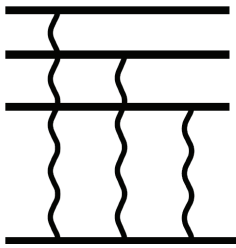
europhysics
conference
abstracts



37th EGAS Conference
Dublin 3 - 6 August 2005

EUROPHYSICS CONFERENCE

37th Conference of the
European Group for Atomic Systems
Dublin City University
Dublin (Ireland), August 3rd – 6th, 2005

BOOK OF ABSTRACTS

Editors: John T. Costello (DCU)
John Dardis (DCU)
Peter van der Burgt (NUIM)

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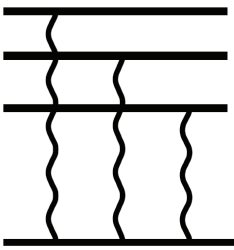

37th EGAS Conference
Dublin 3 - 6 August 2005

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

European
Group for
Atomic
Systems

ABSTRACTS

EDITORS
John T. Costello (DCU), John Dardis (DCU), Peter van der Burgt (NUIM),

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- Posters from the following categories:

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    - Clusters, Quantum Dots, …
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18.00 – 19.00	A. Barany (Einstein Yr Talk)			20.00 -	Conference Banquet *(Dublin Castle)*		

**EGAS General Assembly will be in T101, 12.30 to 13.00 hrs (Lunch 13.00 – 14.30)*

INVITED TALKS

Environmental Monitoring Using Optical Techniques

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Optical spectroscopy, and in particular laser spectroscopy, provides many possibilities for real-world applications. Powerful techniques have been developed for chemical analysis, combustion diagnostics, environmental monitoring and biomedical diagnostics (see, e.g. [1]).

We will here focus on environmental monitoring, and numerous examples from the research performed at the Lund Institute of Technology will be given. Atmospheric monitoring includes the laser radar, the diode laser spectroscopy and the gas correlation imaging methods, while laser-induced fluorescence (LIF) is applied to hydrospheric pollution measurements, vegetation status assessment and building facade monitoring. Non-intrusive measurements in real time are provided, as is characteristic for remote sensing techniques.

The Lund group has been pursuing atmospheric laser radar monitoring for a long time, including industrial and geophysical measurement [2]. Extensive work on the monitoring of mining areas, geothermal fields, and active volcanoes has been performed [3]. Present lidar group activities focus on hydrocarbon monitoring in IR region using optical parametric oscillator (OPO) techniques and difference frequency generation. A passive, imaging technique based on gas correlation imaging has also been developed for hydrocarbon monitoring [4]. The Lund group has also performed extensive fluorescence lidar work regarding water quality, vegetation status, and historical building facades [5].

Diode lasers provide convenient means for certain types of spectroscopic diagnostics. Normally, only line-of-sight path-integrated data are obtained. We recently demonstrated single-mode diode laser spectroscopy in the violet spectral range, frequency-modulation spectroscopy with blue diodes, and also their usefulness in sum-frequency generation to the UV region, accessing the mercury line at 254 nm and sulphur dioxide absorption bands around 300 nm. An emerging new field of diode laser spectroscopy relates to the study of free gas dispersed as bubbles or pore enclosures in scattering materials such as wood, fruits, ceramics foams and insulating materials [6]. Thus, oxygen gas was extensively studied in many materials, with demonstrations of full quantification as well as the potential for pressure measurements and diffusion studies. Recently, first medical applications of this technique were demonstrated. **References**

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Title to be announced

M. Vrakking

Extreme Nonlinear Optics for Coherent X-Ray Generation: Applied Attosecond Science

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By taking concepts of nonlinear optics and ultrashort pulse generation to the extreme, it is now possible to extend coherent light generation to much shorter wavelengths than before by using a process called high harmonic generation (HHG). This process upshifts femtosecond laser light from the near infrared to the extreme-ultraviolet (EUV) and soft x-ray regions of the spectrum. The EUV is a difficult region of the spectrum for nonlinear optics, since traditional frequency-conversion techniques have generally relied on crystalline solids as the nonlinear medium, and solids are not transparent in the EUV. Nevertheless, there is strong motivation to develop EUV light sources - short-wavelength light is useful for many scientific applications, in spectroscopy as a structural and chemical probe, and for possible technological applications such as lithography for chip fabrication. These needs motivated the development of synchrotron light sources, which are the predominant EUV light source used at present. Moreover, laser-based EUV sources can provide unique characteristics, such as ultrashort, femtosecond-to-attosecond, pulse durations.

In this talk, we will explain how high harmonic generation represents an "extreme" limit for nonlinear optics where photons with energy up to nearly 1 keV can be generated through coherent upconversion of visible laser light (i.e. $1-2$ eV photons). This process is radically different from traditional nonlinear optics, where the characteristic time scale of the x-ray emission is much smaller than the optical period of the laser field, i.e. it falls into the attosecond time domain (1 as $= 10^{-18}$ sec). Therefore the inherent attosecond quantum dynamics of the atom-field interaction determines the wavelength range, efficiency, coherence properties, as well as the emitted pulse duration of the generated light. By combining optical pulse shaping technologies with new "EUV photonic structures," these dynamics can be controlled and optimized. This area is therefore an example of the relevance of "attosecond science" for a real-world application: the generation of laser-like, fully spatially and temporally coherent light at short wavelengths that can be used as a stable-top x-ray laser source.

Applications of high harmonic generation as a light source for studying high frequency photo-acoustic responses in materials, for studying ultrafast charge transfer processes on surfaces, and for studying molecular dynamics will also be discussed.

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Atomic and molecular clusters: Matter between molecules and the condensed phase

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The field of atomic and molecular clusters has evolved in a very rapid manner and covers now all types of interactions ranging from van der Waals over hydrogen bonds to covalent, ionic and metal interactions. With the experimental techniques available at present, clusters can be generated for nearly every substance and any size wanted. Because of their finite size and their large surface to volume ratio their properties usually differ from those of the condensed matter, although they exhibit many of their features like collective excitations and phase transitions. Aside from providing interesting research in their own, they open up new approaches to the dynamics and thus a better understanding of the microscopic behaviour of the bulk matter.

In the present contribution we will present examples of typical excitations which range from the intermolecular motions similar to the bulk phonons over the intramolecular vibrations which characterize very sensitively hydrogen bonded networks to the photoluminescence of semiconductor clusters which show pronounced size effects. Examples are reported for argon, water, and silicon clusters, respectively. Then we will present a short account on isomeric and phase transitions and how they are observed in small water and methanol clusters and in larger neon clusters as well. This leads us to the superfluid quantum liquid behaviour of helium clusters which proved to be a very effective ultracold nanolaboratory for the aggregation of other species.

Electron charge and spin in semiconductor quantum dots

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Quantum dots are man-made sub-micron structures in a solid, in which the number of free electrons can be varied from several thousands down to zero. An extra electron can only be added to the dot, if enough energy is provided to overcome the Coulomb repulsion between the electrons. Next to this – purely classical – effect, the confinement in all three directions leads to quantum effects that strongly influence electronic transport at low temperature. In particular, it leads to the formation of a discrete (0D) energy spectrum, resembling that of an atom. This and other similarities have therefore led to the name 'artificial atoms' for quantum dots.

In this talk I discuss electron transport measurements in semiconductor quantum dots. Analogies and differences between quantum dots and real atoms are pointed out. Key phenomena like Coulomb oscillations, Fock-Darwin levels and the Kondo effect are discussed and illustrated by experimental results. By coupling two quantum dots in series, a system is obtained with fundamentally different behavior and possibilities in comparison to a single dot [2]. The interaction of these systems with photon and phonon fields is of particular interest. Finally, I address the relevance of quantum dots for realizing solid state quantum bits (*qubits*).

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Einstein's Nobel Prize

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On January 10, 1923, Albert Einstein writes a letter to Svante Arrhenius. In the letter Einstein expresses his delight in becoming a Nobel Laureate, since now he will never more have to answer the question of why he has not received the Nobel Prize. What he did not mention in the letter is a question that has been one of the most frequent questions asked about Einstein and the Nobel Prize, namely why he did not receive the prize for the theory of relativity. The answer to this second question resides in a fascinating story which involves the three Swedish scientists Svante Arrhenius, Nobel Laureate in Chemistry 1903, Allvar Gullstrand, Nobel Laureate in Physiology or Medicine 1911 and Carl Wilhelm Oseen, Professor of Theoretical Physics at Uppsala University. The story also weaves a thread between the three consecutive Nobel Laureates in Physics, Albert Einstein 1921, Niels Bohr 1922 and Robert Millikan 1923.

Experiments with Bose-Einstein condensates

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The Bose-Einstein condensates represent a peculiar state of matter, with a macroscopic large number of atoms occupying the same quantum mechanical state. Therefore a Bose-Einstein condensate represents a macroscopic system (composed by a number between a thousand and ten million) described by quantum mechanics. An additional characteristic of a condensate is the presence of an atomic interaction whose amplitude depends on the atomic condensate. That atomic interaction modifies the position of the atomic levels and plays an important role when high precision experiments are performed on an atomic condensate. The investigations on Bose-Einstein condensates are in three different directions: i) examine the quantum mechanical properties of a macroscopic sample; ii) investigate new phenomena produced by the nonlinear interaction of the condensate atoms; iii) perform spectroscopic investigations on the condensates. Experimental investigations performed at Pisa will be presented to illustrate the As consequence The properties of Bose-Einstein condensates in lower-dimensional trapping potentials have recently attracted increasing interest. 2D condensates can be created in an array of pancake-shaped traps provided by the periodic potential of a 1D optical lattice. Bose-Einstein condensates within the periodic potential of an optical lattice represent the atomic physics equivalent of solid state problems. The non-linear interactions between the condensate atoms represent a new feature of the Bose-Einstein condensates within a periodic potential. We have investigated Bose-Einstein condensate in an accelerated optical lattice and associated phenomena such as Bloch oscillations and Landau-Zener tunneling. The presence of the nonlinear interactions modifies those phenomena. Furthermore we have investigated the dynamics and phase evolution of Bose-Einstein condensates in 1D optical lattices. The dynamical behavior was studied by adiabatically loading the condensate into the lattice and subsequently switching off the magnetic trap, with the condensate free to expand inside the periodic structure of the optical lattice. The phase evolution of the condensate was studied by non-adiabatically switching on the periodic potential. We observe decays and revivals of the interference pattern after a time-of-flight.

New experimental methods for quantum optics with large molecules

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Recent progress in the development of a variety of new matter wave interference experiments, with electrons, ultra-cold atoms, cold clusters or hot molecules have stimulated the quest for the experimental limitations of de Broglie interference. In particular complex molecules are intriguing as they open new ways for exploring decoherence in the presence of high internal temperatures [1], large polarisabilities [2], permanent electric dipole moments or even chirality. Macromolecule interferometry may also lead to interesting applications in metrology and litho-graphy.

Any molecule interferometer requires a sufficiently efficient source-detector combination as well as a coherent matter manipulation scheme which minimizes the stability requirements and suppresses uncontrolled decoherence.

The recent development of Talbot-Lau (TL) interferometry was crucial for the successful demonstration of the quantum wave-nature of fullerenes, small biodyes and fullerene derivatives [3]. And refined variants of TI-interferometry are believed to be still useful for particles in the mass range well above 10 kDa.

However, experiments up to now were also limited by the lack of sufficiently intense, slow molecular beams which could be detected with high efficiency.

We discuss our recent exploration of thermal beams with particles between 2...7 kDa which yield rather high count rates in electron impact ionization in combination with quadrupole mass spectroscopy.

In an effort to improve on the detection of even larger molecules we have also developed a fluorescence detection scheme which combines the high efficiency of the optical readout with the sub-wavelength position resolution which is intrinsic to the Talbot-Lau scheme.

Using mechanically magnified (MecMag) fluorescence imaging of Talbot-Lau interferences we are able to record high contrast fringes with 100 nm resolution. This novel scheme promises to be very fruitful in combination with dye-labeled biomolecules or fluorescent nanocrystals in the high mass regime. MecMag-imaging is scalable in the sense that its efficiency may even improve with increasing size of the detected particle.

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Modern view on angle- and spin-resolved Auger electron spectroscopy

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Since mid-nineties measurements of the angular anisotropy of Auger- and resonant Auger-electron emission have become a routine method of the studying the dynamics of the Auger process. Also more difficult measurements of Auger-electron spin polarization evolved from being an exotic experiment to a useful tool for investigation of Auger electron dynamics. Spectacular progress in this field has been achieved due to a dramatic increase of the intensity and quality of the beams available at the third-generation synchrotron radiation facilities where most of the modern Auger electron investigations are performed. Examples of modern studies of the angular anisotropy and spin-polarization of Auger electrons which provide spectroscopic and dynamic information will be given in the report.

The ultimate goal of the dynamical studies is to obtain experimental values of the Auger amplitudes, i.e. to realize a so-called complete experiment. Recently, the concept of the complete experiment for Auger decay has been revisited due to establishment of the strict relations connecting anisotropy and spin-polarization parameters [1]. Existence of these relations limits the number of independent parameters which may be obtained from measurements of angular distributions and spin-polarization of Auger electrons.

The advanced modern studies of the Auger processes use a coincidence technique which allows unambiguous separation of the decay channels and provides more differential data in comparison with non-coincidence experiments. We discuss examples of the modern coincidence studies of the Auger-electron cascades and double Auger processes.

Very recently a new direction of investigation of the Auger processes has emerged: a time-resolved study of the Auger decay [2]. The first results and perspectives of the time-resolved investigation of Auger processes will be discussed.

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An Overview of Pump-Probe Experiments in Atomic Photoionization involving Laser- and Synchrotron Radiations

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The combination of laser and synchrotron radiation (SR) has proven to be an ideal experimental approach to study, via a pump-probe excitation scheme, the complex electronic interaction and the dynamics of excited atomic states. The precise manipulation of the electronic cloud of the atom by the first photon makes it possible to influence, in a controlled way, the interaction between the electrons in the atom by changing their direct environment. In particular, such experiments provide access to states of opposite parity to that of the ground state. Using dye lasers, the excited state can be prepared with a well defined set of quantum numbers, including a non-statistical population of the magnetic sublevels when the laser/synchrotron radiation is linearly or circularly polarized. The synchronization of pulsed mode-locked lasers with SR has open the way to time-resolved studies, allowing variable delays to be introduced between the pump- and probe-radiations.

The first experiments taking advantage of the high spectral resolution of the laser and the large tunability range of SR have been developed in the early 80's, using first generation SR sources, namely ACO in Orsay and HASYLAB in Hamburg, and cw dye lasers. Atomic parameters for some excited states of sodium and barium atoms, were measured at that time, allowing to test newly developed many-body theoretical models. Soon afterwards, additional control of the light polarization was achieved in the production of laser-excited sodium atoms, allowing photoionization of oriented- and aligned- atoms to be studied.

The advent of the second generation of SR sources for pump-probe experiments provided monochromatized beams with much higher intensity, which was mostly due to the newly invented undulators devices. With this increased **intensity**, new aspects of photoionization in excited atoms were discovered, such as the strong enhancement of the satellite cross sections in alkali-atoms. Also, the synchrotron became more and more used as the pump and lasers as the probe, sometimes with synchronization techniques. A whole new set of experiments was developed such as measurements of the lifetime of some excited states in rare gas atoms, as well as investigation of doubly-resonant atomic states. Experiments in which the polarization was varied, allowed to deduce the phase difference between two outgoing electron waves in the continuum. Probe of atomic fragments arising from dissociation of molecules was implemented.

The first use of 3^{rd} generation SR sources for pump-probe experiments has considerably improved our understanding of the electronic interactions in highly-correlated atoms. In particular, the high **brilliance** of the Advanced Light Source makes it possible to observe hollow atoms produced by inner-shell excitation of laser-excited lithium atoms. Later, access to the fine structure of an electronic state even after core-excitation was provided. Clear experimental evidence for quasi-forbidden and dynamically forbidden transitions has been obtained in photoionization of laser-excited sodium atoms. Unprecedently achieved resolution in both spectral excitation and electron detection demonstrated the new capabilities offered by these sources for pump-probe experiments.

Ultimately, new Free-Electron-Laser facilities, expected to operate over the 20-200 eV photon energy range, are being tested, e.g. in Hamburg with TESLA. Such new facilities, called 4^{th} generation SR sources, will likely give to a SR pump/probe the fascinating properties of a laser beam.

Resonances in recombination and ionization - a tool for spectroscopy.

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Multiply excited, autoionizing, states are frequently encountered as resonances in atomic processes as ionization or electron-ion recombination. The presence of resonances can change the probability for a process by orders of magnitude and there is thus an obvious interest to be able to describe them and make quantitative predictions of their effects. In addition there are many interesting spectroscopic aspects related to resonances which will be the main topic of this talk.

The probability for the process of electron-ion recombination is in fact often governed by the resonant process of dielectronic recombination and the contribution varies drastically from one charge state to the other since it strongly depends on the density of doubly excited states. The change in electronic configurations when one electron is added or removed can be enough to change the recombination rate coefficients by orders of magnitude. Predictions of the recombination rate requires thus precise spectroscopical knowledge. Of the same reasons, measurements of recombination resonances can in fact be used to access highly accurate information on atomic energy levels, especially for highly charged ions. One among the presently most accurate determinations of an energy splitting in a few electron highly charged ion is obtained from the cross section for recombination with free electrons near the ionization threshold of an highly charged lead ion (Pb^{53+})[1], and several Li-like ions have their most precise determination in this way [2,3]. The spectroscopic principle is that during the formation of a resonance the valence electron is excited by the capture of a free electron into a Rydberg state. The binding energy of the latter can be estimated to excellent accuracy and the excitation energy can then be accessed. The determination of the excitation energy is in many cases sensitive to many-body quantum electrodynamical effects as well as to the hyperfine structure.

Other resonances that will be discussed are those of negative ions. Here there is no long range Coulomb force and as a consequence negative ions have in general very few bound states. The ions show, however, still rich resonance spectra through which they can be studied. During recent years the photodetachment studies of doubly excited states have been extended to photon energies where triply excited states can form. The simplest negative ion that can be triply excited is the pure four-body system He^-, where 40 eV is needed to reach the triply excited states [4,5]. These states are above the threshold for ejection of two-electrons, but they still form with large probability after photoabsorption.

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Interaction of H_2 Rydberg molecule beams with surfaces and travelling electric fields

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Two types of experiment are described which take advantage of the long lifetime and large polarizability of Rydberg states of molecular hydrogen. In both cases two-color excitation (VUV + UV) of H_2 in a supersonic beam is used to produce Rydberg states with principal quantum number in the range $n = 15$–40, and with either 0 or 2 units of rotational angular momentum in the H_2^+ core. In the first set of experiments, the Rydberg molecules interact with a metallic surface at grazing incidence. Tunnelling ionization of the Rydberg electron into the metal occurs and the resultant molecular ions can be pulled away from the surface by application of an electric field. The field required to extract the ions is critically dependent on the distance from the surface at which ionization occurs. This field is measured as a function of initial quantum state populated, and further information obtained by imaging the trajectories of the ions to the detector (which located on an axis perpendicular to the surface). Apart from the expected strong dependence of the distance of ionization with principal quantum number two novel effects are observed; firstly the rotation of the ion core is found to contribute to the process of tunneling ionization, such that the energy of the ion core is given up to the electron in a manner analogous to rotational autoionization. Secondly, the field versus extraction probability profiles show resonance effects with enhancement at specific fields. The profiles also show a strong dependence on the surface roughness, but not on the surface material (Al versus Au)

In the second set of experiments inhomogeneous electric fields are applied to control the translational motion of the molecules [1-4]. In the presence of an electric field, a very large dipole moment can be created in the Rydberg states, exceeding the dipole moments of ground-state molecules by many orders of magnitude. In our experiments the molecules are exposed to the inhomogeneous field of one or more electric dipoles for a fixed period of time ($\sim \mu$s) and their trajectories are monitored by field ionization and ion imaging or time-of-flight measurement. A large decelerating or accelerating force results from the application of the inhomogeneous field resulting from a single dipole oriented perpendicular to the beam direction. The observed acceleration and deceleration are in agreement with those predicted in classical trajectory simulations. Very long lifetimes ~ 100 μs) are observed under certain field and excitation conditions. A two-dipole device is currently being tested in which the Rydberg molecules experience a constant field and constant field gradient as they are decelerated. The purpose of this device is to decelerate and trap Rydberg molecules at temperatures in the milliKelvin range. Progress towards studying collisions of slow H_2 Rydberg molecules with a metal surface will be also be discussed.

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Two Methods Produce Slow Antihydrogen

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The ATRAP Collaboration has developed two methods to produce slow antihydrogen. In the first method, antihydrogen is produced during the positron cooling of antiprotons. In the second, lasers control the production of antihydrogen via a double charge exchange process. The relative merits of the two methods, and the challenges facing antihydrogen experiments, will be discussed.

Project ALPHA and the Future of Antihydrogen Physics

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In 2002, the ATHENA and ATRAP collaborations succeeded in producing antihydrogen atoms from cold plasmas of trapped positrons and antiprotons. Given this and subsequent developments it is natural to contemplate the prospect for trapping the antiatoms, so that they can be studied spectroscopically. Following the completion of the ATHENA project, the ALPHA (Antihydrogen Laser PHysics Apparatus) collaboration has been formed to design and construct a next-generation antihydrogen apparatus at the CERN Antiproton Decelerator (AD). After briefly reviewing the main results of the ATHENA experiment, I will present the design, physics goals, and status of the ALPHA project. The heart of the device is a superconducting magnet system comprising a transverse multipole and mirror coils for trapping antihydrogen. An annihilation vertex detector based on silicon strip modules will diagnose antihydrogen formation and trapping. The collaboration intends to begin antihydrogen production and trapping studies with this device in mid-2006.

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Ground-state hyperfine splitting of antihydrogen

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At CERN's antiproton decelerator (AD), there are two approved experiments, ATRAP and ALPHA, aiming at testing CPT symmetry using high-precision laser spectroscopy of the antihydrogen 1S–2S transition. Our collaboration, ASACUSA, has so far used laser spectroscopy of antiprotonic helium to test CPT [1], but will in the future focus on the measurement of antihydrogen ground-state hyperfine splitting (GS-HFS) [2].

To the leading order, the GS-HFS of antihydrogen is proportional to the spin magnetic moment of the antiproton, $\mu_{\bar{p}}$ which is experimentally known only at the level of 0.3%. Below the level of several ppm accuracy, $\nu_{\rm HF}$ also depends on the electric and magnetic form factors of the antiproton. The measurements of $\nu_{\rm HF}(\bar{H})$ to a relative accuracy of better than 10^{-6} will therefore yield an improvement of the value of $\mu_{\bar{p}}$ by three orders of magnitude, and give some insight into the structure of the antiproton. Furthermore, the only existing phenomenological extension of the standard model that includes CPT violations (the standard model extension of Kostelecky's group [3]) predicts that CPT violation in the 1S–2S transition (for free atom) is cancelled in first order, while for the hyperfine structure it is a leading-order effect [4]. In addition, the parameters introduced by Kostelecky et al. have the dimension of energy (or frequency). Therefore, by measuring a relatively small quantity on an energy scale (like the 1.4 GHz GS-HFS splitting), a smaller relative accuracy is needed to reach the same absolute precision for a CPT test.

