 1 K to below 1 mK. Here, we present details of the scheme such as choice of internal molecular states, selection of suitable molecules and electric trap design. This includes results from first steps taken towards experimental realization of the scheme.

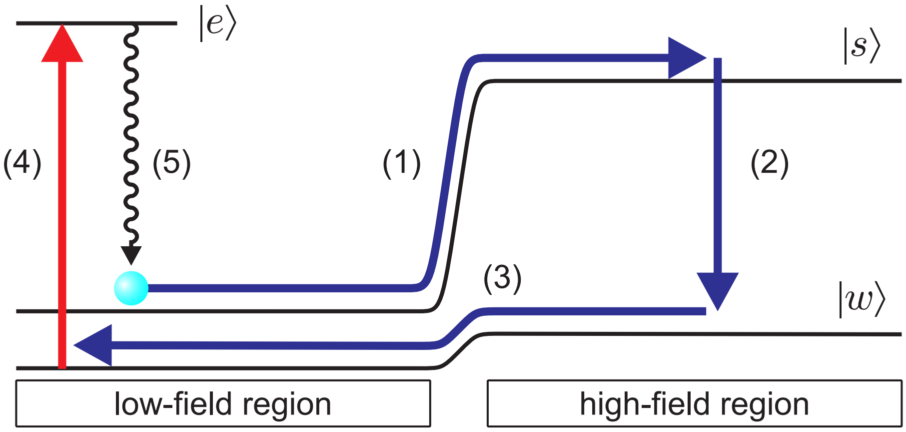

Figure 1: Schematic depiction of opto-electrical cooling. Two internal molecular states $|w\rangle$ and $|s\rangle$ experience a step- potential in an electric trap via two regions with homogeneous but different offset electric fields. By coupling the two states directly in the high-field region and indirectly in the low-field region via spontaneous decay from an excited vibrational state, a Sisyphus-type cooling cycle is achieved.

To provide an initial sample of molecules for opto-electrical cooling, the high-flux beam available from an effusive [2] or cryogenic [3] source is ideally suited. We present some of the latest results from these experiments.

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The FERRUM project: combining laboratory and astrophysical studies reveals rates of forbidden transitions in [Fe II]

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Iron is a highly abundant element in many astrophysical objects and the Fe II spectrum has therefore been studied in much detail through the years. More than 1000 energy levels have been identified [1]. The complex spectrum of Fe II makes the observed spectrum line rich, and the lines are observed in both emission and absorption.

Forbidden lines are very rarely observed in spectra from laboratory sources, due to the levels' sensitivity to collisions. The low radiative rates make the collisional deexcitation the dominating process. However, in the spectra of astrophysical low density plasmas, such as nebulae and HII regions, the forbidden lines are often the strongest lines in the spectrum. The sensitivity to collisions make forbidden lines invaluable probes of physical conditions, e.g. density and temperature, which in many cases can be determined by simple line ratio measurements.

The experimental studies of forbidden transitions in Fe II started in 2001 when the lifetimes of the levels $\mathrm{a}\,^6\mathrm{S}_{5/2}$ and $\mathrm{b}\,^4\mathrm{D}_{7/2}$ were measured by laser probing a stored ion beam [2,3]. The experimental study was continued in 2003 when the same experimental technique was used to measure the lifetimes of two additional metastable levels, $\mathrm{a}\,^4\mathrm{G}_{9/2}$ and $\mathrm{b}\,^2\mathrm{H}_{11/2}$ [4]. The lifetimes of $\mathrm{a}\,^6\mathrm{S}_{5/2}$, $\mathrm{b}\,^4\mathrm{D}_{7/2}$ and $\mathrm{a}\,^4\mathrm{G}_{9/2}$ were also combined with branching fractions (BFs) for forbidden lines derived from astrophysical spectra in order to deduce experimental A-values for forbidden transitions.

In the present work we have extended our experimental work and measured two new levels. The resulting lifetimes of the $3d^6(^3\mathrm{G})4s\ \mathrm{a}\,^4\mathrm{G}_{11/2}$ and the $3d^6(^3\mathrm{D})4s\ \mathrm{b}\,^4\mathrm{D}_{1/2}$ levels are $\tau = 0.75 \pm 0.10\,\mathrm{s}$ and $\tau = 0.54 \pm 0.03\,\mathrm{s}$ respectively. A-values for two forbidden decay channels at 4243.97 and 4346.85 Å from the $3d^6(^3\mathrm{G})4s\ \mathrm{a}\,^4\mathrm{G}_{11/2}$ upper level are 1.05 ± 0.15 and $0.25 \pm 0.05\,\mathrm{s}^{-1}$, respectively. Both the lifetimes and the transition probabilities are compared to previously published calculated values [5,6].

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Relativistic multireference configuration interaction calculations of lifetime of $2s^22p$ $^2P_{3/2}$ level along boron isoelectronic sequence

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Lifetime of $2s^22p$ $^2P_{3/2}$ level along with fine structure separations for the lowest ^2P doublet of Boron-like ions, from Z=14 to Z=30 have been calculated using multireference relativistic configuration interaction(MR RCI) method based on the no-pair Dirac-Coulomb-Breit(DCB) Hamiltonian. Analytic basis sets of Gaussian-type functions are employed to expand the upper and lower components of the Dirac four-spinors in the matrix Dirac-Fock self-consistent field(DF SCF) and relativistic MR CI procedures. Error with respect to variation of basis set parameters was estimated. QED corrections were estimated by evaluation of electron self-energy and vacuum polarisation.

To explain discrepancies between theory and experiment of $2s^22p$ $^2P_{3/2}$ level lifetime for Ar^{+13} ion, the M1 transition amplitude was calculated using electron g-factor for free and bond electron.

Table 1: E2 and M1 transition rates and lifetime of the lowest $^2P_{3/2}$ state for Ar^{+13} ion

Ion	E2(s^{-1})	M1(s^{-1})	τ(ms)	Other	Experimental
Ar^{13+}	1.862e-03	1.044e+02	9.5769	9.582 [2]	9.573(4)(+12/-5)[1]
			9.533[a]	9.5376 [2][a]	
			9.569[b]		

a with anomalous magnetic moment correction for free electron

b with anomalous magnetic moment correction for bond electron

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