We plan to employ a classical atomic-beam method, with a sextupole-magnet beamline and a microwave spin-flip cavity to measure the antihydrogen GS-HFS. In this scheme, it is not necessary to produce very cold (trappable) antihydrogen atoms, but it is important to have a point-like antihydrogen source. A possible method, under development is to use a two-frequency radio-frequency trap, which can simultaneously confine antiprotons and positrons.

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Relativity, atomic clocks and optical links

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It is well-known that, a century after 1905, our physical representation of space and time is based on relativity. The fact that it also involves basic quantum concepts coming from atomic and optical physics is probably less widely appreciated. Accurate time delivered by atomic clocks is nothing but the phase of a quantum oscillator. Meanwhile synchronization, localization or ranging techniques are built on remote distribution of the phase of an electromagnetic field.

Both kinds of phases, which are inescapable ingredients of most recent tests of relativity, are defined from Hamilton's action integrals. For example, global navigation satellite systems (GPS or Galileo) define positions in space and time from a 4-dimensional web of electromagnetic phases labelled by atomic phases. Yet the precise status of time raises questions in quantum theory and its compatibility with relativistic requirements is far from obvious.

Schrödinger and Einstein considered this question as a fundamental problem of the quantum theory. In contrast, a common position states that quantum formalism does not allow for time being treated as an observable, which forbids it to write a energy-time Heisenberg inequality related with a rigorously defined quantum commutation relation. But, if time has a different description from space, it is impossible to conciliate quantum and relativistic requirements for time and space observables.

I will show that relativistic effects and quantum commutators can be given a consistent theoretical description. Observables may indeed be associated with positions in time or space through a reanalysis of synchronization or localization procedures. In particular, a time observable is defined and it follows from the invariance of Maxwell equations under Lorentz transformations and dilatations that this observable is properly conjugated to energy while simultaneously obeying Lorentz transformation properties. Since conformal symmetry includes transformations to accelerated frames, the quantum algebraic framework also leads to quantum expressions of the Einstein redshift laws associated with acceleration and/or gravity.

ORAL SESSION S1

Coherent accumulation induced velocity selective optical pumping of Rb hyperfine lines

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Ultrashort, mode-locked lasers have brought a new insights in different physical phenomena. In the time domain, the femtosecond pulses have been used for probing and manipulation of atomic and molecular dynamic. In a frequency domain, mode-locked, phase-stabilized femtosecond lasers produce a stabilized wide-bandwidth optical frequency combs [1]. The interaction of the fs laser pulse train with the alkali atomic vapor leads to the coherent population accumulation in the excited states [2,3,4].

We present a direct observation of the velocity selective optical pumping of the Rb ground hyperfine levels induced by the coherent accumulation. The coherent accumulation comes as a result of the femtosecond pulse train and rubidium system interaction. The pulse train effects were observed in the frequency domain, corresponding to the different atomic velocity groups, weighted by the Doppler profile. A modified DFCS spectroscopy which, in addition to the fs laser, uses a weak probe laser for monitoring the population distribution between the hyperfine ground state Rb levels was developed. The Liuville equation for the density-matrix elements of a four-level Rb system was employed for the theoretical interpretation of the observed fenomena.

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Attosecond Electron Wave Packet Dynamics

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We present results from some of the first experimental studies of attosecond electron wave packets created via the absorption of extreme ultraviolet light pulses. The light pulses, made via high harmonic generation, form an attosecond pulse train (APT) whose properties we can manipulate by a combination of spatial and spectral filtering. For instance, we show that on-target attosecond pulses of 170 as duration, which at the frequency used is close to the single cycle limit, can be produced [1]. The electron wave packets created when such an APT is used to ionize an atom are different from the tunneling wave packets familiar from strong field ionization. We show, both experimentally and theoretically, how the ionization step and the subsequent electron dynamics can be studied and controlled when atoms are ionized by an APT in the presence of a strong infrared (IR) field. Using an APT with energy close to the ionization threshold of the atoms, the deformation of the atomic potential by the IR field can be studied in real time. We find that the ionization yield is significantly enhanced when both the APT and the IR pulse are present, and that it is modulated as a function of time delay between the pulses. The subsequent electron dynamics can furthermore be studied if the resulting electron spectra are measured. We find that the absorption of energy above the ionization threshold depends strongly on the delay between the APT and the IR pulses [2]. We also demonstrate that altering the properties of the initial electron wave packet by manipulating the APT dramatically changes the subsequent continuum electron dynamics.

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The investigation of NaI photodissociation at 245 - 365 nm: determination of anisotropy parameters and photofragmentation matrix elements.

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Photodissociation is one of the basic elementary processes in the atmosphere of Earth and planets. The investigation of photodissociation reactions can provided detailed information about the electronic structure of a molecule and of the photodissociation dynamics. Recent progress in theory and experiment allows to obtain a set of anisotropy parameters which completely describe the photodissociation process [1,2]. The anisotropy parameters are closely related to the magnitudes and relative phases of the photofragmentation T matrix elements, resulting from *ab initio* calculations [3].

We present the detailed study of NaI photodissociation via the first and the second excited states by Doppler - resolved Faraday technique [4] at different dissociation wavelength in the spectral range 245-365 nm. The experiment has been carried out with a thermal molecular beam in a vacuum chamber using a pulsed tunable circularly polarized photolysis laser. The recoil anisotropy of the produced sodium photofragments and the angular distribution of their spins were probed by cw narrow-band linearly polarized radiation, which frequency was tuned through the photofragment absorption line. By analyzing the absorption and dispersion probe laser profiles we were able to obtain the values of the laboratory frame anisotropy parameters α_1, γ_1 and β and determine the photofragmentation **T** matrix elements.

The paper presents the analysis of the anisotropy parameters wavelength dependence and the interpretation of the underlying photodissociation dynamics.

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ORAL SESSION S2

High resolution Fourier transform spectroscopy and applications to astrophysical spectral analyses

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At Imperial College (IC) we are using our unique VUV high resolution Fourier Transform Spectrometer (FTS) [1] to study spectra of astrophysically important elements. The IC VUV FTS has a MgF_2 beamsplitter which allows the short wavelength cut off to be extended down to a record wavelength of 135 nm [3]. The new generation of high resolution spectrographs on ground-based and space telescopes has led to a demand for improvements in the quality and completeness of atomic data available for analysis of the resulting high resolution astronomical spectra. Wavelengths are needed to at least 1 part in 10^7 and f-values to a few %. Order of magnitude improvements in the accuracy of the atomic data are achievable with the technique of FT spectroscopy which combines both high resolution (IC FTS resolving power = 2 million at 200 nm) and wide spectral range. After calibration, wavelengths of lines of good signal to noise ratio measured in our FT spectra are accurate to a few parts in 10^8. The smoothly varying response of the FTS, together with deuterium and tungsten standard lamps, allows accurate intensity calibration to yield relative line intensities. These can be used to determine branching ratios, which are combined with level lifetimes to yield accurate f-values [2].

We have studied neutral, singly and doubly ionised transition group element spectra, responsible for the majority of the opacity observed in many stars. As light sources we use water cooled hollow cathode lamps for observations of neutral and singly ionised spectra, and a Penning discharge for doubly ionised spectra [1]. Where necessary our VUV, UV and visible spectra are supplemented with IR spectra recorded elsewhere, either with the NIST (National Institute Standards & Technology, USA) FT spectrometer or the Kitt Peak FT spectrometer. Recent results include:

Doubly ionised transition group element spectra: Lines from these spectra dominate in the VUV-UV region of hot star spectra, and the existing atomic data are exceedingly poor. We are continuing our extensive programme of studies, and are undertaking measurements of Mn III, Co III, Cr III and Ni III. The analysis of Fe III is close to completion. We report new measurements of Cr III and Co III recorded at IC and NIST, for determination of accurate line wavelengths and f-values.

Neutral and singly ionised transition group element spectra: Cr I: We have analysed FT spectra of Cr, recorded in the visible-VUV at IC, together with new FT spectra recorded with the Kitt Peak FT spectrometer, to yield a linelist of 18,000 transitions (Cr I & Cr II and buffer gas lines Ne) from 1,800 - 56,000 cm^{-1}, with typical wavenumber accuracy of 1-2 mK (1 mK = 0.001 cm^{-1}). We have reworked the known energy levels, resulting in energy levels with uncertainties of the order of a few mK, and we are searching for new energy levels in Cr I. V I and V II: We have analysed FT spectra from 2,000 - 56,000 cm^{-1} (recorded at IC & Kitt Peak) to yield a linelist with accurate wavenumbers. This linelist has been used to rework the energy levels of V I and V II, and we report new energy levels found using these wavenumbers.

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Isotope shifts in the 3s-3p transitions of ionized Ne

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Neon is a gas commonly used in spectroscopic light sources. It is therefore desirable to have spectral lines of neon available as accurate standards for wavelength calibration. There are three naturally occurring isotopes of neon, $^{20-22}$Ne, with the atmospheric concentrations of 90.48%, 0.27% and 9.25% respectively. When using glow discharge lamps in high resolution spectroscopy, the 3s-3p transitions in Ne I-III show structure due to isotope shifts of the two most abundant isotopes. To use these transitions as accurate standards the structure has to be accounted for, i.e. shifts and positions must be known. Some of the shifts in the 3s-3p transitions of Ne I have been measured by Doppler-free laser spectroscopy, e.g. see [1], producing accurate relative shifts. Shifts in the first two ions of neon are, however, less well studied.

In this work the 3s-3p transitions in Ne II and III have been measured by means of a high-resolution Fourier transform spectrometer. A water-cooled hollow-cathode lamp operated at low currents and neon pressures of 0.05-1.50 torr was used to produce narrow spectral lines. The cathode was made of aluminum, which has good properties when studying gases, such as high thermal conductivity, low sputtering yield and low line density. For the purpose of wavelength calibration argon was added to a level of a few percent of the total gas pressure.

To determine accurate wavelengths and shifts a sum of two Voigt functions were fitted to the line profiles representing the ^{20}Ne and ^{22}Ne isotopes. Due to the low concentration of ^{21}Ne, it starts to affect the fitting first when a transition has a S/N greater than 400. All lines investigated had a S/N below this and the ^{21}Ne contribution was therefore omitted. Apart from the wavelength positions, all parameters were kept the same for the two functions. However, two modifications were made. The areas of the two components were fixed by the ratio of the relative abundances, and due to the difference in mass the Doppler width of ^{22}Ne was reduced by a factor of 0.953. By treating the data this way, isotope shifts as large as 0.4 cm^{-1} in Ne III have been determined.

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Progress in the classification of Ta I and Ta II spectral lines

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We use a combination of different experimental methods (Fourier-Tansform-spectroscopy, conventional specroscopy, laser spectroscopy) in order to classify spectral lines of the tantalum atom (Ta I) and the first tantalum ion (Ta II). Despite of our efforts during the last 15 years, many Ta I and Ta II spectral lines are still not classified, especially in the ultraviolet region. As the main source of information, we use Fourier Transform spectra with high spectral resolution, available for the range 2000 to 50000 Å. For most of the lines, the hyperfine splitting is larger than the Doppler width of the lines and larger than the resolution of the spectra, thus, the hyperfine structure of the spectral lines can be used to identify the involved atomic or ionic levels. Additionally, we use photographic spectra, where we have compared the spectrum of a cw low pressure hollow cathode lamp with the spectrum of a hollow cathode lamp working with pulsed current (pulse current up to 100 A). With the pulsed discharge, most of the ionic lines have much more intensity. This fact allows in most cases to identify if a line belongs to the Ta I or Ta II spectrum. Our list of spectral lines contains now approx. 5900 Ta I lines and approx. 2800 Ta II lines. Among them, still approx. 1500 lines are not classified.

In order to enable the classification of further Ta II lines, we have extracted from the hyperfine structures shown in the FT spectra the hyperfine constants of further 150 Ta II levels.

By combining the wavenumbers of an unclassified line under investigation with the wavenumbers of other unclassified lines, we try to establish a hypothetical new level, including J-value and hyperfine constants, explaining the hyperfine structure of the investigated line. If such a level really exists is proved by explaining not only the wavenumber but also the hyperfine structure of other unclassified lines. A final check is done by laser excitation of a transition from a known lower level to the newly introduced level.

We present here the results of the last year. We could find ca. 30 levels of even parity and ca. 20 levels of odd parity of the tantalum atom and some new levels of the first tantalum ion.

Furter information including line lists and a viewer program one can find via http://iep.tugraz.ac.at/ta.html

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ORAL SESSION S3

Vacuum spark EUV spectrum of tin

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A source of radiation at the extreme ultraviolet (EUV) wavelength of 135 Å will be necessary for next generation of lithography technology. It was shown[1] that high temperature plasma of tin has strong intensity peak close to 135 Å consisting mainly of the $4p^6 4d^k$ - $(4p^6 4d^{k-1} 4f + 4p^5 4d^{k+1})$ transitions in the ions with the ground configuration $4p^6 4d^k$. The spectra of these ions are almost completely unknown. Only four lines have been identified in Sn XIV (k = 1)[2] and a resonance transition array was analyzed in Sn VIII (k = 7)[3]. There are no data on the Sn IX - Sn XIII as well as on the spectra of isoelectronic ions.

The spectrum of tin was excited in a vacuum spark (C =10 - 150 μF, L = 80 - 930 nH, U = 1 - 4 kV) and photographed in a region 100 - 170 Å on a 3-m grazing incidence spectrograph equipped with a holographic grating 3600 l/mm. The spectrograms have a spectral resolution 12,000 and a plate factor 0.25 Å/mm in the 135 Å region.

The spectrum of tin taken at a high current mode of the vacuum spark has distinct groups of the lines in the 155, 147 and 137 Å regions. By a comparison with the calculations by a Cowan code these groups should belong to the transitions respectively in the Sn VIII, Sn IX and Sn X spectra. A group of the lines at 135 Å is a mixture of the Sn XI - Sn XIV spectra. In the group at 155 Å we identified about 100 lines of Sn VIII as the $4d^7$ - $(4d^6 4f + 4p^5 4d^8)$ transitions. On basis of known levels of the ground configuration [3] 37 levels of the excited configurations were found. About 50 lines of the $4d^2$ - $(4d4f + 4p^5 4d^3)$ transitions in Sn XIII were identified in the region 126 - 140 Å and all the $4d^2$ and 28 of the $4d4f + 4p^5 4d^2$ levels were located. The analysis of the Sn XIV spectrum was extended by adding 7 new lines, establishing a splitting of the ground term $4p^6 4d\ ^2D$ and finding the energies of the corresponding levels of the $4p^6 5p + 4p^6 4f + 4p^5 4d^2$ configurations. Also a line 132.751 Å was identified as the $4p^6\ ^1S_0$ - $4p^5 4d\ ^1P_1$ transition in Sn XV. Using these new and available for the Sn VI - Sn VII spectra data the energy matrix parameters were extrapolated to Sn X - Sn XII. By a comparison with the calculations with these parameters the most intense lines in the region 131 - 150 Å are classified.

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Time and Spectrally Resolved Imaging of Colliding Plasmas

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We present a detailed study on the collision of neutral and single charged components of two laser generated plasmas, namely, Li-Li, Ca-Ca and Li-Ca. Our system is composed by a time-resolved gated CCD and a set of band-pass filters and allowed us to follow the temporal and spatial evolution the two plasma plumes from its early time formation until the time when the two plasmas collide.

Concerning the plasma collision, two different regimes can be asserted by its collisionality parameters. One dominated by low velocities and high densities, is known as *stagnation regime* and is characterized by the two plasmas behaving as two fluids. The other one dominated by high velocities and low densities, is known as *interpenetration regime*, and the binary collisions are expected to play a major role on the interaction. In this work, we will discuss and portray the stagnation regime and discuss the conditions to form a plasma collision dominated by interpenetration.

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A statistical approach to tin-based plasmas for 13.5 nm EUV lithography

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Next generation lithography (NGL) schemes based on a 13.5 nm light source are of great importance to the semiconductor industry. From their work with the lanthanides and adjacent related elements using laser-produced plasmas (LPPs), O'Sullivan and Carroll [1,2] reported that the peak wavelength of the $\Delta n = 0$ ($n = 4 \rightarrow n = 4$) unresolved transition array (UTA) emission decreased with increasing atomic number, Z. In tin, the UTA lies near 13.5 nm and is due predominantly to 4d-4f and 4p-4d transitions in a range (Sn^{7+} to Sn^{12+}) of tin ions. A UTA results from thousands of transitions between bands of near-degenerate energy levels [3,4]. Because of the complexity of the configurations, a line-by-line analysis of these transitions is computationally extremely intensive. To identify the contributing ion stages, a steady-state collisional-radiative laser-plasma interaction model is used [5]. Furthermore, to optimise the plasma requirements, a figure of merit is defined as the product of the summed *gf* values (weighted oscillator strengths) for the UTA transitions within each ion stage, weighted by the ion distribution as a function of electron temperature and proposed 13.5 nm, Mo/Si multilayer mirror reflectivity. To simplify radiation transport modelling, the emission profiles of the UTAs for each ion are treated statistically. The results are compared with experimental spectra from tin-based LPPs.

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ORAL SESSION S4

Matter-wave diffraction with an inclined transmission grating: Searching for the elusive Efimov state

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The size of the helium trimer is determined by diffracting a beam of ^{4}He clusters from from a 100 nm period transmission grating inclined by 21°. Due to the thickness of the bars the projected slit width is roughly halved with respect to normal incidence, increasing the sensitivity to the trimer size. The peak intensities measured out to the ±8th order are used to determine the effective slit width for the trimer. From that we find the average trimer bond length to be $\langle r \rangle = 1.1\,{+0.4}/{-0.5}\,\mathrm{nm}$, in good agreement with predictions for the helium trimer ground state. From this the concentration of Efimov state trimers in the beam is estimated to be less than 6%.

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Experimental signatures of the crossed-field double-minimum potential well

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Atomic and molecular systems under the influence of strong external fields can exhibit a range of interesting phenomenon, from those which elucidate the structure of the atom or molecule under investigation, to others which examine the correspondence between classical mechanics and quantum mechanics. The study of strong field effects in laboratory strength electric and magnetic fields is most readily achieved through the excitation of high-lying Rydberg states, since the sensitivity of an atom or molecule to such fields is strongly dependent on the principle quantum number, n. We have taken advantage of this n-dependence to carry out an experimental investigation of the crossed-field double-minimum potential well.

To date, several groups have investigated a range of theoretical aspects of the double-minimum potential well which can be formed when an atom is placed in crossed electric and magnetic fields of suitable strength [1-4]. However, as far as we are aware, our current experiment is the first to provide spectroscopic evidence for the presence of this novel crossed-field feature.

The experimental set-up which we employ is similar to that described in [5], in which an effusive beam of barium atoms is propagated perpendicular to the magnetic field generated in a dipole electromagnet. A crossed electric field is then applied in the remaining perpendicular direction. High-lying barium Rydberg states are excited via a single photon transition from the ground state by single mode, pulsed laser radiation generated in an optical parametric oscillator. This laser radiation propagates through the crossed-field volume, parallel to the magnetic field direction. By altering the polarisation of the laser radiation, using a Soleil-Babinet compensator, and by varying the strength of the crossed electric and magnetic fields, we have been able to identify states which can tunnel through the barrier into the second minimum giving rise to experimental signatures of the double-minimum potential well.

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Ground-state Hanle resonances in cesium vapor confined in Nanoscopic Thin Cell

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Recently, sub-Doppler-width, absorption resonances have been observed in alkali atoms confined in Nanoscopic Thin Cell (NTC, less than one μm length) utilizing the technique based on frequency-tuned single light beam [1]. Due to the extremely short distance between the cell windows, saturation and optical pumping processes can be completed only for slow atoms resulting in observation of sub-Doppler-width spectrum.

In this communication we present an experimental evidence of nonlinear, ground-state Hanle resonances in NTC and propose a theoretical analysis of their behavior. *Cs* atoms, confined in NTC (with no buffer gas added) are irradiated by circularly polarized light which is successively frequency tuned in resonance with everyone of the three allowed hyperfine (hf) transitions starting from the ground-state hf level $Fg = 4$ of D_2 line of *Cs*. The transmitted through the cell beam is registered in dependence on a perpendicular to the laser beam magnetic field B, scanned around B=0. Determined by the degeneracy of the involved levels, for the $Fg = 4 \rightarrow Fe = 5$ transition Electromagnetically Induced Absorption (EIA) while for the two $Fg = 4 \rightarrow Fe = 3{,}4$ transitions Electromagnetically Induced Transparency (EIT) were expected. However, for all transitions, the experiment has shown EIT resonances of similar behavior. At all hf transitions of *Cs* D_2 line also EIT resonances have been reported, for *Cs* atoms in ordinary (5cm long) gas-buffered cell [2]. There, the EIA resonance sign reversal is attributed to the excited state magnetic sublevel population mixing due to the *Cs* buffer-gas-atom collisions.

The nonlinear Hanle effect in NTC was analyzed by means of Zeeman coherence rate equations [3], which for stationary excitation is equivalent to optical Bloch (Liuville) equations but are simpler to solve. Assumptions of redistribution of atoms among the magnetic sublevels of the excited state and atomic coherence relaxation are incorporated in a form similar to one used in [2]. In addition here we assume that relaxation rate depends on energy separation between magnetic sublevels. We believe that reason for atom redistribution among Zeeman sublevels of the excited state is a long range interaction of atoms with the walls of the NTC. Theoretical and experimental resonance profiles comparison, made at the strongest ($Fg = 4 \rightarrow Fe = 4, 5$) hf transitions, shows a qualitative agreement. Moreover, experiment supports predicted by the theory linear dependence between the light intensity and the squire of the Rabi frequency.

The obtained results are important for the study of the dynamics of ground-state atom coherence, atom-atom and atom-surface collisions, atom velocity distribution and atom-surface interaction, for atoms confined in nanoscopic-width vapor layers.

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ORAL SESSION S5

Spectroscopy of Rb_2 and KRb on He nanodroplets

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Beams of cold (0.4 K) superfluid helium droplets complement photoassociation for the production and spectroscopic investigation of cold molecules. The droplets pass through a pickup cell containing alkali atom vapor, and each may capture one or more atoms. The atoms remain on the surface of the droplet, where they move freely and form bound complexes. Because the binding energy is dissipated into the He droplet, weakly bound molecules are preferentially formed: in our case alkali dimers in their lowest high-spin (triplet) state.

The measured electronic absorption spectra are only weakly perturbed by the droplets and can normally be assigned from the simulated spectra of the free species. Because the presence of the droplet does not quench the fluorescence from the excited molecules, emission spectra are also easily measured; in most cases emission occurs from free molecules which have come to separate from the droplet upon excitation.

We have investigated the electronic absorption and emission spectra of Rb_2 and KRb thus formed. As expected, the obtained spectra show that the energy levels of the molecules are only weakly perturbed. Conversely, the droplets strongly affect the accessible states, as well as the dynamics of the molecules after excitation.

Enhanced, Site–Specific Loading of Optical Lattices Using Light–Shift Engineering of an Atomic Excited State.

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We report on a method of light–shift engineering where an auxiliary laser is used to tune the atomic transition frequency [1]. The technique is used both to selectively load a specific region of an optical lattice and to enhance the loading of an optical dipole trap.

We examine the loading of ultra–cold ^{85}Rb from a magneto–optical trap (MOT) into an optical lattice based on standing wave created by a CO_2 laser ($\lambda = 10.6$ μm). We show that by focussing an additional laser (a Nd:YAG, $\lambda = 1.064$ μm) on specific sites of the optical lattice we can selectively load only these sites.

We explain the effect by calculating the differential light–shifts of the relevant ground and excited states in the presence of the two laser fields. We have performed theoretical calculations of the frequency dependent polarizabilities of the states concerned and have shown that the addition of a second laser field induces a splitting of the hyperfine levels of the excited state which is crucial in determining the efficiency of loading into the combined trap.

We suggest how the technique could be applied to load a single-site in 3D CO_2 lattice, with the interesting prospect of creating a Bose–Einstein condensate (BEC) in the limit of high trap frequency. In addition one could adapt the technique to perform patterned loading of optical lattices [2] for applications in QIP experiments.

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Development of a diode-laser-based sensor for chloridic and fluoridic acid detection in proximity of a waste incinerator

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The problem of atmospheric pollution has become increasingly important in recent years. The composition of atmosphere is changing rapidly, as result of energy overuse for industrial purposes and lack of control of industrial emission in most countries. Some atmospheric pollutants, such as nitrogen oxides, can have a significant impact on the environment and on human safety even in small concentration. Their detection and the identification of their sources require the development of high sensitive techniques for real and in-situ measurements. Laser-based systems have attained a increasing attention in recent years, due to their high sensitivity and selectivity. In particular, laser sensors based on the use of diode lasers emitting both in the near- and in the mid-IR region, are the best choice to achieve a very good sensitivity with a relatively cheap system. In this work, we present the development of a new compact sensor, based on the use of two different diode lasers, for continuous monitoring of chluoridric and fluoridric acid from a waste incinerators.

In our system, all the optical elements are fixed on a breadboard and they have been properly designed to reduced as much as possible the dimensions (60x75 cm^2) and the mechanical instability. HCl concentration is monitored by investigating the P(4) line at 1.7 μm in the ν_2 overtone vibrational band, while HF is detected observing the absorption of the R(3) line at 1.3 μm. Both lines have a line strength of the order of 10^{-21} cm/mol and 10^{-20} cm/mol. The measurement technique is based on the Lambert-Beer law for the absorption combined with the use of a multi-pass cell (total optical path 50 m) and phase-sensitive detection techniques (TTFMS). This type of detection reduces significantly the electronical noise. Optical noise, due to interference fringes, is still present and becomes predominant at very low concentration levels. We strongly reduced this noise by means of digital filtering. The minimum detectable concentration obtained with this system is about 8 ppbV for both gases.

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ORAL SESSION S6

Relativistic calculations of Ba^+ atomic properties

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The interest in calculating the energy levels and transition rates of Ba^+ ion is motivated by the possibility to study the parity non-conservation (PNC) with a single trapped ion. The study of PNC in heavy atoms provides atomic-physics tests of the Standard Model and allows to measure nuclear anapole moment. There is an ongoing theoretical and experimental effort for precise calculations and measurements of the PNC transition amplitudes. We compute the energy levels and transition amplitudes of Ba^+ ion using the relativistic all-order method. The lifetimes of several excited states are calculated and the results are found to be in good agreement with the experimental values. The static electric-dipole and electric-quadrupole polarizabilities of the Ba^+ ion in its ground state are calculated and compared with recent experimental values. We investigate the significant disagreement between the theoretical and experimental values of the ground state quadrupole polarizability. A consistency study of the lifetime and polarizability measurements in Ba^+ is conducted.

QED corrections to the parity-nonconserving 6s-7s amplitude in ^{133}Cs

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The complete gauge-invariant set of the one-loop QED corrections to the parity-nonconserving 6s-7s amplitude in ^{133}Cs is evaluated to all orders in αZ using a local version of the Dirac-Hartree-Fock potential. The calculations are peformed in both length and velocity gauges for the absorbed photon. The total binding QED correction is found to be -0.27(3)%, which differs from previous evaluations of this effect. This correction is combined with other contributions to get the total 6s-7s PNC transition amplitude in ^{133}Cs. Using the experimental value for $E_{\rm PNC}/\beta$ [1], where $E_{\rm PNC}$ is the PNC transition amplitude and β is the vector transition polarizabilty, the weak charge of ^{133}Cs is derived to be

$$Q_W = -72.57(29)_{\rm exp}(36)_{\rm th}$$

for $\beta = 26.957(51)a_{\rm B}^3$ [2,3] and

$$Q_W = -73.09(39)_{\rm exp}(37)_{\rm th}$$

for $\beta = 27.15(11)a_{\rm B}^3$ [3-5]. The first value deviates by 1.1σ from the prediction of the Standard Model, while the second one is in perfect agreement with it.

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Fine and Hyperfine Structure Calculations for Odd Configurations of Neutral Lanthanum

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The neutral Lanthanum atom, the first element of the rare-earth series in the periodic table, has interested a number of authors over the years for various reasons. Because of its complicated atomic-structure, neutral La has a very complex spectrum. In the course of time, many investigations of hyperfine structure (hfs) of ^{139}La have been carried out. Early theoretical studies are concentrated on the even-parity levels. Although some hfs data have been obtained of the odd-parity levels of ^{139}La, the very strong mixing between the odd parity configurations requires more data for a detailed analysis of the hfs. Lanthanum has two stable isotopes ^{138}La and ^{139}La with nuclear spins 5 and 7/2 respectively. Their magnetic moments are $3.7139\mu_N$ and $2.7832\mu_N$.

In our present study, a parametric analysis of the fine structure for the five La odd-parity configurations *5d6s6p*, *4f6s*^{2}, *6s*^{2}*6p*, *5d*^{2}*6p* and *4f5d6s* has been done in a multi-configuration fit using the program code of Cowan [1] in SL-coupling scheme. For the parametric fine structure calculations 50 parameters are required, eight for *5d6s6p* , each two for *4f6s*^{2} and *6s*^{2}*6p*, each ten for *5d*^{2}*6p* and *4f5d6s* configurations as well as eighteen configuration interaction parameters. The five configurations are comprised of 111 theoretical fine structure levels up to the ionization limit. Although, 97 experimental energy levels are known [2], the terms of 33 levels were unknown and the configurations of 15 levels were uncertain.

Based on the results of our fine structure calculation and experimental hfs data from literature, the magnetic dipole hfs was analysed using our HFSAC and HFSFIT programmes [3,4]. For the parametric analysis of these configurations, 26 experimental A constants are available. One-electron parameters are determined and theoretical predictions for the magnetic dipole hyperfine structure constants A for all levels of the configurations *5d6s6p*, *4f6s*^{2}, *6s*^{2}*6p*, *5d*^{2}*6p* and *4f5d6s* are calculated.

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ORAL SESSION S7

H_2^+ and D_2^+ Ions in Intense Ultrashort Laser Pulses

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Molecular dynamics in ultrafast intense laser pulses is a topic of considerable current interest largely driven by the quest to control simple chemical reactions. This is becoming increasingly more feasible as few cycle phase stabilised pulses are realised. In addition there is an opportunity to enhance our knowledge of fundamental processes in this inherantly non-linear regime. To this end much work has been carried out on the simplest molecular ion H_2^+, albeit with an incident neutral H_2 target. This has the disadvantage that the initial ionization step in the laser pulse requires such high intensities that the H_2^+ fragmentation dynamics proceeds at the field strength far away from threshold.

Recently measurements have been repeated where H_2^+ ions have been prepared remotely by electron impact, and a beam transported to the interaction region [1,2]. This removes the precursor stage with the inherant possibility of electron rescattering contribution, permitting pure field-dissociation effects to be studies over a broad range of intensities. We have carried out an experiment of this type, using an intensity selective scanning technique [3], measuring the momentum of fast H atom products through their time-of-flight. Fragmentation energy spectra for a range of intensities covering $5\text{x}10^{12}$ - $2\text{x}10^{14}$ Wcm^{-2} are observed, with the H atom peak shifting towards lower energy values as the pulse intensity increases. Whereas H_2 neutral precursors have been shown to field ionize into an extremely skewed vibrational distribution [4], H_2^+ ions formed by electron impact are known to be well represented by a Frank-Condon distribution [5]. The results will be described in these terms, where comparison with a calculation using a two-state approximation will be made.

Experimental techniques, results on D_2^+ and analysis procedures will be presented at the conference.

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How to measure the electron mass with two protons?

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The vibrational energy levels of the $H_2{}^+$ molecular ion mainly depends on the very well known Rydberg constant and on the electron to proton mass ratio m_e/M_p. It is thus possible to measure directly this mass ratio from a spectroscopy experiment between to vibrational levels. Because $H_2{}^+$ is an homonuclear ion, one must use two photon spectroscopy. We have shown [1] that one of the most favourable transition is the J=0, v=0 to v=1 infra red transition at 9.13 microns. We have built a RF Paul trap for $H_2{}^+$ ion trapping. The v = 0 ions can be selected by UV photodissociation of the v>0 levels. The transition to the v=1 level will be excited using laser light at 9.13 microns and detected by UV photodissociation. We are currently developping the 9.13 microns laser source. It is a quantum cascade laser (QCL) frequency locked to a stabilised $C0_2$ laser. Recent HD^+ calculations have shown that this molecular ion may be a better candidate for the determination of the mass ratio m_e/M_p.

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Anticrossing spectroscopy of He atoms excited by electron capture in 30 keV-He^+-H_2 collisions

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Anticrossing spectroscopy provides a convenient experimental technique for analysing collisionally excited He atoms. By measuring the intensity of He I spectral lines as a function of an electric field F_z applied parallel and antiparallel to the projectile beam, the coherence parameters for the excitation of 1snl states with different l quantum numbers can be determined. The asymmetry of the intensity functions with respect to the sign of the electric field reflects a forward-backward asymmetry of the charge distribution, in particular, an electric dipole moment of the collisionally excited state. Prominent features of these intensity functions are resonance structures at singlet-triplet anticrossings of 1snl $^1\Lambda \times {}^3\Lambda$ Stark sublevels.

This experimental technique has been used previously for analysing He I states produced by direct excitation of He atoms by proton and He^+ impact and electron capture in He^+-He collisions[1]. In this contribution we present first results obtained for 30 keV-He^+-H_2 collisions. We investigated both He I spectral lines emitted by projectile atoms formed by electron capture and H I spectral lines resulting from direct excitation and dissociation of hydrogen molecules.

Both spectra are highly asymmetric with respect to the sign of the electric field F_z. This leads again to the conclusion that immediately after the collision both the He and the H atoms have an electric dipole moment due to the excitation process. These results clearly show that the dipole moment of the He atoms is parallel to the direction of the projectile beam whereas the dipole moment of the H atoms is antiparallel.

Most remarkable, however, is the fact that the measured intensity functions of the He atoms produced by electron capture from H_2-molecules show a significant similarity to those measured in He^+-He collisions. As far as yet discovered, the relative amplitudes of the HeI spectra differ little from those measured in He^+-He collisions. The measured anticrossing spectra lead also to the conclusion that the singlet states are significantly more occupied than the triplet states. This result was quite unexpected and will be discussed at the conference.

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ORAL SESSION S8

Photoionization of Atmospherically Important Atoms at the Elettra Synchrotron Source

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As part of a larger programme to study the photoionization behaviour of reactive intermediates with synchrotron radiation, atomic oxygen, nitrogen and sulphur have been studied at the Elettra synchrotron source using angle resolved photoelectron spectroscopy (PES) and constant-ionic-state (CIS) measurements. In each case, relative partial photoionization cross-sections and angular distributions have been measured from threshold up to at least 21.0 eV. Results on O, N and S will be presented. For example, the natural width G, line shape parameters q and r2 and discrete oscillator strengths f have been measured for the members of the N*[2s2p3 (5S), np] (4P)N(4S) autoionizing resonances for n= 5 to 10. The n = 5 parameters calculated in this work are in good agreement with the values obtained previously whereas for the resonances with n = 6 to 10 the values of these parameters are reported for the first time. The asymmetry parameter (b) for the first band of N atoms, the N+(3P) N(4S) ionization, has also been measured in the photon energy range of the above autoionizing resonances. For S, the angular distribution parameter and relative photoionization cross-section for the S+(4S) S(3P), S+(2D) S(3P) and S+(2P) S(3P) (3p)-1 ionizations have been measured as a function of photon energy from threshold to 31eV. Inspection of the CIS spectra recorded for the S+(2D) S(3P) and S+(2P) S(3P) ionizations shows that all bands can be assigned to excitation to known Rydberg states. Rydberg states converging to the fourth ionization limit, corresponding to a (3s)-1 ionization, have been observed for the first time and assignments were proposed based on the observed resonance positions and asymmetry parameter measurements.

Photoelectron studies of laser excited and aligned alkali atoms

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Photoelectron spectroscopy is a standard tool for exploring the details of the atomic structure. So far photoelectron spectroscopy has been mostly performed on atoms in the ground state or thermally excited states. Much more information of atomic and molecular interactions with light can be gained if the target can be prepared into an excited [1] and/or polarized [2] initial state. Therefore we set up a continuous wave laser system at the soft x-ray undulator beamline I411 at the storage ring MAX II in Lund (Sweden). This setup provides laser radiation from the near infra-red (1000 nm) to the blue and near ultra-violet range. It will be possible to excite a variety of atoms and molecules both in the gas phase and on solid samples.

In this presentation we will give an overview over the first experiments that have been performed with the setup. Atomic beams of the alkali metals sodium, potassium and rubidium have been excited with laser light tuned to the first s→p transition of the valence electron. Fine structure resolved photoelectron spectra have been taken from the outermost filled p-shell with 60 eV synchrotron radiation. Recently D. Cubaynes and coworkers [1] have reported fine-structure resolved photoelectron spectra of the 2p photoemission from laser excited sodium. They showed that the spectra from the $^2P_{1/2}$ and $^2P_{3/2}$ initial state give considerable different fine structures. These studies give deep insight into the photoionization process and allow for detailed tests of the theoretical models. Furthermore the combination of laser excitation with photoelectron spectroscopy widens the information one can get from both the initial and final state and thereby improves the interpretation of the spectra. We have explored similar effects in the 3p photoemission of laser excited potassium and in the 4p photoemission of laser excited rubidium. In all spectra conjugate shakedown lines were visible.

This presentation will give an overview over photoelectron spectroscopy of laser excited alkali atoms. The comparison of the different atoms gives insight into effects of the different coupling schemes (LS-coupling for Na, jK-coupling for Rb) and the influence of the 4s–3d (K) and 5s–4d (Rb) configuration interaction in the final state. The comparison of photoemission from the $^2P_{1/2}$ and $^2P_{3/2}$ excited states with the conjugate shakeup excitation of the same final states give additional information on the process of photoionization.

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ORAL SESSION S9

Neutral Titanium and Manganese Laboratory Oscillator Strengths Applied to Low Mass Star Studies.

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A full understanding of the properties of low mass stars (LMS) and substellar objects (SSO) such as brown dwarfs and extrasolar planets is one of the major challenges facing astrophysics. In particular, the determination of mass, abundance, gravity and temperature are crucial in the understanding of LMS and SSO. The key problem is that LMSs and SSOs emit their observable radiation in the infrared region of the spectrum where the current knowledge of atomic line broadening effects and f–values is poor.

Our current project concentrates on the atomic data needs for LMS analysis. These differ from those used routinely (and already available) for hot star spectra. Due to the low temperature of the LMS atmospheres, the atomic opacity is dominated by neutral spectra. Because of the lack of experimental atomic data, stellar spectrum analyses are currently based on calculated atomic data. Although a great deal of effort has gone into trying to calculate accurately atomic data for LMS models, uncertainties in the calculated oscillator strengths for some lines (in particular Ti I, Mn I, Na I, and K I) are still large enough to affect seriously the interpretation of the observed line strengths [1].

The Low Mass Star project at Imperial College focusses on the accurate laboratory measurement of line wavenumbers (1:10^7), line broadening (hyperfine structure) [2], and f–values for Ti I, Mn I, Na I, and K I. The new spectra have been recorded using the high resolution Imperial College UV and VUV Fourier Transform (FT) spectrometers, with a wavenumber resolution of the order of 0.03 cm^{-1} (0.0002 Å at 2000 Å) [3]. Further spectra have also been recorded with the high resolution IR FT spectrometer at the National Institute of Standards and Technology (NIST), USA, with a wavenumber resolution of the order of 0.005 cm^{-1} [4]. Accurate intensity calibration of all the new spectra and the broad spectral range of the measurements (5.5 μ m to 140 nm) enables branching fractions (BF) to be determined with an uncertainty of the order of 10 %. Oscillator strengths are determined (with an uncertainty of the order of 10 to 15%) by combining the BFs with radiative lifetime values. We report on our results for Ti I and Mn I and their application to exciting new work on LMS analysis.

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Laser Spectroscopy of radioactive yttrium isotopes.

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The isotopes $^{86-100}$Y were produced by proton and deuteron induced reactions on a ^{89}Y target and proton induced fission of uranium at the IGISOL facility at the University of Jyväskylä. The extracted ions have been studied by collinear laser spectroscopy using 363 nm light to excite the $5s^2\ ^1S_0$ ground state to the $4d5p\ ^1P_1$ excited state at 27516.691 cm^{-1}. Nuclear moments have been extracted from the observed hyperfine structures, using the known moments of the ^{89,90}Y ground states for calibration. Isotope shifts were extracted from the centroids of the hyperfine structure. A King plot analysis using modified mean square charge radii, $\delta\langle r^2\rangle$, values from neighbouring isotope chains [1–3] was used to obtain the mass and field shift factors for the transition. The mass and field shift factors obtained from the systematics of the isotope shifts for nuclei close to stability provide the calibration needed to determine the nuclear charge radii for yttrium isotopes in the mass ∼100 region, where the sudden onset of nuclear deformation has been seen in the isotopes of neighbouring elements [2–4]. Also, as yttrium has odd Z (Z=39), many of its isotopes and isomers have nuclear spins greater than 1/2. This allows the electric quadrupole moment to be measured via the hyperfine structure, giving a direct measure of the static nuclear deformation. This can then be compared with the deformation inferred from the $\delta\langle r^2\rangle$ values, which are sensitive to both static and dynamic deformation contributions, giving a measure of the rigidity of the nuclear shape.

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Determination of the Nuclear Charge Radii of the Radioactive Lithium Isotopes ^{8}Li und ^{9}Li

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The measurement of the isotope shift of atomic transitions is the only model-independent access to determine nuclear charge radii of short-lived isotopes. However, this was limited to isotopes with nuclear charge of $Z \geq 10$ because the nuclear volume effect of the isotope shift is dominated by the mass shift by several orders of magnitude for the light isotopes. Here we report a novel method to measure charge radii of short-lived lithium isotopes. It is based on an accurate measurement of an atomic transition combined with recently performed theoretical calculation of the mass shift [1]. The calculations have a high accuracy of 10^{-9} and the predicted shifts show excellent agreement with the results of isotope-shift measurements on stable lithium isotopes [2] and known nuclear charge radii from electron scattering [3] as well as absolute transition energies [2]. The experimental method meets the requested efficiency of $> 10^{-4}$ and the required accuracy of < 200 kHz. This is achieved by Doppler-free two-photon spectroscopy in a thermal atomic beam followed by resonance ionization and detection by quadrupole mass spectrometry [4]. The excitation scheme is

$$2s\,^2S_{1/2} \;\rightarrow\; 3s\,^2S_{1/2} \;\rightarrow\; 2p\,^2P_{1/2,3/2}\,, \;\; 2p\,^2P_{3/2} \;\rightarrow\; 3d\,^2D_{3/2,5/2} \;\rightarrow\; \mathrm{Li}^+,$$

where the light for the two-photon step at 735 nm is provided by a titanium-sapphire laser. The efficient excitation is decoupled from this part to avoid strong AC-Stark broadening and shift by spontaneous decay to the $2p$ states. The light for the $2p \rightarrow 3d$ excitation at 610 nm is provided by a dye laser, whereas both lasers contribute to the non-resonant ionization. Relatively high laser power is needed for the first and final step. Therefore both lasers are enhanced in a resonant optical cavity. A reference frequency is provided by frequency-modulation saturation spectroscopy on iodine. A description of the stabilization chain is given in [5].

The isotope shifts of the isotopes ^{6}Li to ^{9}Li were determined at the online mass separator at GSI with an accuracy better than 180 kHz. The extracted nuclear charge radii decrease monotonically. This can be explained by the strong $\alpha + d$ clustering of ^{6}Li, which diminishes with the increasing number of neutrons. The results are compared to predictions of different nuclear models and improve the understanding of the structure of these nuclei. With this experiment, the foundation is laid to determine the charge radius of ^{11}Li.

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ORAL SESSION S10

On the Construction and Evaluation of a Information Theory Based Similarity Index for Atoms from Numerical Hartree Fock Wave Functions

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In our work we investigate Quantum Similarity for atoms from electron densities and shape functions. Our goal is to construct a Similarity Index that reveals the periodicity of the physical and chemical properties through the Mendeleev's periodic table. Earlier work showed that the mear application of the Carbo Similarity Index[1], used for comparing molecular systems, does not show the sought characteristics, masking indeed periodicity. Inspired by some recent publications we introduced the concept of Information Entropy in this framework[2]. We found that evaluating this information theory based functional for each atom, with its core as reference, uncovers the expected periodicity through Mendeleev's Table. Improved results are obtained when the shape function is used to evaluate the Entropy functional. This confirms and strengthens the fundamental role of the shape function as carrier of information[3].

We are currently devising a similarity index, based on the entropy functional, aiming for a periodic similarity index. The density and shape functions are evaluated for the atomic systems under investigation from non-relativistic numerical Hartree-Fock wave functions calculated by using the Hartree-Fock code extended to partially filled f-subshells[4], needed in the rare-earth elements. We are planning to investigate the relativistic effects on the similarity of the atomic systems through the Similarity Index, using fully relativistic wave functions calculated with the Multiconfiguration Dirac-Fock package[5].

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Photoionization with excitation and double photoionization of Li^+ ions

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Photoionization of atoms and ions resulting in the ejection of two or even more electrons cannot occur in the absence of electron-electron correlations due to the single-particle nature of the dipole interaction. This is the reason why double and multiple photoionization processes serve as sensitive probes of electron-electron correlations in both the initial bound and final continuum state. The most basic of all these processes is double photoionization of two-electron systems such as He atoms and Li^+ ions. This process is known as the three-body Coulomb problem and, in full, requires an accurate description of the correlated motion of two electrons in the long-range Coulomb field of the residual stripped atom and ion, respectively. Although this process comprises the interaction of just three charged particles, it can only be handled numerically.

While double photoionization of He has been thoroughly investigated both experimentally and theoretically, the situation for double photoionization of ions of the He isoelectronic sequence, which are of importance in plasma physics and astrophysics, is much less advanced, primarily due to difficulties in attaining target densities sufficient to carry out experiments. Nonetheless, plans are afoot to do extensive experimental studies on Li^+ [1].

To guide experimentalists, we have calculated partial cross sections for photoionization with excitation of Li^+ leaving the remaining bound electron in the 1s, 2s, 2p, 3s, 3p, and 3d states and total cross sections for double photoionization employing the well established time-dependent close-coupling method [2, 3]. The six-dimensional total wavefunction is propagated in time using a numerical lattice for the two radial coordinates and coupled channel expansions for the four angular coordinates. The calculations include both the ground state $1s^2\ ^1S$ and the two lowest metastable excited states $1s2s\ ^{1,3}S$. Photon energies below and up to about 200 eV above the respective thresholds for double ionization are considered. Comparisons are drawn mainly with convergent close-coupling results [4] and B-spline based R-matrix results [5].

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Two-photon inner-shell detachment: Li^-

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The dynamics of negative ions is of great interest to atomic physicists as the binding of the extra electron is strongly influenced by electron-electron interactions. In recent years, investigations of the properties of negative ions have been extended to study the photodetachment of inner-shell electrons. One of the ions for which this process has been investigated is Li^-. After detachment of a 1s electron, the residual Li atom is left in a doubly excited state, which decays through autoionization. The end result of the inner-shell photodetachment process is thus a Li^+ ion. Experimental yields for Li^+ creation following photodetachment of a 1s electron from Li^- have been compared to theoretical cross sections for inner-shell photodetachment [1,2]. Good agreement between experiment and theory was found except close to thresholds, where the photoelectron leaves with very small energy. The reason for this difference was subsequently found to be recapture of this slow electron by the Li^+ ion created after autoionization [3].

Recent developments in X-ray laser sources will enable the study of inner-shell processes at higher intensities and enable multiphoton processes to take place. Recently, free-electron lasers have been used to study the dynamics of small clusters in intense VUV light fields [4], but the aim is to develop free-electron lasers capable of generating intense light fields with photon energies approaching 200 eV. These fields would enable the simultaneous absorption of many X-ray photons. In these high-frequency fields, one cannot ignore the response of the inner electrons to the laser field. However, multiphoton processes have at present only been investigated for valence-shell electrons. The reason for this is obvious: with several orbitals significantly influenced by the laser field, accurate calculcations demand an explicit multi-electron approach. Hence we apply the R-matrix Floquet approach, which uses R-matrix theory to account for the atomic structure, and the Floquet-Fourier Ansatz to account for the laser field [5].

Using the R-matrix Floquet approach, we have determined two-photon detachment rates for the 1s electron in Li^-. The two-photon spectra show significant structure just above the three lowest doubly-excited thresholds of Li, $1s2s^2\ {}^2S^e$, $1s(2s2p\ {}^3P^o)\ {}^2P^o$, and $1s(2s2p\ {}^1P^o)\ {}^2P^o$, while little structure is seen above the higher three thresholds included in the calculations. Two-photon detachment of the 1s electron with excitation of the $1s2s^2\ {}^2S^e$ threshold is dominated by the emission of s electrons, since the emission of d electrons is suppressed due to the angular momentum barrier. We also investigate whether it is possible to observe this two-photon detachment of an inner electron experimentally.

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KLL dielectronic recombination of highly charged $Hg^{75+...78+}$ ions

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The photorecombination of highly charged (few-electron) mercury ions was studied theoretically and compared to experimental data measured at the Heidelberg electron beam ion trap (EBIT). In the two-step process of dielectronic recombination (DR) a free electron is captured into an ion with the simultaneous excitation of a bound electron. The energy E_{res} of the free electron at resonance fulfills the energy conservation condition $E_{res} = E_d - E_i$, with E_i being the energy of the initial ionic bound state (N electrons) and E_d being the energy of the excited intermediate state d with $N + 1$ electrons. In the range of 46 to 52 keV one finds DR resonance peaks associated with KLL transitions. Here a free electron is captured into the $n = 2$ shell while an $n = 1$ electron is lifted to the $n = 2$ shell. In the second step the excited electronic state decays to a bound final state f under emission of x-ray photons of energy $E_d - E_f$.

We present results for KLL DR resonance energies and x-ray energies for initial charge states ranging from He-like to B-like. The multiconfiguration Dirac-Fock (MCDF) method [1] was applied to calculate relativistic level energies for the ground states, singly- and doubly excited states involved in the process. We used the GRASP (General-Purpose Relativistic Atomic Structure Program) [2] implementation of the MCDF method. The convergence of self-consistent field calculations was analyzed by systematically extending the basis of configuration states [1] for the individual levels.

Experimental excitation energies have been determined [3,4] in the EBIT [5] with uncertainties as small as ±5 eV, allowing to clearly identify several individual KLL resonances. X-ray energy measurements have error bars of 14 eV at 70 keV. The experimental results for excitation energies, fine-structure splittings of doubly-excited states and radiative transition energies show a good agreement with theory. The spectral information enhances our understanding of a number of physical effects such as electron correlation in relativistic systems, finite nuclear size effects as well as QED contributions.

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POSTER SESSION P1

Mn II transitions of astrophysical importance

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We present results of extensive configuration interaction calculations of absorption oscillator strengths for transitions in Mn II from the $a\,^7S_3$ ground state to the lower $^7P^o_J$ and $^5P^o_J$ states. Of particular importance are the weak transitions to the $y\,^7P^o_J$ and $x\,^7P^o_J$ levels, which themselves strongly interact. These weaker lines are crucial in defining the interstellar abundance of Mn. Due to their proximity, we investigate their respective labelling to see if the $3d^4 4s4p$ does lie below the $3d^5 5p$, as claimed by [1]. A selection of these results is shown in the following table:

Table 1: Comparison of f-values and A-values for $a^7S_3 -^7 P^o_J$ transitions

g_l	g_u	ΔE (cm^{-1})	f-values		A-values ($\times 10^8\,\mathrm{s}^{-1}$)	
			Present	[2]	Present	[2]
$a\,^7S_3 - z\,^7P^o_J$						
7	5	38366.18	0.216	0.198	2.96	2.72
7	7	38543.08	0.304	0.280	3.00	2.78
7	9	38806.67	0.394	0.361	3.08	2.82
$a\,^7S_3 - y\,^7P^o_J$						
7	5	83255.79	0.084	0.121	5.40	7.85
7	7	83375.63	0.116	0.169	5.38	7.85
7	9	83529.33	0.148	0.181	5.36	7.85
$a\,^7S_3 - x\,^7P^o_J$						
7	5	85895.30	0.0083	0.0047	0.569	0.324
7	7	85960.43	0.0126	0.0072	0.623	0.355
7	9	86057.44	0.0180	0.0102	0.690	0.390

Comparisons have been made with atomic data quoted by Kurucz [2], with significant discrepancies being found in the two weaker lines. We have also extended these calculations to examine intercombination lines of the form $a\,^7S_3 - {}^5P^o_J$, and again comparisons have been made with [2], as well as another examination of the ordering of the higher states.

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$4d$ photoabsorption spectra of indium ions (In II -In IV)

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Indium and its ions have received much interest due to numerous applications such as solid state laser media, as an optical frequency standard [1] and as transparent electrodes, for example indium-tin-oxide (ITO) in liquid crystal displays. Future applications in the semiconductor industry include thin-film solar cells such as $CuInS_2$ [2] in which indium plays a crucial role. Previous studies along the indium isonuclear sequence include optical emission [3] and photoabsorption [4] in In II and emission in In III [5-7] and In IV [8,9]. Analysis of the Ag I isoelectronic sequence [10] and the Pd I isoelectronic sequence [11] suggested strong configuration interaction was present in In III and In IV.

The photoabsorption spectra of singly to triply ionized indium has been recorded using the dual laser plasma (DLP) technique [12]. Photoexcitation from the $4d$ subshell is the dominant process in the 24.5 - 55 eV photon energy range. With the aid of Hartree-Fock calculations [13] the lines recorded in the photoabsorption spectra of In II - In IV are identified as $3p^6 4d^{10} 5s^x \rightarrow 3p^6 4d^9 5s^x \, np \, , mf$ where $x = 2$ for In II, $x = 1$ for In III and $x = 0$ for In IV and $n = 6 \rightarrow 11$, $m = 5 \rightarrow 13$. The data substantiate and add to previously classified lines in In II and In IV while many new lines are identified in In III for the first time.

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The 3p photoabsorption spectra of Mn IV

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Atomic photoionization of free iron-group elements in the region of inner shell 3p-3d giant resonances has received much interest in the past. EUV photoabsorption and photoion spectra of singly charged ions of chromium [1,2,3], manganese [4,1,6] and theoretical studies [7,8] gave rise to much debate. A recent photoabsorption experiment by Kilbane et al [9] confirmed Dolmatov's predictions [7], that between Mn^{+} and Mn^{2+}, not only do the 3p-4s resonances swap over to the high energy side of the giant 3p-3d resonance but also that this reordering has significant effects on the resonance profiles. Recently there have been many studies on the electronic structure and magnetic properties of compounds containing transition-metals, e.g. a perovskite manganite such as $LaMn0_3$ [10]. The starting point of a theoretical description of such manganites is knowledge of the electronic structure of the free Mn^{3+} ion.

Here we investigate the spatial and temporal evolution of a manganese plasma while concentrating on the Mn^{3+} ion. The dual laser plasma (DLP) technique [11] was used to record the Mn^{3+} spectra in this experiment. Isolation of this ion was achieved at an optimum position of 1 mm from the optic axis and time delay of 30 ns. The main features of the experimental spectrum are reproduced using configuration-interaction Hartree-Fock calculations [12]. The synthetic spectra allow for absorption from excited states of the Mn^{3+} ground state configuration weighted by an appropriate plasma temperature.

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Disentanglement of magnetic field mixing reveals the spontaneous M2 decay rate for a metastable level in Xe^+

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We have investigated the radiative decay of the metastable level 5d $4D_{7/2}$ in Xe+ both experimentally and theoretically. The calculations show unexpectedly that the decay is heavily dominated by an M2 transition and not by M1/E2 transitions as previously anticipated. Experimental determination of the radiative lifetime in an ion storage ring is difficult in this case since its population is strongly quenched by magnetic mixing between the metastable and a short-lived level. Careful measurements of decay rates by laser probing technique [1] were performed at different magnetic field strengths (B) in CRYRING and made it possible to extract the radiative lifetime. Due to the strong magnetic quenching, the extraordinary situation occurs that requires both the linear and quadratic dependence on the magnetic field to be considered. From such a non-linear extrapolation to B=0, an experimental lifetime of 2.4 0.8 s was obtained in good agreement with the calculated value of 2.3 s, but two orders of magnitude smaller than previously estimated [2,3].

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Fine-structure energy levels, oscillator strengths and lifetimes in Co XV

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Energy splittings of 54 fine-structure levels as well as oscillator strengths and transition probabilities for all 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, $3s^24$s, $3s^24$p, $3s^24$d, $3s^24$f and 3s3p4s configurations of Al-like cobalt are calculated using extensive configuration-interaction wave functions obtained using the CIV3 computer code of Hibbert [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. Our excitation energies, including their ordering, are in excellent agreement with the available experimental results [3,4], also predicting new data for several levels where there are no theoretical and/or experimental results available. The mixing among several fine-structure levels is found to be very strong.

From our transition probabilities, we have also calculated radiative lifetimes of some fine-structure levels and the results are compared with the experimental data and the other available calculations. Our calculated lifetimes (in ns) of 3s3$p^2(^4P_{0.5,1.5,2.5})$ levels (18.58; 106.94; 25.96) are in excellent agreement with the corresponding experimental values (18±1; — ; 26±1.5) of Trabert et al. [5] and the theoretical results (20.1; 107; 26.9) of Huang [6].

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Extended fine structure analysis of the even configuration system of Pr I

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Praseodymium belongs to the lanthanide group, where spectroscopic properties are determined by the fact that the binding energies of 4f, 5d, 6s, and 6p electrons are of the same magnitude. This gives rise to several overlapping configurations and strong configuration mixing effects arising in the fine and the hyperfine structure of Pr. For these reasons the apparently simple interpretation of relatively low lying levels becomes complicated and requires very systematic analysis performed in a many-configuration approximation.

The even-parity configuration system of Pr I has been considered on the basis of the experimental data available. Our fine structure analysis of the system consisting of the 15 even configurations

$$\sum_{n=6}^{8} 4f^3 6snp + \sum_{n'=5}^{7} 4f^3 6sn'f + \sum_{n''=6}^{8} 4f^3 5dn''p + 4f^2 5d6s^2 +$$

$$+4f^2 5d^2 6s + 4f^2 5d^3 + 4f^2 6d6s^2 + 4f^2 6p^2 6s + 4f^2 5d6s7s$$

has been performed with the use of a semi-empirical method. The fine structure parameters have been determined, the wavefunctions of the even energy levels have been evaluated and more than 500 observed levels have been classified. Extremely strong configuration mixing effects have been observed and will be discussed.

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Multiconfiguration calculation of the hyperfine structure of Vanadium

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The hyperfine structure of the low lying levels of Vanadium are known from experiment. Semiempirical calculations for the hyperfine structure exist resembling the experimental results within some MHz. Pure *ab initio* calculations are under survey by our group in order to gain deeper understanding of the correlation and relativistic effects of the $3d$ metals. The aim is not only to calculate the hyperfine structure to higher accuracy but also to compare the interactions with diagram techniques used in semiempirical and perturbational calculations. We use the multiconfiguration approach based on the improved ATSP MCHF [1, 2, 3] package and GRASP92 [4].

The ground state of Vanadium has the configuration $[Ne]3s^2 3p^6 3d^3 4s^2$. Valence, core, valencevalence, corevalence and corecore correlaton effects are examined by orbit to orbit excitations to extended complex. Combinations of these correlations are calculated and compared with configuration interaction calculations. Nonrelativistic and relativistic calculations are compared.

The method used allows to track down the most important orbital correlations and effects of the correlations with each other. The influence on the hyperfine structure constants can be observed and relativistic effect deduced.

While semiempirical calculations [5] suggest a strong interaction of $3d^{3+m}4s^m$ $m = 0, 1, 2$ configurations, it is unimportant for the nonrelativistic MCHF calculation for the groundstate ^4F. Dominant influence is due to single valence excitations to complex $\{4\}$ and $\{5\}$. The core excitations alone has an influence mainly for complex $\{5\}$ but show strong interaction with the valence correlation. On the other hand the valence correlation is almost not affected by core correlation, a result verified also by configuration interaction calculation. Valencevalence correlation is of minor importance while corecore and valencecore are unimportant. Some analogies with diagram techniques are drawn.

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Transitions in Gallium II

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This poster reports extensive CI calculations of the lifetimes of the 4s4p $^{1,3}P^o_1$ in Ga II. Results were previously calculated by Fleming and Hibbert [1] using a model potential to represent the core-valence interaction. However more recent results by Karlsson and Brage [2] using the MCHF+BP method of Froese Fischer [3] suggest that the calculations of [1] may not be as accurate as required. Karlsson and Brage [2] calculated their results from an ab initio MCHF calculation. They allowed the n=3 shell to be open and so including core polarisation by means of explicit CI.

In this work we report large scale systematic calculations using the CIV3 [4] code. We have also refined the ab initio calculation by making small adjustments to the Hamiltonian matrix in order to produce the experimental energy separations and so improve the accuracy of the results. Relativistic effects were introduced using the Breit-Pauli Hamiltonian. Some of the results are shown below.

Comparison of lifetimes (ns)

	4s4p $^1P^o_1$	4s4p $^3P^o_1$	4s5s $^1S_0$
Calculations			
This work	0.528	3090	2.73
[2]	0.527	2955	2.83
[1]	0.493	2445	
[5]		3090	
Experiment			
[6]	0.48±0.12		2.55±0.15

Oscillator strengths of a number of other transitions were also calculated and will also be included on the poster.

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Vacuum-UV absorption spectra from a laser-produced chromium plasma: 3p-subshell photoabsorption of Cr^{3+}

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The photoionisation spectra of the iron group elements have been the subject of intensive research [1,2], not just because there is an intrinsic interest in the sensitivity of 3d wavefunction localization here, but also photoionisation data from the iron group elements have practical importance, for example, in providing insights into the electronic and magnetic properties of surfaces and thin films [3]. The following report presents the time resolved vacuum-UV photoabsorption spectra of chromium ions in a plasma obtained by employing the dual laser plasma technique [4].

Past studies on neutral and singly ionized chromium [5,6], resulted in theoretical debates on the assignment of structure in the experimental data. The presence of metastables was introduced to this debate which added to the complexity of the Cr^+ spectrum. In this report the photoabsorption measurements of Cr^{3+} ions were taken at photon energies from 40 to 70eV, where the dominant absorption mechanism is excitation from the 3p subshell. Performing Hartree-Fock (HF) calculations using the Cowan suite of codes [7], discrete structure due to 3p - 4s, 5s excitations were identified, while the broad resonance was ascribed to 3p - 3d excitations.

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Autoionizing Ne($2p^5_{1/2}np', J = 0$) Rydberg series: Comparison of experiment and *ab initio* theory

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The importance of maintaining the orthogonality between the wave functions of the ground state and excited states with the same symmetry is illustrated by comparison of ab initio computations of the shape of autoionizing $2p^5_{1/2}np'$ J = 0 resonances in Ne with experiment. The reduced width Γ_r and the quantum defect μ_p, computed for the $2p^5_{1/2}13p'$ J = 0 resonance within the CIPFCP approach [1,2], are $\Gamma_r = 6431$ cm^{-1} and $\mu_p = 0.7634$ with the requirement $\left\langle 2p^5_{1/2}np' \text{ J} = 0 \right| \textit{ground state} \rangle = 0$ (realized via a technique described in [3,4]). These results differ strongly from the values $\Gamma_r = 1887$ cm^{-1} and $\mu_p = 0.7850$, computed without the orthogonality condition. Another aspect of the present calculation are the positions of Cooper minima (modified by many-electron correlations) located close to the $2p^5_{1/2}np'$ J = 1, 2 resonances; they provide a sensitive test of the theoretical approach.

The $2p^5_{1/2}np'$ J = 0, 1, 2 autoionizing Rydberg states (ARS) have been studied by two-step two-color ionization of ground-state neon atoms via the intermediate states $2p^5_{3/2}3s$ J = 1 and $2p^5_{1/2}3s'$ J = 1 followed by time-of-flight ion detection [5]. The intermediate state was populated by narrow-band vacuum ultraviolet radiation obtained by four-wave mixing of the frequency-doubled and -tripled output of two pulsed dye lasers. The ARS were then accessed by the frequency-doubled output of another pulsed dye laser (UV bandwidth 0.15 and 0.06 cm^{-1}, respectively). The spectra can be fully accounted for by multichannel quantum defect theory (MQDT) using known MQDT parameters and the relative values of the transition moments derived from measurements of the radiative lifetimes of the intermediate states.

The measured lineshape of the np' J = 0 resonances is also in very good agreement with the ab initio computation: a Fano-type lineshape analysis yields $\Gamma = 5334$ cm^{-1} and $\mu_p = 0.7662$, which clearly shows the importance of the above mentioned orthogonality condition. The reduced widths and quantum defects for the np' J = 1, 2 resonances are in good agreement with our previous finding [6]. Comparison between measured and computed relative intensities of the np' J = 0 and np' J = 1, 2 resonances leads to the conclusion that our previously used core polarization potential [6] is slightly too weak.

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Competition between multiphoton emission of the 1s and 2s electron from the 1s2s ^{1}S state of He

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He is the simplest atom in which the interaction between electrons plays an important role. These interactions continue to play an important role when He is subjected to an intense laser pulse. One of the most striking observations of the influence of the electronic interaction has been the increased probability for double ionization beyond single-active-electron models [1]. The development of X-ray laser sources will provide a new approach to studying laser-matter interactions, as demonstrated for example in [2]. In high-frequency laser fields, the electron-electron interaction will continue to play a major role through, for example, the possibility of exciting doubly excited or triply excited states.

R-matrix Floquet theory has proven to be very successful in accurately describing the interaction between intense laser fields and atoms. R-matrix Floquet theory uses R-matrix theory to describe the atomic structure and the Floquet-Fourier Ansatz to describe the interaction with the laser field [3]. Typical outcomes of an R-matrix Floquet calculation are the energy and width, including a breakdown into partial widths, of a state of the atom at a particular choice of frequency and intensity. Recent studies employing R-matrix Floquet theory include the investigation of two-photon double ionization of He [4], and multiphoton ionization studies of Ca, K^-, Ne and Ar [5-7]. As these studies demonstrate, the theory can in principle be applied to any atomic system. One of our present interests is thus the investigation of multiphoton processes in X-ray laser fields, including the excitation and emission of inner-shell electrons.

In the present study, we investigate the simplest system which contains an outer and an inner electron: the 1s2s ^{1}S state of He. When He in this state is subjected to a intense X-ray laser field, both the 1s and the 2s electron can be emitted. In the present investigation, we compare multiphoton emission rates of the 1s electron with multiphoton emission rates of the 2s electron for the same number of absorbed photons. We demonstrate that for single-photon and two-photon ionization, emission of the 1s electron is more likely than emission of the 2s electron, while the opposite is seen for three- and four-photon ionization.

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Multiphoton ionization of neon and argon at 390 nm

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The experimental study of the atomic response to intense laser fields has mainly focused on three atoms, He, Ne and Ar. Most theoretical investigations investigating the atomic dynamics in intense laser fields have, however, focused only on the helium atom, since the most common approach used to study the dynamics is the time-dependent solution of the Schrödinger equation. While this approach is capable of providing results with excellent accuracy for two-electron systems [1], it is very difficult to extend this approach to atoms with more than two electrons. On the other hand, the R-matrix Floquet approach [2], which transforms the time-dependent Schrödinger equation into a time-independent one, is an approach well suited to describe complex multi-electron systems in intense laser fields as it is designed to do so. A recent application of the R-matrix Floquet approach was a comparison of photoionization rates for He subjected to 390 nm light with rates obtained by the most sophisticated time-dependent approach to solving the intense-field Schrödinger equation for He [3]. While photoionization, at intensities above 9×10^{13} W/cm^2 requires absorption of at least nine photons, the agreement between both approaches is typically within 10%.

The most detailed R-matrix Floquet study of Ne and Ar has been an investigation of harmonic generation at the KrF wavelength [4], while at QUB we have carried out a study of two- and three-photon ionization [5]. This latter study demonstrated that the Rydberg series converging onto the $3s3p^6$ threshold need to be included for two-photon ionization of Ar, as the $3s3p^6n\ell$ Rydberg states appear prominently in the two-photon ionization spectrum. For three-photon ionization, some small effects due to these excited states are still noticeable, but their influence is greatly reduced.

In the present investigation, we extend our previous work on multiphoton ionization of Ne and Ar to a wavelength of 390 nm at intensities around 10^{14} W/cm^2. Near this intensity, the minimum number of photons that need to be absorbed to achieve ionization is 8 for Ne and 6 for Ar. Because of the increased number of photons that need to be absorbed to achieve ionization, the Floquet expansion needs to be expanded, both in terms of the number of Floquet blocks and number of angular momenta retained. As a consequence, the atomic structure description needs to be reduced in order to keep the size of the calculations manageable: we use a single target state for Ar^+. The influence of this reduction is examined for six-photon ionization of Ar at low intensities, and is found to be insignificant. We compare our photoionization rates with photoionization rates obtained through the ADK formalism [6] to assess whether this formalism is capable of predicting ionization yields accurately.

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Kr in Intense Ultrashort Laser Pulses: Effects of Ellipticity on NonSequential Ionization

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The phenomenon of non-sequential double ionization is a continuing area of research. Presented here is a study of recollision in Kr^{2+} ions, produced in an intense ($>10^{16}$Wcm^{-2}) ultrafast (55fs) laser field. It is well documented that recollision occurs when the laser field is linearly polarized, but not when it is circularly polarized [1]. An ionized electron can be driven back along its path to the nucleus and cause further ionization if the field is linearly polarized. However if the field is circular, the electron will be deflected from its path and be unable to return to the nucleus. This experiment uses elliptically polarized light to control the motion of the electron wavepacket in a laser field.

Neutral Kr atoms were ionized in the interaction region of a time-of-flight mass spectrometer. A detailed description of the experimental apparatus is given elsewhere [2]. An Intensity Selective Scanning (ISS) technique [3] was used to produce results with high spatial resolution. The ion yields of Kr^+ with linear and circular polarizations were normalized using effective intensity matching [4]. Ion yields for elliptical polarization were also intensity matched using this method to enable a direct comparison of all results.

Secondary ionization due to recollision is extracted from the data by subtracting the circular from the linear Kr^{2+} yield. This removes contributions from both primary ($\hbar\nu$ + Kr $\rightarrow$ Kr^+ + e) and sequential ($\hbar\nu$ + Kr^+ $\rightarrow$ Kr^{2+} + 2e) ionization. Thus non-sequential contributions are obtained as a function of ellipticity. The results will be presented at the conference, demonstrating that the returning electron becomes increasingly efficient at re-ionizing the nucleus as the field changes from circular to linear.

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Partial wave analysis of interfering resonance Auger (RA) transitions in the Raman regime with special emphasis of the contribution from direct processes

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The experimental dependence of the orientation parameter O_{10} of the Kr+ $3p^4(^1D)5p^2P_{3/2}$ state, populated in the decay of the Kr $3d^9{}_{5/2}5p_{3/2}$, $3d^9{}_{3/2}5p_{1/2}$, $3d^9{}_{3/2}5p_{3/2}$, $3d^9{}_{5/2}6p_{3/2}$ resonances, was measured for energies between 90.8 eV and 92.65 eV. The bandwidth of the exciting circularly polarized undulator radiation was 15 meV allowing a study of the energy dependence within the natural line width of the absorption resonances of about 80 meV.

The experiments were carried out at the UE56/PGM beam lines of BESSY II applying photon-induced polarization fluorescence spectroscopy. This technique allows the determination of the relative contribution of the three contributing electron partial waves through the measurement of the alignment parameter A_{20} and orientation parameter O_{10} of the photoion [1].

The comparison of the experimental values with calculations [2] confirms the interference between the resonant and the non-resonant direct excitation process. This interference was predicted to be observable for ion states with total angular momentum J = 3/2. Ion states with J > 3/2 show interference of partial waves from resonances overlapping due to lifetime broadening. For the studied $3p^4(^1D)5p^2P_{3/2}$ state both interference mechanism contribute which manifests itself in a different energy dependence of the orientation parameter when compared to the observed behaviour of the $3p^4(^1D)5p^2D_{5/2}$ state.

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Accurate laboratory UV wavelengths from seven species of interest to the investigation of a possible space-time variation of the fine structure constant

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The quality of astronomical spectra is now so high that the accuracy of the laboratory data is getting more important for the analysis and interpretation. One of the methods of investigating possible space-time variations of the fine structure constant, $\alpha = (1/\hbar c)(e^2/4\pi\epsilon_0)$, is the many multiplet method. The use of this method requires very accurate laboratory wavelengths of several spectral lines visible in high redshift QSO absorption spectra. A change in α could be detected as a shift in wavelengths of atomic transitions in the QSO systems. For this purpose laboratory wavelengths and wavenumbers of 23 UV lines from Mg I, Mg II, Ti II, Cr II, Mn II, Fe II and Zn II have been measured using high-resolution Fourier transform spectrometry. The spectra of the different ions (except for one Fe II line, one Mg I line and the Ti II lines) are all measured simultaneously in the same FTS recording by using a composite hollow cathode as a light source. This increases the relative accuracies of all the wavenumbers.

The calibration accuracy is limited by the standard of the Ar II calibration lines, by possible pressure shifts and by effects of illumination. To ensure a minimization of pressure shifts of the calibration lines, only 4s-4p transitions of Ar II [1] are used. The absolute wavenumber uncertainties are ± 0.001 and ± 0.002 cm^{-1} for the symmetric lines with good signal to noise ratio, ± 0.010 cm^{-1} for the weaker lines and ± 0.005 cm^{-1} for the asymmetric, hyperfine affected Mn II lines. The relative wavenumbers are for the strong lines determined with an uncertainty of ± 0.0005 cm^{-1} or better, depending mostly on the uncertainty of the line fitting.

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4d photoabsorption spectra of neutral and low ion stages of Sn at the EUVL source wavelength, 13.5 nm

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A laser produced Sn plasma is currently one of the major contenders as a high-power source for future high-volume-manufacturing extreme ultraviolet lithography (EUVL) systems based on the requirement of high radiation intensities at 13.5 nm [1], the wavelength of choice for EUVL. Alternative sources include laser produced plasmas or pulsed discharge plasmas containing either xenon or lithium. However it has recently been shown that higher conversion efficiencies can be obtained with tin based plasmas within this wavelength regime [2], thereby making it the source with most future promise.The demand for photoabsorption spectra of the low ion stages of tin in the aforementioned spectral region is motivated mainly by the need for such data in current radiation transport models of Sn laser produced plasmas. It is known that EUV photoabsorption due to 4d $\rightarrow \epsilon$f shape resonances within the lower ion stages of xenon reduces the photon flux from a xenon source[3]. The corresponding resonances for Sn I - IV have been recorded by means of the time honoured dual laser plasma (DLP) technique[4] whereby the ions produced by one laser pulse are backlit by EUV continuum radiation from a second laser pulse.It is also found that above the 4d ionization threshold the spectra of Sn I - IV are dominated by a 4d $\rightarrow \epsilon$f shape resonance which peaks at close to 65 eV in eachcase. A transfer of oscillator strength from the shape resonance to pseudo - discrete 4d $\rightarrow$ nf transitions with increasing ionization is clearly evident. Hartree Fock with configuration interaction and many body relativistic time dependent local density approximation calculations successfully account for this behaviour and also allows the identification of the discrete features.

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Exact Nondipole Kramers-Henneberger Form of the Light-Atom Hamiltonian: An Application to Atomic Stabilization and Photoelectron Energy Spectra

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The exact nondipole minimal-coupling Hamiltonian for an atom interacting with an explicitly time- and space-dependent laser field is transformed into the rest frame of a classical free electron in the laser field, i.e., into the Kramers-Henneberger frame. The new form of the Hamiltonian is used to study nondipole effects in the high-intensity, high-frequency regime. Fully three dimensional nondipole *ab initio* wavepacket calculations show that the ionization probability may decrease for increasing field strength. We identify a unique signature for the onset of this dynamical stabilization effect in the photoelectron spectrum.

Doppler-free Two-Photon Spectroscopy of the $6D_{3/2} \leftarrow 6S_{1/2}$ Transition in Cesium Using a Titanium Sapphire Laser

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Many researchers have investigated the hyperfine structure of the higher states in various atoms and molecules to find a frequency standard for developing an optical frequency stabilized laser system[1],[2]. The two-photon method, nonlinear spectroscopic technique, is very effective for obtaining Doppler-free spectra, and can be used a frequency standard because the spectral lines are narrow enough to be used as discrimination signals[3]. This method eliminates the Doppler effect and reduces frequency shifts caused by closed lines. Spectroscopic forbidden transitions can also be observed, whose selection rules are $\Delta J = \pm 2$ or $\Delta F = \pm 2$.

Doppler-free two-photon spectra for the $6D_{3/2}(F' = 2 \text{ to } 5) \leftarrow 6S_{1/2}(F'' = 3)$, $6D_{3/2}(F' = 2 \text{ to } 5) \leftarrow 6S_{1/2}(F'' = 4)$, $6D_{5/2}(F' = 5 \text{ to } 1) \leftarrow 6S_{1/2}(F'' = 3)$ and $6D_{5/2}(F' = 6 \text{ to } 2) \leftarrow 6S_{1/2}(F'' = 4)$ transitions in cesium were observed using a titanium-sapphire laser. These spectra can be used as an optical frequency standard.

The splittings of the spectral liens were detemined by the side band signals generated by EOM. Table 1 shows the hyperfine splitting for the $6D_{3/2}$ and $6D_{5/2}$ excited states.

Table 2: Hyperfine splitting of the $6D_{3/2}$ and $6D_{5/2}$ excited states in cesium. Units are in MHz.

$6D_{3/2}$				$6D_{5/2}$			
F''	F'	Obs.	Diff.	F''	F'	Obs.	Diff.
4	5-4	81.15(84)	0.22	4	6-5	-27.93(35)	-0.51
	4-3	64.18(51)	-0.46		5-4	-22.40(8)	0.43
	3-2	48.76(64)	0.33		4-3	-18.57(21)	-0.40
					3-2	- -	
3	5-4	81.17(41)	0.33	3	5-4	-22.57(31)	0.25
	4-3	64.02(51)	-0.62		4-3	-17.85(12)	0.32
	3-2	49.02(85)	0.60		3-2	-14.07(36)	-0.49
					2-1	-8.97(39)	0.11

The hyperfine coupling constants of A (magnetic dipole constant) and B (electric quadrupole constant) were determined using the spectral line splittings, giving $A = 16.17(17)$ MHz and $B = 0.11(127)$ MHz for the $6D_{3/2}$ state and $A = -4.56(9)$ MHz and $B = -0.35(183)$ MHz for the $6D_{5/2}$ state.

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Atomic data for Os I and Os II

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Transition rates in neutral and ionized osmium are still very sparse. In Os I, the only f-values available are those of Corliss and Bozman [1], those derived from the lifetime measurements of Kwiatkowski *et al.* [2] and a recent determination for 18 transitions by Ivarsson *et al.* [3]. Some compilations have also been reported by Doidge [4] for resonance lines and by Morton [5] for transitions of astrophysical interest longward of the Lyman limit. In Os II, the Corliss and Bozman [1] measurements have been superseded by more accurate results obtained by Leckrone *et al.* [6] and, more recently, by Ivarsson *et al.* [7]. In the latter case, oscillator strengths of 27 Os II transitions have been determined by combining experimental radiative lifetimes obtained by laser spectroscopy with branching fractions measured using a Fourier transform spectrometer.

In the present work, radiative lifetime measurements have been performed, with a time-resolved laser-induced fluorescence technique, for 12 levels of Os I and for 9 levels of Os II. For 9 levels of Os I and 4 levels of Os II, there were no previous experimental data available. From a comparison with new theoretical calculations, taking configuration interactions and core-polarization effects into account, it has been possible to deduce oscillator strengths for 129 transitions of Os I and 137 transitions of Os II of astrophysical interest appearing in the wavelength range 180 - 870 nm.

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Radiative lifetimes and transition probabilities in singly ionized rhenium (Re II)

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There has been, during the past few years, strong motivations for investigating the abundances of heavy elements in chemically peculiar stars in relation with their interest for nucleosynthesis. The high resolution ultraviolet spectra of some stars (e.g. the HgMn-type star χLupi) made available with the Hubble Space Telescope Goddard High Resolution Spectrograph (GHRS) have given a strong impulse to the analysis of the chemical composition of such stars [1].

Among the heavy elements of the periodic table, rhenium has been little investigated in stellar spectra. This is directly related to the rather poor knowledge of the energy level structures of Re I and Re II and to the lack of radiative data. In addition, many Re II lines are occuring in the far UV region where little observational material was available until recently.

In the present contribution, we extend the set of lines usable for stellar abundance determinations by providing new atomic data for 45 UV transitions of Re II. The transition probabilities are deduced from a combination of lifetime measurements for 7 levels of Re II obtained using the technique of laser-induced fluorescence and theoretical branching fractions for the lines depopulating the levels of interest. These last ones have been obtained through a Hartree-Fock approach [2] taking relativistic and core-polarization effects into account.

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Photodetachment of the ground and excited states of P^-

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A high resolution measurement of the electron affinity and excited states of P^- was carried out by means of laser photodetachment. In the experiment a beam of negative ions were merged in a collinear geometry with an infra red laser beam and the wavelength of the laser was scanned across the photodetachment threshold region. We observed the photodetachment of P^- from its ground and excited states, $^3P_{2,1,0,}$ through detection of the neutral atom, $^4S_{3/2}$. A comparison with previous measurements, both theory and experiment is made. The experiment having been carried out by Slater and Lineberger [1], although significant improvements have been made in the accuracy of the measurement due to developments in experimental apparatus, not least the use of a collinear geometry.

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EIT in rubidium mismatched V-type system

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Electromagnetically induced transparency (EIT) has been the subject of many experimental and theoretical papers emerged since its first demonstration by Harris and co-workers in 1991 [1]. Different aspects of this phenomena such as realization of EIT in cascade, Λ and V-type schemes, lasing without inversion etc. have been published [2].

We investigated EIT in rubidium system using the ECDL lasers in mismatched wavelength V-type scheme where the probe beam operated at 420nm and the coupling wavelength was locked at the ^{85}Rb $5S_{1/2}$(F=2) - $5P_{3/2}$ transition. EIT was observed by monitoring the Rb $6P_{3/2}$ laser induced fluorescence (LIF). The dependence upon the power of the coupling and probe laser beams of the EIT signal was determined. In addition, temperature, external magnetic field strength and laser beams polarization dependencies were also examined.

Strong optical pumping effect was observed due to the low ground-state collisional mixing rate (the rubidium cell temperature was up to 80°C). The experimental results showed good agreement with the steady-state solution of the four-level atomic system Liouville's equation [3].

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Detection of heteronuclear molecules at thermal, cold and ultracold conditions

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Recently heteronuclear molecules have been detected at ultra cold conditions and some very interesting laser spectroscopy has been carried out for those molecules under conditions of magneto-optical traps. Heavy alkali heteronuclear molecules became very attractive recently and their observation on helium clusters is desirable, since triplet states are most prominent features in nano-cryostat conditions.

Potential curves for heteronuclear molecules are becoming better known in both cases with and without spin-orbit interaction taken into account. Singlet transitions are better known than triplet transitions in usual laser spectroscopy. However, at ultra low temperatures triplet states become more accessible and thus analysis reveal the structure of the potential curves for triplet manifold. Optical transitions within triplet states, sometimes called diffuse bands, may be used for two-photon resonance ionization scheme.

We shall discuss absorption spectra at high density alkali vapor mixture at thermal conditions, in the case of excitations from the He droplets, and under ultra cold conditions. Recent observations may contribute to the final interpretation of heteronuclear diffuse bands in the broad spectral region.

PFI ZEKE photoelectron spectroscopy of ND_3

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The pulsed-field-ionisation zero-kinetic-energy (PFI-ZEKE) photoelectron spectrum of ND_3 has been recorded in the vicinity of the first ionisation threshold following single-photon excitation from the ground state. The spectrum consists of rotationally resolved bands corresponding to transitions to the first three vibrational levels of ND_3^+ associated with the umbrella mode ($v_2^+ = 0$, 1, 2).

The rotational structure of bands with an odd v_2^+ value strongly differs from that of bands with an even v_2^+ value and are modelled theoretically using different approximations for the ionisation dynamics.

The spectra are compared with photoionisation spectra and their simulation by multi-channel quantum defect theory (MQDT). The comparison with similar spectra recorded for NH_3 [1] reveals the importance of channel interactions in the photoionisation of ammonia and its isotopomers.

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Fourier transform spectroscopy of the first triplet state of KRb

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The first triplet state $a^3\Sigma^+$ in KRb was studied for the first time by high resolution Fourier transform spectroscopy. This state plays an important role in producing and trapping of cold KRb molecules [1,2], hence its accurate spectroscopic characterisation is of actual interest.

The KRb molecules were formed in a heat-pipe oven loaded with about 5 g K and 5 g Rb (natural composition of isotopes for both elements). The strongly coupled complex of the $B^1\Pi$-$c^3\Sigma^+$-$b^3\Pi$ states [3] was excited with a single mode CR-599 dye laser (DCM dye). The laser induced fluorescence spectra to the $a^3\Sigma^+$ state in the region around 11000 cm^{-1} were recorded with a IFS120 Fourier transform spectrometer with a typical resolution of 0.015 – 0.03 cm^{-1}. More than 1400 transitions to the $a^3\Sigma^+$ state were assigned. All observed transitions in the triplet band exhibited partially resolved structure reflecting hyperfine splitting (hfs) in the $a^3\Sigma^+$ state. The hfs basically can be described within the $b_{\beta S}$ coupling scheme with dominating atomic Fermi contact interaction. However, numerous deviations from the expected hfs pattern were observed.

The presence of experimental data for the $^{39}K^{85}Rb$ and $^{39}K^{87}Rb$ isotopomers allowed us to establish the absolute vibrational numbering of the observed $a^3\Sigma^+$ state levels. Current data field covers a range of vibrational quantum numbers from v''=1 to 22 and rotational quantum numbers from N'' =12 to 124. Using these data a preliminary IPA potential [4] was constructed. Present status of the study is presented.

We would like to thank Dr. P. Staanum for the assistance in the experiments. The work is supported by DFG through SFB 407 and GRK 665. The Riga team acknowledges the support by the NATO SfP 978029 Optical Field Mapping grant and by the EC 5th Frame "Competitive and Sustainable Growth " grant G1MA-CT-2002-04063, as well as by Latvian Science Council grant No. 04.1308 and Latvian Government grants ES 03-40 and TOP 04-44. J.Z. acknowledges the support from the European Social Fund.

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Use of absorbing potentials for the calculation of partial cross sections for photofragmentation processes

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In the present contribution we investigate a variant of the method proposed by Seideman [1] for calculating partial cross sections in molecular photodissociation processes. It is based on the use of a discrete variable representation (DVR) for the dissociating coordinate and the introduction of absorbing potentials in the asymptotic region in order to provide correct boundary conditions. While the calculation of the total cross section involves only the initial bound state diagonal matrix element of the Green operator, the calculation of partial cross sections involves matrix elements between the bound and free scattering states for each specific fragmentation channel. For small systems direct diagonalization methods can be used to calculate these matrix elements but for large systems the use of various iterative procedures is necessary.

We shall present results of detailed comparisons with an exactly solvable, two-channel model problem, proposed previously by Han and Reinhardt [2] in their study of the application of the complex coordinate method in calculations of partial photoionization cross sections. This model assumes the final states of the photofragmentation process to be the eigen states of two coupled square-well potentials and allows for an analytic solution for all partial cross sections. It also illustrates excellent examples of Feshbach resonances and non-analytic (cusp) shapes of the open-channel cross sections in the threshold region.

In our recent total near-threshold photodissociation cross-section calculations of CH^+ [3] it was found that the form and characteristics of the absorbing potential become crucial as the photon frequency approaches the threshold region. The optimal choices of absorbing potentials should also be very important in their applications in super cold collisions. After testing various forms of absorbing potentials in the above mentioned model problem, we have found that the best performance in the near- threshold region is provided by the recently proposed transmission-free absorbing potential of Manolopoulos [4].

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Incoherent broad-band cavity-enhanced absorption spectroscopy of liquid samples

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A new application of incoherent broad-band cavity enhanced absorption spectroscopy (IBBCEAS) [1] to weak transitions in solution through a very straightforward modification of commercially available double-beam UV/VIS absorption spectrometers is reported [2]. The improved sensitivity of the new approach is demonstrated on basis of the weak Franck-Condon inhibited absorption of the fifth, sixth and seventh C-H stretch overtone in liquid benzene. The theoretical limits of the enhancement of the signal-to-noise ratio of IBBCEAS in comparison with single pass absorption experiments are discussed for a set of given experimental cavity parameters. The optical loss properties of a typical transparent cuvette window in the cavity are also presented.

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The influence of non-elastic processes in $H^*(n) + H$ collisions to the Rydberg states population of hydrogen atom in laboratory and astrophysical plasmas

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The influence of two groups of non-elastic processes in $H^*(n) + H(1s)$ collisions to the Rydberg states populations of hydrogen atoms in weakly ionized plasmas was investigated here. The first group consists of the chemi-ionization and chemi-recombination processes

$$H(1s) + H^*(n) \leftrightarrow \vec{e} + \begin{cases} H^+ + H(1s), \\ H_2^+, \end{cases} \tag{1}$$

and the second group - the excitation and de-excitation processes

$$H^*(n) + H(1s) \leftrightarrow \begin{cases} H^*(n' = n + p) + H(1s), \\ H(1s) + H^*(n' = n + p), \end{cases} , \tag{2}$$

where $\vec{e}$ and H_2^+ denote the free electron and the hydrogen molecular ion in the ground electronic state, the principal quantum number $n \geq 4$ and $p \geq 1$. The rate coefficients of these processes were determined, on the base of already developed semi-classical method [1], for weakly ionized laboratory and astrophysical hydrogen plasmas (ionization degree less then 10^{-3}). With help of these rate coefficients the efficiency of the mentioned processes was compared with the efficiency of the other relevant ionization/recombination and excitation/de-excitation processes. It was shown that the exchange between the excited state atom populations within the lower part of the Rydberg region of n is determined by the processes (2) while the exchange between the mentioned group of Rydberg states as a wholeness and the continuum is determined by the chemi-ionization/recombination processes (1). It is important that all mentioned is related to the plasma of the part of Sun's photosphere and lower chromosphere (the region with $T < 6000K$) [2].

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Electron collisions with Fe IV ions

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Modelling of spectra and their interpretation require both accurate transition probabilities in addition to accurate rate coefficients or effective collision strengths. Detailed electron-ion collision data are essential for the understanding of the behaviour of plasmas and for identifying electron-impact excited lines in various astronomical objects from gaseous nebulae such as Orion , symbiotic nova , quasars, Seyfert galaxies, supernovae to the Sun and enable the evaluation of electron densities, temperatures and abundances. UV and optical lines in low ionization stages of Fe have all been detected in supernovae remnants. In interstellar dust grains, the predominant destruction process is via shocks driven by supernova explosions. It is important to determine whether the observed bow shocks in the working surfaces of Herbig-Haro (HH) outflows have led to a destruction of dust grains and to a change in the gas-phase metal abundances (eg Fe) in the cooling regions of HH bow shocks. For various applications in astrophysical and laboratory plasmas it is the transitions within the $3d^5$ manifold of the Fe IV ion that are of prime interest and importance. In fact triply ionized iron Fe^{3+} is one of the dominant ionized states of iron that exist in planetary nebulae including H II regions.

Electron-impact excitation collision strengths of the Fe-peak element Fe IV are calculated in the close-coupling approximation using the R-matrix suite of codes PRMAT designed for parallel processors. One hundred and eight LS - coupled states arising from the $3d^5$, $3d^4 4s$ and $3d^4 4p$ configurations of Fe IV, are retained in the present calculations. Detailed multi-configuration interaction target wavefunctions are used with the aid of $3p^2 \rightarrow 3d^2$ electron promotions and a $4\overline{d}$ correlation orbital in the present calculations.

Effective collision strengths for optically forbidden transitions, which are extremely important in the analysis of lines in the Fe IV spectra, are obtained by averaging the electron collision strengths for a wide range of incident electron energies, over a Maxwellian distribution of velocities. Results are presented for electron temperatures (T_e in degrees Kelvin) in the range $3.3 \leq \mathrm{Log}\ T_e \leq 6.0$ applicable to many laboratory and astrophysical plasmas for transitions within the $3d^5$ manifold. The present results[1,2] compared to previous investigations[3] provide improved results for important lines in the Fe IV spectrum.

Further details of the calculations will be presented at the conference along with a complete set of results.

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Measurements of mean charge values of heavy atoms on Dubna gas-filled recoil separator

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We measured the mean electronic charge $< q >$ of heavy ions with atomic numbers Z=89 through 118 traversing dilute hydrogen gas with velocities ranging from 1 to 2.6 times the Bohr velocity[1,2]. We observe a strong linear dependence of the average charge on the velocity of the ions, and only a weak dependence on their atomic number Z. A more detailed examination of the experimental results shows that the $< q >$ values reflect the influence of the 5f electron shell on the properties of these elements.

Our new data on mean charge values of latest synthesized superheavy elements with Z=115[3] confirm previous findings.

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Laser spectroscopic investigations of Pr I and Pr II lines

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We report on our current laser spectroscopic investigation of the praseodymium spectrum in the wavelength region from 420 nm to 450 nm (stilben 3). Using a hollow cathode lamp filled with metallic praseodymium the Pr I and Pr II lines of interest were excited by tunable single mode cw laser light. Chopping the laser beam the intensity modulation of selected fluorescence lines was used as monitor for the laser resonant signal during the laser scan (LIF detection method). In that way the hyperfine structure of 30 Pr I lines and 10 Pr II lines has been determined. By evaluating the hyperfine structure a dozen of new Pr I levels and two new Pr II levels were discovered.

Especially the Pr II results reveal an urgent need for the determination of new Pr II levels (with priority an low J-values; J = 0, 1, 2 and 3). The results of our evaluation: J-values, hyperfine constants and - if possible - the level energies are presented. Further research is in progress.

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Stochastic dynamics in the Associative Ionization of Rydberg atoms

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Stochastic theory of associative ionization (AI) in collisions of alkali Rydberg atoms with ground state atoms is presented. It treats the ionization as excitation of the Rydberg electron to continuum by the electric dipole field generated by exchange interaction within the quasi-molecular ion. Redistribution of population prior to ionization over a range of Rydberg states due to non-adiabatic processes in overlapping multiple level crossings of quasi-molecular Rydberg states is described as stochastic diffusion of electrons in the Rydberg energy spectrum using a Fokker-Planck type equation. A consequence of such diffusion is the onset of global chaos in dynamical evolution of the Rydberg electron. The basic concepts of the stochastic theory for alkali A**(nl) + A systems are described in [1,2]. The present study [3] is an elaboration of this theory and it involves the following essential modifications of the earlier theories [4, 5, 6] by taking into account: (i) influence of *twisting effect* on the efficiency of AI channel of the ionization; (ii) l-mixing of Rydberg levels; (iii) stochastic phenomena occurring during the passage of the colliding A** + A complex through the zone of multiple overlapping level crossings. The choice of the collision velocity distribution is shown to be important, while the divergence of atomic beams can strongly modify the intra beam velocity distributions. Theoretical rate constants were calculated for Na**(nl) + Na associative ionization, with n=5-25 and l = S, P and D for crossed and single beam conditions. A good agreement between the predictions of our stochastic theory and the available experimental data [4,7] is found.

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Two-photon excitation of the $1S-2S$ transition in atomic hydrogen in presence of the photo ionization

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The frequency of the $1S-2S$ transition in atomic hydrogen plays an important role for the accurate determination of the Rydberg constant and the ground-state Lamb shift [1]. A comparison between two high-precision frequency measurements opened an opportunity to set a stringent limit on the drift of the fine structure constant [2]. Presently, the $1S-2S$ transition frequency is determined with a relative accuracy of $1.5 \cdot 10^{-14}$ [2].

Besides the data statistics, one of the important limiting factors for the experimental accuracy is the accuracy of the line shape model [3]. The model has been implemented to correct for the 2nd order Doppler effect and the dynamic Stark shift which are responsible for shifts of the $1S-2S$ transition frequency in the beam experiment. One of the processes accompanying the excitation of the hydrogen atom in the light field with λ =243 nm is the decay of the excited $2S$ level via photoionization to the continuum. At intensities necessary for effective excitation of the $2S$ level (a few MW/m^2), the ionization rate reaches a level of 1 kHz which significantly reduces the lifetime of the excited level (the natural life is 140 ms). This process modifies the dynamics of the excitation and should be taken into account in future experiments to reduce the uncertainty of the $1S-2S$ frequency.

We have calculated the line profile of the $1S-2S$ transition in different regimes in presence of ionization losses using damped master equations for a two-level system. To compare with experimental data, we used a Monte-Carlo simulation for an ensemble of atoms moving through a spatially inhomogeneous field in the excitation region. The ionization results in a modification of the velocity distribution of metastable atoms reaching the detector and significantly contributes to the line broadening of the $1S-2S$ along with other broadening mechanisms.

The intensity-dependent part of the line broadening and the shift of the line frequency observed in the experiment [2] are in a good agreement with simulated values. Such an analysis opens an opportunity to increase the accuracy of the line shape model due to better understanding of the excitation process. Moreover it allows for an indirect experimental validation of the two-photon matrix element as well as of the ionization cross-section.

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Measurements of the $Ar^-(3p^5\ 4s^2)$ and $N_2^-(^2\Sigma_g^+)$ Feshbach resonances at 5 meV energy resolution

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Using a novel electron scattering apparatus [1,2] involving a laser photoelectron source and a highly collimated supersonic target beam, we have investigated angle-differential elastic electron scattering from argon atoms and nitrogen molecules in the energy range of the low-lying Feshbach resonances [3-6] at energy widths around 5 meV. The scattered electrons are simultaneously detected by five retarding field analyzers with channel electron multipliers at angles of 22.5°, 45°, 90°, 112.5° and 135°. An additional channel electron multiplier, mounted at the kinematically appropriate position, detects long-lived excited species. Comparing the measured metastable Ar^* yield near onset with a Wigner-type threshold cross section, convoluted with a Gaussian resolution function of fitted energy width, allows for a precise determination of both the absolute electron energy scale and the effective energy width of the scattering experiment.

Thus the properties of the $Ar^-(3p^5 4s^2\ ^2P_{3/2,1/2})$ resonances have been measured with unprecedented accuracy: The position of the $^2P_{3/2}$ resonance was determined as 11.103 eV in agreement with [4], the energy separation between the two fine structure components as 172.7 meV, and the natural width of the resonances as 2.4 meV, in agreement with the value recommended in [3], but in disharmony with that obtained in [4].

The energy of the $N_2^-(^2\Sigma_g^+)$ resonance was determined as 11.497 eV by calibration against the $Ar^-(^2P_{3/2})$ resonance in an experiment with a mixed Ar/N_2 beam. The N_2^- resonance was further studied in both elastic scattering and in vibrational excitation channels using an optimized apparatus with hemispherical monochromator and energy analyzer at 13 meV resolution. A preliminary analysis of the two N_2 data sets yields a new value of 1.0 meV for the width of the $N_2^-(^2\Sigma_g^+)$ resonance.

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Nonlinear Optics in Coherently Prepared Media

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The efficient generation of short-wavelength, i.e. vacuumultraviolet (VUV) radiation (λ <185 nm) is of considerable interest for scientific and technical application, e.g. in spectroscopy, laser lithography or high resolution microscopy. Nonlinear optical frequency conversion processes, e.g. third-harmonic generation or four-wave mixing, usually implemented in rare gases and metal vapors, are typical techniques to provide coherent VUV radiation. However, such frequency conversion processes suffer from poor conversion efficiencies due to the small nonlinear susceptibilities. To overcome these difficulties, coherent preparation of the nonlinear optical medium prior to the frequency conversion process serves to significantly enhance the conversion efficiency.

The nonlinear optical response of an atomic medium is determined by the atomic coherences, i.e. the non-diagonal elements of the density matrix, which describes the system. Coherent techniques like electromagnetically-induced transparency (EIT) [1], Stark-chirped rapid adiabatic passage (SCRAP) and stimulated Raman adiabatic passage (STIRAP) [2] serve to prepare a *maximum coherence*, i.e. maximum nonlinear optical polarization, in the medium. The maximum coherence acts like an strong local oscillator. When a probe laser is introduced in the system to beat with the atomic local oscillator, most efficient generation of radiation at sum- or difference-frequency modes takes place.

Strong enhancement of third-harmonic generation to provide VUV radiation at $\lambda_{VUV} = 71$ nm has been demonstrated experimentally in coherently prepared krypton atoms [3]. The atoms were driven to maximum coherence by interaction with two radiation fields : the pump laser pulse at $\lambda_P = 213$ nm driving a two-photon transition from the ground state to an excited state, slightly detuned from exact two-photon resonance; a second, strong laser pulse at λ_{St} =1064 nm, inducing dynamic Stark-shifts of the atomic transition frequency. Thus, the atoms were driven in a Stark-chirped rapid adiabatic passage (SCRAP) process to the excited state and a transient maximum coherence was prepared during the transfer process. The transient coherence beats with the pump laser pulse to yield enhanced generation of VUV radiation at the third harmonic frequency of the pump laser. The conversion efficiency is enhanced by as much as a factor of 22 compared with a conventional third-harmonic generation process.

We also investigate experimentally the enhancement of VUV generation in a medium, driven to maximum coherence by an alternative coherent technique, stimulated Raman adiabatic passage (STIRAP). A heat pipe with mercury vapor at high densities serves as an efficient nonlinear optical medium. Coherent population transfer is driven by a pump laser pulse (at $\lambda_P = 254$ nm) and a Stokes laser pulse (at $\lambda_S = 408$ nm) in a ladder-type level scheme. In this case a high amount of internal energy is stored in the coherently prepared mercury vapor. Subsequent sum-frequency mixing of a probe laser pulse (at $\lambda_{Pr} = 532$ nm) with the atomic maximum coherence permits the generation of short-wavelength radiation (at $\lambda_{VUV} = 121$ nm). In contrast to expectations based on conventional frequency mixing, the conversion efficiency reaches a maximum, when the laser pulses do not coincide in time, but are arranged in a counterintuitive pulse sequence (STIRAP case : Stokes preceding pump pulse).

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Grid mapping procedure based on the reduced variable substitution for the radial coordinate

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A rigorous exploration of the photoassociation experiments, calculation of formation rates for ultracold molecules, determination of the scattering lengths and of collision cross sections at subKelvin temperatures requires highly accurate quantum models based on a numerical solution of a large set of close-coupling (CC) radial equations. A mapping grid procedure using an adaptive coordinate $z(r)$ has been proved to be an efficient tool for the problem solution [1,2]. We offer to transform the CC equations using the reduced variable representation (RVR) $z \equiv (r^\alpha - r_e^\alpha)/(r^\alpha + \beta r_e^\alpha)$ (where $\alpha, \beta, r_e > 0$ are the free parameters) which is often used to reproduce the diatomic potential energy curve $V(r)$ [3]. The above substitution reduce an infinity interval of the radial coordinate r to the finite one $z \in [-1/\beta, 1]$ while the $g \equiv dz/dr > 0$ and hence the inverse function $r = f^{-1}(z)$ could be easily found in the closed form. The corresponding radial equation is transformed to the form:

$$\left(\frac{d^2}{2\mu dz^2} + [E - \tilde{V}(z)]/g^2\right)\phi(z) = 0; \qquad \phi(z) = \sqrt{g}\psi(r) \tag{1}$$

where

$$\tilde{V} = V + \frac{g''}{2g} - \frac{3}{4}\left(\frac{g'}{g}\right)^2 \tag{2}$$

is the effective potential and the symbol prime denotes the first derivative with respect to r.

Direct integration methods such as Numerov finite-difference schema could be applied straightforwardly to solve the equation (1) while variation approaches lead to the generalized eigenvalue problem $\mathbf{A}\phi = E\mathbf{B}\phi$, where $\mathbf{B}$ is the symmetric positive defined diagonal matrix. The most efficient uniformed Fourier grid method (FGM) [1,2] yields the symmetric $\mathbf{A}$ matrix. Then, the $\varphi = \mathbf{B}^{\frac{1}{2}}\phi$ substitution based on trivial LU decomposition: $\mathbf{B} = \mathbf{B}^{\frac{1}{2}}\mathbf{B}^{-\frac{1}{2}}$ provides the ordinary eigenvalue problem for the symmetric and easily evaluated matrix $[\mathbf{gAg}]\varphi = E\varphi$, where $\mathbf{g}$ is the diagonal matrix and $\varphi(z) = \psi(r)/\sqrt{g}$. Optimal in a particular energy region E parameters of the substitution α, β and r_e could be found by solving of the equation: $g^2(r) \approx |E - \tilde{V}(r)|$.

Numerical tests performed on the CC set of Morse oscillators demonstrated that a combination of the RVR mapping and FGM procedures decreases significantly the boundary condition effect at $r \to \infty$ and improves an accuracy of the solution by 4-5 orders of magnitude for the same computational effort.

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Nonadiabatic treatment of the $A^2\Pi \sim B^2\Sigma^+$ complex of the $ArLi^{6,7}$ isotopomers near dissociation threshold

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Comprehensive deperturbation analysis of the rovibronic termvalues of the $A^2\Pi \sim B^2\Sigma^+$ complex of the $ArLi^{6,7}$ isotopomers obtained by the sub Doppler absorption laser spectroscopy [1] have been performed in the framework of the inverted close coupling approach (ICCA) [2] adopted implicitly to a simultaneous treatment of both strong-local and weak-regular mutual perturbations without reducing the dimensionality. Influence of the remote electronic states was taken account by the perturbation theory (PT) calculations using the approximate vibronic sum rules. The adiabatic potentials derived for the well-bound $A^2\Pi$ and shallow $B^2\Sigma^+$ states together with relevant $A \sim B$ nonadibatic coupling parameters as functions of the internuclear distance R restore the experimental termvalues of the $ArLi^7$ isotopomer with the rms 0.003 cm^{-1}. The deperturbed electronic parameters were involved in a direct close coupling calculations of the termvalues manifold for the $ArLi^6$ isotopomer by a substitution for the reduced mass only. The predicted termvalue positions coincide with their experimental counterparts within 0.004 cm^{-1}. The conventional p, q and γ splitting parameters of the $A^2\Pi$, $B^2\Sigma^+$ and $X^2\Sigma^+$ states were evaluated for both isotopomers as well to compare with the available experimental data [1].

The required $A^2\Pi \sim X, B^2\Sigma^+$ spin-orbit coupling matrix elements and spin-orbit splitting of the $A^2\Pi$ state were evaluated in the framework of the relativistic shape-consistent core pseudopotential approximation [3] combined with many-body multi-partitioning perturbation theory (MPPT) [4] calculations. The electronic angular coupling matrix elements between the $A^2\Pi$ and $X, B, C^2\Sigma^+$ states were obtained by the extensive multi-reference configuration interaction (MRCI) calculations. The *ab initio* results were supported by the one-channel quantum defect theory (QDT) treatment of the low-lying Rydberg electronic states. The correct long range behavior of the calculated electronic matrix elements near the $Ar(^1S)+Li(^2P)$ dissociation threshold was attained by appropriate analytical forms using the reduced variable representation (RVR) of the radial coordinate R. Overall set of the initial parameters was optimized by nonlinear least square method based on the ICCA procedure. Mapped grid procedure based on the RVR transformation allowed us to decrease the boundary condition effect at $R \to \infty$ as well as to improve accuracy of a tedious numerical solution of the coupling radial equations by 4-5 orders of magnitude for the same computational effort.

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Dynamic and Coherent Manipulation of Calcium ions in a Penning Trap

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We will report on experiments to improve the localisation and control of ions held in a Penning trap. Our goal is to show that the Penning trap, with its purely static fields, is a viable and indeed ideal system in which to perform Quantum Information Processing (QIP) using trapped ions. As such the work reported is part of a wider project aimed at performing sideband cooling of Ca^+ ions in a Penning trap, measuring the decoherence rate in this system, and moving on to perform key QIP operations.

We have extended the technique of axialisation, which we first demonstrated using Mg^+ ions, to the Ca^+ system. Axialisation overcomes some of the problems associated with laser cooling in a Penning trap. The radial motion in this type of trap consists of an epicyclic superposition of a fast (modified) cyclotron motion and a slower $\mathbf{E} \times \mathbf{B}$ circular drift motion about the centre of the trap (the magnetron motion). The magnetron motion is difficult to laser cool since it is unstable — energy must be added to this degree of freedom to allow the ion to climb a potential hill and move towards the centre of the trap. The cyclotron motion, however, is not unstable and behaves normally with regard to laser cooling. Axialisation works by applying a weak oscillating drive to the trap electrodes which couples the magnetron and cyclotron motions so that the efficient cooling of the cyclotron motion is extended to the magnetron motion. This gives improved laser cooling and localisation of ions in the trap.

We measure cooling rates by studying the phase of the ions' motion relative to a driving electric field at a frequency close to the motion frequency. The cooling rate is given by the frquency width of the π phase change across resonance. We have recently measured enhanced magnetron cooling rates with axialisation. We have also observed shifts in the motional frequencies due to a coupling between the magnetron motion and the modified cyclotron motion ('dressed' by the axialisation drive at the cyclotron frequency). Theory predicts that when the dressed modified cyclotron frequency is degenerate with the magnetron frequency, a classical avoided crossing results. We have confirmed this interpretation by measuring the predicted avoided crossing.

"Magic" wavelengths for optical frequency standards on laser cooled alkaline-earth atoms in 3D-optical lattice

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As a prime candidate for an optical frequency standards in neutral atoms, laser cooling of alkaline earth atoms have been studied in Mg, Ca, Sr and Yb atoms (see, for example [1-2]). It is important to note, that optical frequency standards can be developed based on narrow transitions that allow exceptionally high Q-factor, that are orders of magnitude higher than in Cs-fountains. Besides, the atomic configuration of two outer electrons introduces a unique complexity in their energy structure, specifically, the spin-singlet ground state and the spin-forbidden triplet excited states.In this paper we consider light shifts in the optical frequency standards based on the 3D-optical lattice for alkaline-earth atoms in the Lamb-Dicke confinement. We have examined theoretically the effect of the light shift cancelation in the vicinity of the "magic" wavelengths of the trapping laser radiation. In order to provide theoretical support for these measurements employing a"light shift cancelation technique", we here report results of calculations for the light shift for the S-P hfs-induced singlet-triplet transition 0-0 in Be, Mg, Ca, Sr, Yb and Hg atoms as prime candidates for an optical frequency standards in neutralatoms.In our calculations we have used the general theory of [3-4] for consecutive estimates for the higher-order light-shift contributions(described by ac hyperpolarizabilities, magnetic dipole and electric quadrupole terms in addition to the electric-dipolepolarizability). For the accurate calculations of these quantities we have applied the Fues' model potential method [4]. The key point is that it is consistent to use analytical wave functions for the evaluation of radial matrix elements, together with experimental ionization energies. Quite simple presentation for the Green's function enables us to evaluate the contribution of the higher excited states (including continuum) which are neglected in the finite-sum approach. As a result, the precise calculations of ac susceptibilities for the 0-0 clock transitions indicate that the contribution of the higher-order light shifts can be reduced to less than 1 mHz,allowing for a projected accuracy of better than 10^{-17}.

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Stark level crossing signals in 7, 9, $10^2D_{3/2}$ Cs at two-step laser excitation

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We have studied the coherently excited magnetic sublevel crossings at the stepwise two-laser excitation $6S_{1/2} \rightarrow 6P_{3/2} \rightarrow nD_{3/2}$ of the $7D_{3/2}$, $9D_{3/2}$ and $10D_{3/2}$ levels of atomic cesium in the presence of an external dc electric field. The experiment was aimed at detecting resonance signals in the fluorescence from the $nD_{3/2}$ level measured as a function of the electric field strength. Positions of these resonances correspond to the magnetic sublevel crossings.

Cesium vapor was produced in a sealed glass cell kept at room temperature. An electric field up to E_{el} = 2400 V/cm was applied via transparent Stark electrodes separated by a 2.5 mm gap. For the first step, the 852.1 nm beam of the diode laser (LD-0850-100sm laser diode) was used to excite the $6^2P_{3/2}$ state. The laser beam $\mathbf{e}_1$ was linearly polarized along the external electric field $\mathbf{E}_{el}$ direction ($\mathbf{e}_1 \parallel \mathbf{z}$). The second laser beam $\mathbf{e}_2$ polarized as $\mathbf{e}_2 \parallel \mathbf{y}$ was sent in a contra-propagating direction to induce either the $6P_{3/2} \rightarrow 7D_{3/2}$ transition at 698.3 nm (using a Hitachi HL6738MG laser diode) or the $6P_{3/2} \rightarrow 9D_{3/2}$ transition at 584.7 nm and the $6P_{3/2} \rightarrow 10D_{3/2}$ transition at 563.6 nm (using a Coherent CR699-21 dye laser). The laser induced fluorescence (LIF) $nD_{3/2} \rightarrow 6P_{1/2}$ was observed along the **z**-axis. The LIF was dispersed by a monochromator with 1.3 nm/mm inversed dispersion and detected with a photomultiplier tube operated in photon counting regime. The intensity I(**y**) of LIF linearly polarized along **y** axis was detected as a function of E_{el}. The experiment reveals two resonance signals centered at the positions of coherently excited magnetic sublevels crossings with Δm_F = +/- 2 at ca. 1300 and 1800 V/cm for $7D_{3/2}$, at 180 and 250 V/cm for $9D_{3/2}$, and at 85 and 120 V/cm for $10D_{3/2}$ states. These measured level crossing positions are in a good agreement with the calculated crossing points. The Stark energies for magnetic sublevels m_F of the hyperfine F=2,3,4,5 levels of states under study was calculated based on the Cs atom D state polarizabilities from [1]. The resonance signal shapes and amplitudes are in an excellent agreement with simulated signals that were obtained by applying the density matrix rate equations [2] for Zeeman coherences.

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Sub-Doppler spectroscopy of Xenon atom in the mid-infrared

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The mid-infrared (mid-IR) spectral region is particularly interesting for several spectroscopic features. For instance, in many applications related to trace-gas analysis, the mid-IR is very attractive since strong absorption bands connected to fundamental vibrations of most molecular species lie just in this spectral region. Moreover, high-resolution laser spectroscopy in the mid-IR is interesting to get detailed information about atomic and molecular structures and to provide new frequency standards, since a limited number of absolute frequency measurements have been made in this region. Recently new tunable coherent sources have been developed, such as Optical Parametric Oscillators (OPO), Difference-Frequency Generators (DFG) [1], and Quantum Cascade Diode Lasers (QCDL). All these sources have been extensively used in many high sensitivity detection studies of molecular species and in few Doppler-free investigations of molecular lines. In this work we report, according to our knowledge, the first Doppler-free spectroscopy of an atomic species (xenon atom) by using low-power difference-frequency radiation. Xenon atom (Z=54) is of particular interest for Doppler-free analysis: it has nine stable isotopes in natural abundances accessible to high sensitivity laser spectroscopy techniques (^{124}Xe: 0.0096%, ^{126}Xe: 0.0090%, ^{128}Xe: 1.92%, ^{129}Xe: 26.4%, ^{130}Xe:4.1%, ^{131}Xe:21.1%, ^{132}Xe:26.9%, ^{134} Xe:10.4%, and ^{134} Xe:8.9%), and, hence, is suitable for isotope shifts analysis. In addition, the nuclei of two of these isotopes have a spin (^{129}Xe:I=1/2 and ^{131}Xe:I=3/2) which gives rise to a hyperfine splitting of the levels. Finally, the series of Xe isotopes crosses the closed neutron shell N=82 (^{129}Xe is a magic nucleus), and this can result in interesting anomalies in the isotope shifts. Moreover, since for atoms with atomic number Z between 30 and 60 the mass shift and field shift contribution are of the same order of magnitude and can also exhibit different sign [12], expected isotope shifts for xenon (Z=54) are quite small, and. therefore, quite hard to investigate. The transition investigated in the present work is the 6p 3/2 $[1\ 1/2]_2 \rightarrow$5d 3/2 $[3\ 1/2]_3$ which is the strongest atomic line in the mid-IR region accessible to the tunability of our apparatus. A part the famous He-Ne transition at 3.39 μm used by Evenson for his historical measurement of the speed of light, we think this is the first atomic line in the mid-IR investigated with Doppler-free techniques. The experiment was realized by generating about 60 μW mid-IR radiation through difference-frequency mixing in a periodically poled lithium niobate (PPLN) optical crystal. Sub-Doppler saturation spectra were observed by retroreflecting the laser beam back through the discharge cell. Preliminary results about the isotope shifts and hyperfine structure are discussed.

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Extreme-ultraviolet generation from molecules in intense infrared lasers

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Very recently the prospect of imaging, resolving and manipulating electronic dynamics by creating ultrashort extreme UV pulses has been advanced. To realise spatial and temporal resolution of electronic transitions within materials requires intense coherent light that switches on attosecond (10^{-18}s) timescales with wavelengths in the extreme ultraviolet or soft x-ray spectrum, $\lambda = 0.1 - 10$nm. One of the most promising schemes for producing such light is through high-harmonic generation from intense infrared lasers [1].

We have analysed such processes for simple molecules subjected to intense infrared light. For ultrashort IR pulses of duration 10-50 fs or less, rotational or bending motion is frozen. However for hydrogenated molecules the vibrational stretch time is comparable with the cycle time of the laser, and hence the period of the forced oscillation of the electronic wavepacket [2]. Thus the electronic and nuclear motions are strongly coupled. Very recently we have shown that this is extremely important for the process of ionization in light molecules [3]. In this paper we show that the effect on harmonic generation is even more extreme.

We have carried out quantal and semiclassical simulations of harmonic generation in hydrogen molecules subjected to intense Ti:sapphire ($\lambda \sim 790$nm) radiation allowing for dissociation and ionization processes. We find that molecular vibration controls the electron release and rescattering process and enhances the production of high-frequency harmonics. Typically for an intensity $I \sim 5 \times 10^{14}$W cm^{-2}, quantal vibration enhances UV efficiency (up to the 150th harmonic) by a factor of 100 in comparison to the atomic model.

At intensities of the infrared laser above $I \sim 10^{14}$W cm^{-2}, the corresponding spectum for harmonic intensity does not have the conventional plateau associated with atomic systems. Rather the spectral density shows a steady slow decrease with increasing harmonic order. The primary reason for these features is the increase in ionization via dynamic tunnelling [3]. One could cite this as an extreme example of phonon-assisted tunneling. Another factor is the quantum enhancement of bremsstrahlung due to nuclear wave packet expansion and dispersion increasing the cross section for electron-ion scattering.

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Stimulated emission in Calcium vapour pumped by UV laser radiation.

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Several visible stimulated emission lines are observed in both forward and backward direction when Calcium vapour is irradiated by resonant UV light. The latter is delivered by the frequency doubled output of a Nd:YAG pumped nsec dye laser and induces the $4s^2\ {}^1S_0 \longrightarrow 4snp\ {}^1P_1$ single-photon transitions with n = 7 and 8 (wavelengths ∼220 nm and ∼215 nm respectively). Calcium undergoes continuous evaporation within a T-shaped heated quartz cell maintained at temperatures 750-820 ^{o}C corresponding to atomic densities 10^{15} - 10^{16} cm^{-3}. For preventing Ca vapour to coat the fused silica windows as well as for studying collisionally induced processes the cell is filled with 10 to 300 torr He buffer gas. Stimulated emission in the forward direction is analyzed by a CCD-camera-equipped monochromator (400-750 nm) while fluorescence emitted perpendicularly to the laser beam is observed by another monochromator (200-540 nm) and detected by a photomultiplier. Stimulated emission spectra are recorded as a function of Ca density, laser intensity, and buffer gas pressure.

Eleven stimulated emission lines are observed for both n=7 and 8 including those recorded previously for n=5 [1]. Ionization of Ca is also made evident through the side detection of $Ca^+\ 4p_{1/2,3/2} \longrightarrow 4s_{1/2}$ transitions. However the most interesting aspect of the present study is the observation of a stimulated emission line (beam divergence below 4 mrad) at 6449.8 Å for n=7 but not for n=8. This line is carefully calibrated with a commercial Neon lamp and unambiguously attributed to the singlet-triplet $3d4p\ {}^1D_2 \longrightarrow 3d4s\ {}^3D_1$ transition. Moreover, with increasing buffer gas pressure its intensity decreases in favour of the line at 6163.7 Å due to the $4s5p\ {}^3P_1 \longrightarrow 3d4s\ {}^3D_1$ transition. This fact suggests that the upper $3d4p\ {}^1D_2$ level is not predominantly populated by collisions between excited Ca atoms and He buffer gas atoms. It furthermore suggests the existence of a state-specific transfer pathway to that upper state, associated perhaps with the presence of bound doubly excited state perturbers. Further discussion on observations and population mechanisms for all the observed stimulated emission lines will presented at the conference.

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Time-resolved spectroscopy using a microcalorimeter at an electron beam ion trap

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Spectroscopy in the soft-x-ray range usually employs time-integrated data acquisition with a spectrograph (equipped with a position-sensitive detector like a CCD camera), or time-resolved data recording with a single-channel detector on a monochromator. However, there are physics problems that require time resolution while at the same time observation would be benefiting greatly from the spectral coverage offered by a spectrograph.

We have studied the metastable $3d^9 4s\ ^3D_3$ level in Ni-like Xe^{26+} at the Livermore electron beam ion trap. This level can decay only by a magnetic octupole (M3) transition. Such a transition has been reported before only from Ni-like ions of Th and U [1]. For high resolution soft-x-ray spectroscopy, we used a flat-field spectrograph [2] equipped with a CCD camera. The time-integrated spectra thus gained were complemented by data collected using a microcalorimeter (Goddard XRS with 16 active pixels) that has a somewhat lower spectral resolving power (line width 6 eV), but which permits the time-stamping of individual counts and thus the creation of scatter plots of photon energy vs. time. We operated the electron beam ion trap in a cyclic pattern with periods of the electron beam on and off. When the electron beam is on (for about 50 ms), ions are produced and are being ionized further, as long as the electron beam energy is higher than the ionization potential of a given charge state. When the electron beam is stopped, excitation and therefore also prompt emission end. Emission during the electron beam off periods (some 50 to 70 ms) originates from either long-lived levels or from charge exchange reactions.

At an electron beam energy of 1.5 keV, Ni-like Xe ions are readily produced, but no higher charge states should be reached, except for the presence of the aforementioned metastable level acting as a stepping stone. Indeed, the 3d-4f transitions of Co-like Xe^{27+} arise as soon as the 3d-4f transitions of Ni-like Xe^{26+} are excited. A scatter plot of the microcalorimeter signal reveals the $3d^9 4s\ ^3D_3$ level at 590 eV [3] as the only long-lived excited level, with a level lifetime of about 11 ms. Theoretical predictions range from 14 to about 19 ms.

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New electron affinity measurements with the photodetachment microscope.

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New photodetachment microscopy experiments have been performed on a beam of $^{32}S^-$ ions. Analysing the electron images obtained, we find that the electron affinity measurements performed with the photodetachment microscope contain a small bias, due to the difference between the actual and assumed values of the applied electric field. Having a measure of this bias, we can reanalyse older data recorded on the negative ions O^- and Si^- along similar lines. As a consequence, the values of the electron affinities of Oxygen, Silicon and Sulfur can be given with an improved accuracy. The recommended values (with expanded uncertainties) are now 11 784.676(7) cm^{-1} for ^{16}O, 11 207.246(8) cm^{-1} for ^{28}Si, and 16 752.974(5) cm^{-1} for ^{32}S, i.e. 1.461 113 5(12), 1.389 521 3(13) and 2.077 104 0(9) eV, respectively. These are today the most accurate of all atomic and molecular electron affinities. The possibility for going to still improved accuracies, by e.g. an active control of the residual magnetic field in the photodetachment region, will be discussed at the conference.

EUV spectroscopy of Xenon ions created using and electron beam ion trap

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The present experimental studies on xenon were performed at the NIST Electron Beam Ion Trap (EBIT) [1]. Radiation from xenon ions in the spectral range from 4 nm to 20 nm has been measured, using a flat field spectrometer [2]. It is well known that xenon emits strongly in the 10 nm to 11 nm wavelength region of the spectrum with this emission arising from a number of adjacent ion stages that merge to form an unresolved transition array UTA [3]. Operating EBIT with electron beam energies between 200 eV and 500 eV allows sampling of the charge states that contribute to this UTA. The analysis of the spectra is based on spectroscopic modelling using the COWAN suite of atomic structure codes [4]. Initial calculations have used the basic UTA approach [5], in which the UTA is considered as a statistical distribution of lines, each with an energy and weight (equal to the line intensity, gA) calculated using the COWAN codes. The mean wavelength and the spectral width of the transition array are then calculated using the UTA model. However, the EBIT operates in a low-collisional regime where the level populations and consequently the line intensities are not proportional to gA but depend instead on the rates at which ions are excited. A different set of calculations are needed, using density dependant collisional-radiative line intensities instead of simply gA values, and the results will be compared to the measured spectra. [6]. This work has been motivated by the recent interest in using the EUV radiation emitted by xenon or tin as a light source for lithography and the associated need to fully understand the origin of this radiation.

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On the influence of collisions with charged particles on Cr I lines in stellar atmospheres

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Using the semiclassical perturbation method, electron-, proton-, and ionized helium-impact line widths and shifts for the nine Crı spectral lines from the $4p^7P^0 - 4d^7D$ multiplet, have been calculated for a perturbed density of 10^{14} cm^{-3} and temperatures T = 2,500 − 50,000 K. The obtained results have been used to investigate the influence of Stark broadening effect in the Cr-rich Ap star β CrB atmosphere on line shapes of these lines.

From our investigation we can conclude:

(i) The calculated value of Stark widths as well as of shifts can be quiet different for the different lines, although these belong to the same multiplet.

(ii) The contribution of the proton and HeII collisions to the line width and shift is significant, and it is comparable and sometimes (depending of the electron temperature) even larger than electron-impact contribution.

(iii) Depending on the electron-, proton-, and HeII density in stellar atmosphere the Stark shift may contribute to the blue as well as to the red asymmetry of the same line.

(iv) To fit well Cr ı line wings we need to decrease the calculated Stark widths by 60-70%, which is the same order of overestimation as for Si ı lines [1]. The approximation formula of Cowley [2], used in the cases where the adequate semiclassical calculation is not possible due to the lack of reliable atomic data, predicts also overestimated influence of Stark broadening in comparison with observations.

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Measurement of Stark shifts in Xe III.

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This work reports a collection of 10 high precision measurements of Stark shifts of Xe III spectral lines. These Stark parameters were measured in a pulsed plasma, a detailed description of the experimental apparatus and the diagnostic methods can be seen elsewhere [1,2]. The excitation unit has a capacitor bank of 20 μF charged up to 9.2 kV approximately. The mixture of He-Xe at a pressure of $3.0 \cdot 10^3$ Pa continuously flows through the discharge lamp. The plasma electron density (0.2 to $1.6 \cdot 10^{23}\, m^{-3}$) has been determined by two-wavelength interferometry within an error band lower than 10%.

Spectra were recorded with a spectrometer equipped with an optical multichannel analyzer (O.M.A.) detector with 512 channels. Exposure times for the spectra were usually 5 μs. The spectral measurements were taken in first order of diffraction and the spectral interval ranged from 300 nm to 650 nm. The linear dispersion changes from 3 pm/channel to 6 pm/channel in this spectral interval. The excitation temperature (17000 - 29000 K) was calculated by Boltzmann-plot techniques.

Original spectra were corrected to self-absorption effects when necessary and the transmittance of the detector system was considered. Stark shifts were obtained from a linear extrapolation of line center position as a function of electron density. In this experiment, more than 60 lines were analyzed, more than 30 of them being acceptable for Stark shift measurements. We selected the lines which showed a very clear linear dependence. From the linear fits, the resulting values at electron density of $10^{23}\, m^{-3}$ were determined. These Stark shifts results have been compared with previous existing data [3].

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Quantum and classical calculations of ground state properties of parabolic quantum dots with up to 20 electrons

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We calculate the electronic ground state of parabolically confined quantum dots in two dimensions for up to 20 electrons based on the quantum Monte Carlo method. Effects of the electron-electron interaction and the response to a magnetic field are exposed. The wavefunctions and the ground state energies are compared with purely classical calculations. A close correspondence in electron density is found even for small number of electrons.

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Transition energies and probabilities for F-like ions with $10 \leq Z \leq 49$

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Much attention has been devoted to the study of highly charged atoms, due to its importance for several fields in physics, namely the diagnostics of plasmas, laser physics and also astrophysics. As far as the F-like ions spectrum are concerned, the transitions are important for laser produced plasmas and astrophysics [1].

In the present work, we continue [2] the calculation of relativistic transition energies and probabilities for several F-like ions with $10 \leq Z0 \leq 49$. The lines considered correspond to transitions between levels of $2p^4 3s$, $2p^4 3p$ and $2p^4 3d$ configurations. The spectral fine structure is taken into consideration and the results for individual lines are given. We start from a Dirac-Fock calculation with Breit interaction included self-consistently. Higher-order retardation and one-electron radiative corrections are also included and the screening of the self-energy is evaluated using Welton approximation. Correlation is added within the Multi-Configuration Dirac-Fock method (MCDF). The present results are in good agreement with the available experimental results.

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Thermal Decomposition of Unstable Molecules by Ultraviolet Photoelectron Spectroscopy (UVPES) and Matrix Isolation Infrared Spectroscopy

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Azide compounds play important roles in a number of industrial processes. For instance, the use of reactive molecules containing the azido group as precursors in surface nitridation processes in microelectronics industry is well known. Azides are also used as synthesis tools for cancer research and AIDS, as reagents for organic synthesis and as having great relevance in the design of new magnetic materials. Their applications also include production of molecular nitrogen in situ in space vehicles and in car air bags. However, due to their high instability most of their properties are quite difficult to be measured and the mechanisms of their decomposition are largely unknown. UVPES is a well established technique to study the azides and their thermal decomposition pathways [1] which needs to be supported by Infrared Matrix Isolation Spectroscopy.

Azidoacetonitrile, N_3CH_2CN, 2-azidopropionitrile, N_3CHCH_3CN, 3-azidopropionitrile, $N_3CH_2CH_2CN$, methyl azidoformate, N_3COOCH_3, and ethyl azidoformate, $N_3COOCH_2CH_3$, as well as their decompositions products were studied by both UVPES and Infrared Matrix Isolation Spectroscopy. The experimental measurements were supported by the results of molecular orbital calculations, which are used to compute the relative energies of different decomposition channels, and the electronic structure, ionisation energies and vibrational frequencies of possible decomposition products.

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Helium photoionization beyond the dipole approximation: partial cross sections and asymmetry parameters between the N=2 and N=4 thresholds.

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Dipole (E1) and quadrupole (E2) contribution to photoionization cross sections of $1s^2\,{}^1S$, $1s2s\,{}^3S$, $1s2s\,{}^1S$ helium states between the $n = 2$ and $n = 4$ thresholds (65.4−75.61 eV) are investigated. The ${}^1P^o$, ${}^3P^o$, ${}^1D^e$ and ${}^3D^e$ continua are determined using a K-matrix method [1] with 10 channels. Both atomic and continuum orbitals are expanded on a B-spline basis.

Results include partial and total photoionization cross-sections as well as asymmetry parameters β, δ and γ[2], and position and widths of the autoionizing states. Magnetic dipole (M1) amplitudes to P^e continua are found to be completely negligible.

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A study of the competition between the dissociation and autoionizaton in small molecules following photoexcitation using synchrotron radiation.

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The present study was carried out at the Advanced Light Source on the undulator beamline 10.0.1, which is used for high-resolution atomic, molecular, and optical physics and photoemission studies of highly correlated materials. The data sets were obtained using the technique of two dimensional photoelectron spectroscopy. This is a process by which ionized photoelectron intensities are measured as a function of both photon energy and electron kinetic energy[1]. The tuneable monochromatic photon source is used to build up the two-dimensional spectra by recording many conventional spectra at photon energies that are generally separated by a few meV. The resultant data sets are acquired over a broad range of photon energies and resemble a topographic map. These two dimensional spectra can reveal resonant features at discrete photon energies which may not be otherwise apparent in one dimensional spectra.

The main focus of this investigation are the processes following the photoexcitation of dissociative resonance states. Recent studies have shown that the narrow bandwidth property of synchrotron radiation can be exploited for the purpose of detuning away from resonant states which has the effect of shortening the duration time of the core excitation de-excitation process. This consequently results in the rapid molecular decay process getting stronger in comparison to the late Auger decay from the dissociated atomic fragments[2].

The two step process of fast dissociation followed by fragment autoionization was first observed for inner shell excitation in HBr[3] and gives rise to sharp peaks in the photoelectron spectrum at electron energies that correspond to transitions in the excited fragment. The sharp peaks may also contain contributions from resonant Auger decay before the fragmentation is complete if the energy separation between the two potential curves becomes constant before the dissociation limit. Alternatively, broader spectral features are associated with electron emission before or during fragmentation, when there is not a constant separation between the potential curves. The existence of indistinguishable channels gives rise to the possibility of observing interference phenomena in the photoelectron spectrum.

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Novel inexpensive two-dimensional magneto-optical trap for efficient loading of a moving optical molasses

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Slow beam sources represent a useful tool for many applications: atom interferometers, atomic clocks, Bose-Einstein condensation and atom optics experiments. In the case of atomic clocks, continuous fountains [1] have the advantage of a lower atomic density for a given signal-to-noise ratio than their pulsed counterparts, which helps minimise collisional shifts. Furthermore, the use of such a fountain enables one to eliminate the intermodulation (*i.g.* Dick) effect associated with local oscillator noise [2]. In order to take full advantage of the continuous fountain approach, however, we need to increase the useful flux. One way is to launch more atoms to begin with. This can be achieved by loading the moving optical molasses source from a slow beam rather than by capture from the low velocity tail of a vapour at 10^{-8} mbar.

Slow beam sources can be produced in various ways. Zeeman slowing of an atomic beam allows a continuous source but is cumbersome while chirp slowing provides only packets of atoms. Here we report on a much simpler solution, namely the development and characterization of a 2D magneto-optical trap (MOT) of cesium atoms producing a continuous low velocity beam ($v \simeq$20 m/s). While 2D MOT's have already been employed elsewhere, the devices in question are somewhat expensive, requiring many polarising large beam splitter cubes, half- and quarter-wave plates, all of which are anti-reflection coated [3]. Furthermore, the laser power is divided at each stage so several hundred milliwatts are necessary at the input.

In our own version, gold-coated prisms replace mirrors and quarter-wave plates and the optical power (<200 mW) is recycled. The net result is a considerable saving both in complexity and financial cost without degrading performance as regards the useful flux extracted from the source. We plan to use this flux to load a moving molasses that feeds our cold atom continuous fountain clock. We have already obtained an order of magnitude increase in flux compared with a vapour-filled molasses (about 10^9 at/s), even without the use of a pusher beam to provide a more intense MOT pre-source (*i.e.* a so-called $2D^+$ configuration). Current work is centered on characterisation of the slow beam (longitudinal and transverse velocity distribution, spatial profile) and the optimisation of various parameters (laser power and polarisation, magnetic field gradient, laser detuning, cesium vapour pressure).

Latest results will be presented at the conference.

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Measuring the hyperfine shift in Cu-like ^{207}Pb by electron scattering resonances

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The hyperfine structure (hfs) in atoms reflects fundamental effects in the interaction between the bound electrons and the nucleus. The energy shift contains contributions from Quantum Electrodynamics (QED) and from the nuclear charge and magnetic moment distribution. These effects have been studied over decades by spectroscopy, mainly on neutral atoms or singly charged ions. In such many-electron systems, the atomic structure is complex. The theoretical predictions are further hampered by unprecise knowledge of nuclear magnetic moments. Only recently, experimental approaches to measure the hyperfine structure of heavy highly-charged systems were opened giving a new way to obtain nuclear moments and to test QED in a new regime. Here we present a measurement of the hyperfine splittings in the $4p_{1/2}$ and $4s_{1/2}$ states of Cu-like ^{207}Pb isotopes by a new method. Instead of the generally applied optical spectroscopy, the splitting was observed in dielectronic resonances in low-energy electron-ion recombination. This opens new possibilities to measure hfs in new energy ranges and ionization stages.

The spectroscopic principle is that during the formation of a resonance the valence electron is excited by the capture of a free electron into a Rydberg state. The binding energy of the latter can be estimated to excellent accuracy and the excitation energy can then be accessed. In the present measurement, carried out at the heavy-ion storage ring CRYRING, the recombination goes through resonances in Pb^{52+},

$$^{207}\mathrm{Pb}^{53+}\left(4\mathrm{s}_{1/2}\right)+\mathrm{e}^{-}\rightarrow{}^{207}\mathrm{Pb}^{52+}\left(4\mathrm{p}_{1/2}18\ell_{\mathrm{j}}\right)\rightarrow{}^{207}\mathrm{Pb}^{52+}\left(4\mathrm{s}_{1/2}18\ell_{\mathrm{j}}\right)+\mathrm{h}\nu.$$

After electron cooling of the ion beam the recombination rates are measured as a function of the electron-ion relative energy and the energy positions of the resonances are determined. The contribution due to hfs is clearly seen by comparing the DR resonances with those of $^{208}Pb^{53+}$ where no hyperfine splitting exists.

We have evaluated the isotope dependent contributions using both Relativistic Many-Body Perturbation Theory and the Multi-Configuration Dirac-Fock method, and combined this with the previously calculated resonance pattern for $^{208}Pb^{52+}$[1]. To test the hfs-sensitivity we generate also synthetic spectra with slightly shifted values for the the hyperfine splitting constant, a, defined through $\Delta E_{HFS} = a/2[F(F+1)-I(I+1)-J(J+1)]$. The spectrum generated from the calculated shifts seems to fit the data best. Different peaks in the spectrum are rather differently affected when a is shifted, reflecting the non-linear shift of the resonances.

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Applications of polarizability calculations: from quantum computation to parity nonconservation

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We calculate the frequency-dependent polarizabilities in all alkali-metal atoms and Ba^+. The quadrupole polarizabilities are also calculated for Si^{3+} and Ba^+. In our work, the polarizability calculations are reduced to the calculations of the electric-dipole and electric-quadrupole matrix elements. The matrix elements which give the dominant contributions are evaluated using the relativistic all-order method with single and double excitations of Dirac-Fock wave functions included to all orders in many-body perturbation theory. The resulting polarizability values are used for a variety of the applications from reducing the decoherence in quantum logic gates to the discovery of the inconsistency in the experimental studies of Cs. Our alkali-metal atom polarizability calculations can be used to predict the oscillation frequencies of optically-trapped atoms, and particularly the ratios of frequencies of different species held in the same trap. We identify wavelengths at which two different alkali atoms have the same oscillation frequency. Our Rb calculations also led to the solution of the problem of motional heating in the fast two-qubit quantum gate with neutral atoms. In Cs, we use our calculations to demonstrate that the experimental $5d$ lifetime data are inconsistent with the $6s - 6p$ experimental Stark shift data. Our *ab initio* calculated $6p$ polarizabilities in Cs agree well with experimental determinations of the Stark shifts. Our calculation of the Ba+ polarizabilities is motivated by the possibility to study the parity non-conservation (PNC) with a single trapped ion and by recent measurements of the Ba^+ dipole and quadrupole polarizabilities and light shift ratio. The study of PNC in heavy atoms provides atomic-physics tests of the Standard Model and allows to measure nuclear anapole moment. The results of our Ba^+ calculations will be reported at the conference.

Radiative lifetimes and transition probabilities in Zr III

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Experimental investigations of radiative constants of excited levels of multiply charged ions are important because of the recent achievements in astrophysics and high temperature plasma devices. In the present contribution, radiative lifetimes and transition probabilities of Zr III excited states are reported.

Radiative lifetimes of 5 levels belonging to the 4d5p configuration ($^1D_2$, $^3D_{1,2,3}$ and $^3F_2$) have been measured for the first time using the Time-Resolved Laser-Induced Fluorescence (TRLIF) technique[1]. Free ionized zirconium atoms have been generated by laser ablation and laser excitation was used to populate the levels under study.

The ions were populated either in the ground state or in metastable states and the number of ions is strongly dependent on the presence of an external magnetic field. Selecting of the proper field is proved to be decisive when using the TRLIF technique for the lifetime measurements of highly charged ions. In this way, plasma diagnostics regarding the dependence on the magnetic field is also obtained.

Transition probabilities for spectral lines originating from the above states have been deduced by combining the experimental lifetimes and measurement of branching fractions of Zr III transitions using, as a source of Zr III ions, a plasma produced by laser ablation.

A good agreement between these results and those obtained with a multiconfigurational relativistic Hartree-Fock calculation is observed.

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Investigations on Coherent population trapping resonances with coherently coupled lasers

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Coherent population trapping (CPT) is a resonance phenomenon due to a quantum mechanical interference effect in an atomic system. The resonantly driven atomic level population is being trapped into a superpositional dark state, yielding the atomic medium transparent for the exciting electromagnetic fields. The observation of this effect requires a special electronic structure ($\Lambda-$System) and suitable lifetimes which can be found e.g. in alkali atoms. The vanishing absorption leads to a reduction of fluorescence light intensity and the atomic vapor appears darker, therefore the designation as a 'dark resonance'. The width of these CPT-resonances can be extremely small, so that they are of particular interest in precision measurements as well as in applications in magnetometry or as a CPT-atomic clock.

A condition for observation of narrow CPT-resonances is a coherent bichromatic light field. Therefore an optical phase lock loop (OPLL) laser system[1] is used. This system consists of a pair of phase stable coupled lasers. With a special design of the OPLL servo electronics a good phase noise performance and thus a good signal to noise ratio of the CPT dark resonances is achieved.

In our experiments investigations on CPT-resonances in buffered ^{87}Rb thermal vapor cells were made. We studied the behavior of CPT-resonances using magnetic hyperfine sublevels of the ^{87}Rb D_1 line in dependence of the transmitted laser power for different beam diameters and cell temperatures. In these experiments CPT-resonance line widths down to 25 Hz were achieved. In the latter case the width of the CPT-resonance is mostly limited by time of flight broadening effects of the diffusive motion of the Rubidium atoms in the buffergas (40 Torr Ne in our case). The dependence of the CPT-resonance width on the temperature can be qualitatively explained by spin exchange collisions and a line narrowing due to optical thickness.

The presented data material is interesting in fields like magnetometry or CPT atomic clocks where optimized parameters of the CPT-resonances - on the ^{87}Rb D_1 line - are needed in order to reach maximum performance.

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Experimental Hyperfine Structure Investigation in Cobalt I

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In continuation of our hyperfine structure studies of elements of the iron group [1,2,3] experimental investigations of the hyperfine structure in the spectrum of atomic Cobalt have been performed. The element Cobalt possesses just one stable isotope of mass number 59, whose nuclear spin is I = 7/2. The most recent hyperfine structure measurements on Cobalt were done by Pickering in 1996 [4] using high-resolution Fourier transform spectrometry in the region from 222 nm to 3000 nm. She published the magnetic dipole hyperfine interaction constants A for 297 energy levels.

In the present work we used laser spectroscopy methods to investigate the hyperfine structure: six transitions from 640 nm up to 660 nm have been measured using a cw ring-dye laser and optogalvanic detection in a gas discharge of a hollow cathode lamp [5]. The magnetic dipole hyperfine constants A of the six levels of odd and four levels of even parity have been evaluated. These values are compared with the values in reference [4].

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Spectator fluorescence of n_cp^{4}nℓ n$'\ell'$ doubly excited states in KrI and ArI below the satellite threshold

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Cross sections for the production of n_cp^{4}nℓ ($\ell = $ s, d) satellites in singly charged rare gas ions can be determined utilizing the photon induced fluorescence spectroscopy (PIFS) [1] via measured fluorescence intensities emitted on $n\ell \rightarrow n_c$p transitions. The $n\ell \rightarrow n_c$p fluorescence in the doubly-excited n_cp^{4}nℓ n$'\ell'$ configurations of the atom becomes important in the proximity of the satellite threshold when the $n\ell n'\ell' - n_c$p$\varepsilon\ell''$ Auger decay competes with the $n\ell \rightarrow n_c$p radiative decay. The fluorescence with the $n'\ell'-$ electron as a spectator is observed as a 'shift' of the satellites' threshold measured by the PIFS technique. This 'shift' can be used for measuring the ratio of the Auger and radiation rates in case the 'real' position of threshold is known. The latter quantity can be either taken from photoelectron measurements or from energies of the members of the Rydberg series measured via PIFS [2].

In the present paper the cross sections for the production of 3p^4 (^{3}P)4s ^{2}P$_J$, 3p^4 (^{3}P)4s ^{4}P$_J$ satellites in ArII and 4p^4 (^{3}P)5s ^{2}P$_J$, 4p^4 (^{3}P)5s ^{4}P$_J$ satellites in KrII were measured by PIFS. The positions of the thresholds for the n_cp^{4}ns ^{2}P$_J$ satellites were measured as the convergence point for the n_cp^{4}ns ^{2}P$_J$ n$'$p Rydberg series. The spectator ns $\rightarrow$ n$_c$p fluorescence in n_cp^4 (^{3}P)ns ^{2}P$_J$ n$'$p doubly-excited states of ArI and KrI was measured for the first time. The 'shift' of the threshold due to the spectator fluorescence in Ar and Kr amounts to 1–6 meV. This value is less than the 'radiation shift' of the Ne 2s– threshold estimated using the data of [3] as 16 meV.

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Fine structure of even configuration system of lanthanum atom

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The fine structure (fs) analysis of the even levels of lanthanum atom has been performed with the method of level-fitting procedure for the extended system of the 52 interacting configurations : $5d^3$, $5d^2n's(n'=6\text{-}11)$, $5d^2n''d(n''=6\text{-}11)$, $5d^2n'''g(n'''=5,6)$, $5d6s^2$, $5d6sn's(n'=7\text{-}11)$, $5d6sn''d(n''=6\text{-}11)$, 5d5g6s, 5d6s6g, $5d6p^2$, 5d6p7p, 5d5f6p, 4f5d6p, 4f6p6d, $6s6p^2$, 6s6p7p, 4f6s6p, 4f6s7p, 4f6p7s, 5f6s6p, $6s^2n's(n'=7\text{-}11)$, $6s^2n''d(n''=6\text{-}11)$, $4f^26s$.

Our semi-empirical method includes, beside the electrostatic and spin-dependent interactions (represented by the Slater integrals F^k, G^k, the spin-orbit integrals ζ_{nl} and radial integrals R^k, characterizing interconfiguration electrostatic interactions), also the interactions with distant configurations. The second-order effects were represented by three-body parameters T_2, T_3, Ts and by electrostatically correlated spin-orbit interaction parameters $E-C^k$, Q^k. The energy matrix for the system given above consists of 9 J-submatrices (maximum rank of the J-submatrix is 368) and includes 3359 electrostatic and spin-orbit radial parameters, which can be taken into account as free, dependent or fixed parameters. The number of free parameters has been reduced to 58 by applying the relations based on the effective quantum numbers. In the fitting procedure of 130 experimental energy levels [1] good agreement between observed and calculated values of energy and g_J Lande factors was achevied.

The fine-structure analysis enables to determine quantitatively the effects of the interactions between the configurations constructing the system under study.

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The calculations were partially performed at Poznan Supercomputing and Networking Center.

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Hyperfine structure investigations of europium atom

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The hyperfine structure (hfs) and the isotope shift (IS) of more than 100 transitions between $4f^7 5d6s$ configuration and some even configurations of ^{151}Eu and ^{153}Eu have been studied with the method of laser induced fluorescence (LIF) in the hollow cathode discharge. For each of the transitions investigated the LIF signal in selected fluorescence channels has been recorded.

The investigated transitions within two spectral ranges have been excited by stabilized tunable single-mode ring dye lasers (Coherent, model 699-21), operating on Rhodamine 6G in the spectral range of 570-605 nm, and on Stilbene 3 in the spectral range of 410-460 nm. Fluorescence channels have been selected by a grating monochromator.

The upper even levels have been chosen on the basis of the fine and hyperfine structure interpretation of extended configurations system of Eu I performed by Dembczynski [1].

The hfs magnetic dipole A and electric quadrupole B constants of more than 30 even levels for both isotopes have been determined for the first time. A good agreement between experimental and calculated [1] values of hfs A constants was observed.

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Analysis of the configuration interactions in the hyperfine structure of La atom

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High precision measurements of the hyperfine structure (hfs) splittings of electronic levels, especially by rf-spectroscopic methods make it possible to study even fairly complicated aspects of the interaction between electron shells and the nucleus, which can result in determination of the nuclear moments with high accuracy. We report the parametrization method of the hyperfine structure which takes into account simultaneously one and two-body effects appearing in the second order perturbation theory. The analysis of the hfs of the even configurations of La atom was performed in the basis of 16 configurations. The number of independent radial parameters was reduced by applying the relations between spin-orbit parameters or effective quantum numbers. In order to include the J-off-diagonal effects in the hyperfine structure, direct diagonalization of the matrix containing J-diagonal as well as J-off-diagonal elements was performed. For 21 energy levels with precisely measured hfs A and B constants [1-3], the corrected values of A and B were calculated. For the magnetic dipole hfs interactions, 14 independent parameters were used in the least-square fit of 29 experimental and calculated hfs A constants. The predicted values of the A constants were calculated for all levels in the energy region up to 40000 cm^{-1}. For the electric quadrupole hfs interactions, we use 7 parameters and 19 hfs B values respectively. The values of some second-order hfs parameters were determined.

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Observation of Alignment-to-Orientation Conversion in the Presence of an External Electric Field

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We have observed alignment-to-orientation conversion in cesium atoms under the influence of an external electric field. The effect results from the evolution of coherently excited atomic sublevels. The magnitude of the effect depends on the degree of mixing between these sublevels, and is therefore also a function of the Stark splitting of these sublevels in an external electric field. In our experiment, two counter-propagating laser beams excite the cesium atoms, first from $6^2S_{1/2}$ to $6^2P_{3/2}$, and then from $6^2P_{3/2}$ to $7^2D_{3/2}, 9^2D_{3/2}$, or $10^2D_{3/2}$. We observe the fluorescence from the excited states to $6^2P_{1/2}$ in the same direction as the exciting lasers. The first laser (852.35 nm) is polarized parallel to the electric field. The second laser is polarized at an angle of $\frac{\pi}{4}$ with respect to the first. These linearly polarized laser beams initially create an *aligned* ensemble of atoms. Alignment can be both longitudinal and transverse. Longitudinal alignment implies that the population of the magnetic sublevels varies with $|m_J|$. Transverse alignment refers to the coherence that is created between magnetic sublevels with $\Delta m = \pm 2$. On the other hand, an *oriented* ensemble of atoms shows an imbalance in the population of the $+m_J$ and $-m_J$ sublevels (longitudinal orientation) and a coherence between magnetic sublevels with $\Delta m_J = \pm 1$ (transverse orientation). We demonstrate the alignment-to-orientation conversion by observing that the fluorescence is circularly polarized. In our case, transverse alignment in an electric field is converted into transverse orientation. A similar effect in diatomic molecules was predicted in [1]. The fluorescence is observed with a PMT in photon-counting mode mounted behind a monochromator. Circularly polarized fluorescence light is converted to linearly polarized light by an achromatic quarter-wave plate. Behind the quarter-wave plate is an analysing polarizer, which is switched between vertical and horizontal polarization by computer control. The degree of circularity of the fluorescence is defined as the normalized difference between the intensities of vertically and horizontally polarized light detected after the quarter-wave plate. A computer varies the electric field throughout the experiment and the fluorescence intensity, electric field, and analysing polarizer position are recorded for analysis. We compare our measurements with the results of numerical calculations. Our model is based on a modification of the optical Bloch equations for two-step excitations. It is cast into the form of rate equations for Zeeman coherences [2]. The measured signals are in reasonably good agreement with our model. The calculations and measurements together shed light on the parameters governing the Stark splitting of the magnetic hyper-fine sublevels of cesium.

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Light storing in a medium of atoms in the tripod configuration

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Light propagation and storing in a medium of atoms in a tripod configuration i.e. one including three low-lying states coupled with the single upper state, driven by two control pulses are investigated theoretically in terms of two polaritons [1] and numerically. Contrary to the case of lambda system, which is usually examined in storage experiments [2], for the tripod configuration a single pulse is stored in a form of two atomic coherences. This enriches the dynamics and open new possibilities of a coherent control of light pulses. In particular light releasing in a case of a tripod system may be performed at a few stages and in a more flexible way then for a double lambda system [3]. It is shown that magnetic field switched on at the pulse storage state changes the phase relations between the atomic coherences due to the stored pulse, which leads to an essential modification of the released pulse.

In the present paper the system of the Maxwell-Bloch equations is presented and their approximate solutions are discussed in terms of two polaritons. An evolution due to an additional interaction at the storage stage, which does not cause transitions but changes the phase of the coherences, cannot be described in term of polaritons but its creates new initial conditions for polariton's evolution at the release stage. For proportional control pulses we give simple analytical predictions of the released pulse and for the values of the coherences which will remain trapped in the medium. The numerical illustration of the theoretical results and the verifications of our predictions in the case of ^{87}Rb in the situation in which the additional interaction is due to a constant magnetic field parallel to the direction of propagation are presented. We also demonstrate the pulse evolution if at the release stage the two control pulses are not switched on simultaneously.

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Dark resonances in the D_2 line of ^{87}Rb in the vapor cell with co- and counter-propagating waves

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We have tested experimentally the recent theoretical predictions [1] of high contrast electromagnetically induced transparency (EIT) in ^{87}Rb with counterpropagating σ^+ and σ^- bichromatic waves. According to the calculations, the resonance amplitude on the D_1 line increases nearly ten times at laser intensities of about 10 mW/cm^2, compared to the running circular waves [1]. Because of the periodic spatial dependence of the resonance amplitude the phenomenon can be seen only if the cell length is shorter then the period of the amplitude modulation, i.e., $\pi/(k_1 - k_2)$. It is assumed that k_1 and k_2 are wave vectors of two beams that couple booth ground hyperfine levels to the common excited state hyperfine level. In this work, we have compared the EIT amplitudes, obtained in a Λ system between degenerate two hyperfine levels of the ^{87}Rb and the same excited $^2P_{3/2}$ level. Bichromatic co-propagating and counter-propagating (standing wave) schemes where used.

In the experiment, the pump laser is locked to the F=2 - F'=2 transition, while the probe scans F=1 - $^2P_{3/2}$ transition. Beams propagate through the gas cell with pure ^{87}Rb, held at a room temperature. The length of the cell is 10 mm. The pump and the probe laser intensities were 7 mW/cm^2 and 8.9 mW/cm^2, respectively. We have examined three configurations: when both lasers are linearly polarized and co-propagating; when lasers are σ^+ and σ^- polarized and co-propagating; and with σ^+ and σ^- counter-propagating waves. In the last case, the quarter-wave plate is placed between the Rb cell and the mirror that reflects most of the light back towards the cell. This allowes excitation of the Rb atoms by four beams. The transmission of booth beams (pump and probe) was measured with the photodetector.

The beams polarization induces the double Λ if both beams are offset by the hyperfine structure of the ground level, while coupling the common F'=2 excited level. The results revealed similar EIT amplitude in all three cases. Therefore, for laser intensities used in the experiment we could not measure an increase of the amplitude of the EIT with σ^+ and σ^- beams counter-propagating through the cell. The benefits from the counter-propagating scheme may not be present in the D_2 line where the EIT contrast is only few percents of the linear absorption. We have observed small spatial variation (less then 25%) of the EIT amplitude if the distance of the retro-reflecting mirror from the Rb cell is changed in the counter-propagating scheme. The period of the modulation is larger then 2.5 cm, as expected for the two wave vectors. In the configuration with the two linearly polarized traveling lights and at such high laser intensities, the EIT resonance starts to split into two peaks, i.e. into the double-dark resonance [2].

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Switching from electromagnetically induced absorption to transmission in CPT-Hanle experiment in ^{85}Rb

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We study experimentally and theoretically a coherent population trapping (CPT), electromagnetically induced transparency (EIT) and absorption (EIA) induced between Zeeman sublevels of the ground hyperfine level by the fixed frequency laser, locked to the transition to $^2P_{3/2}$ in ^{85}Rb, while magnetic field varies around zero.

Experimentally, the beam from the laser locked to either closed F=3 - F'=4 or open F=2 - F'=3 transition passes through the Rb cell placed inside the tube made of a double layer of μ metal. The solenoid around the cell determines the axial magnetic field. The laser polarization before the cell was either linear or σ. We investigate the Hanle-CPT effect detected in the laser light transmitted through the cell, while the magnetic field varies between - 500 mG to +500 mG.

The experiment have shown, for the closed transition and linearly polarized light, the onset of the transition from the EIA to the EIT at laser intensity of 2.6 mW/cm^2. The full transformation to the narrow EIT or dark resonance (with the full width about 100 mG) is achieved at 7.3 mW/cm^2. We are not aware of previous experimental reports on such transformations of resonances in CPT-Hanle effects using linearly polarized light. Previous calculations [1] have shown a disappearance of an EIA but not appearance of a dark resonance. The theoretical investigations [2] of an EIA, in closed degenerate two-level transition, have shown that under specific polarization of pump and probe laser (σ - σ or σ - π) and at higher pump laser intensity, an EIA peak splits into two absorption peaks and a transmission maximum in between. In the experiment the EIT is observed for the open F=2 - F'=3 transition. The width of the EIT changes from 120 mG to 530 mG (5.6 and 25 MHz, respectively) if laser intensity changes from 0.35 mW/cm^2 to 16.5 mW/cm^2. Circularly polarized light, at the closed transition, shows EIT peak whose width did not change noticeable with the laser intensity. In the case of the open transition and the circularly polarized light the dark state (EIT) is accompanied by a lateral bright state or the EIA. The amplitude of the EIA part of the spectrum is getting smaller as the laser intensity increases.

We use a semiclassical model of an atom and electromagnetic field, based on optical Bloch equations to calculate laser absorption for the closed atomic system. The full system of coupled equations for the coefficients of the density matrix for magnetic sublevels of F=3 - F'=4 is solved. The presence of magnetic field is included through the splitting of the Zeeman sublevels of the ground and excited hyperfine levels and corresponding Raman detuning from the resonant m_F=0 - $m_{F'}$=0 transition. The Doppler broadening was not included. The calculations show transition from the EIA to the EIT as well.

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Coherent manipulation and optical cooling of molecules

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Optical cooling and trapping of atoms has brought huge advances in the fields of spectroscopy: atom optics, atom interferometry, collision studies and quantum information processing. The step from atoms to molecules is complicated by the manifolds of rotational and vibrational molecular energy levels. Conventional magneto-optical trapping requires relaxation into a definite initial state, whereas population loss over the manifolds of rovibrational energy levels reduces the effectiveness of this technique for molecules. Previous attempts to create cold molecules have used: Feshbach resonances photo-associating pre-cooled atoms [1], cooling via a buffer gas [2] or time varying electric fields [3]. We hope to establish an all-optical approach to cool molecules directly.

We plan to investigate experimental techniques of manipulating atoms and molecules using coherent interactions, such as π-pulses to invert populations [4]. Doppler cooling can be amplified by coherently driving the molecules before spontaneous emission can occur. When used with a velocity selective interaction, this has the effect of 'folding' the velocity distribution instead of 'herding' the molecules from the edges of the distribution as in normal Doppler cooling. Another experiment involves *Interferometric cooling*[5]. In this scheme, atoms or molecules placed in a superposition using $\frac{\pi}{2}$-pulses, will have different phase evolution depending on their energy (including the kinetic term). By controlling the timing of $\frac{\pi}{2}$ pulses, the atomic states can be chosen to interfere constructively or destructively. This leads to a velocity selective force which can be used to cool the atoms or molecules. This will be the first experimental investigation of this recently proposed mechanism. The sequence of coherent quantum manipulations can be interpreted as quantum computing processes. It has been shown that one dimensional radiative coupling of momentum states produces a full set of quantum computing operations of a *Momentum state quantum computer* [6]. The quantum operation 'divide-by-two' acting on a velocity distribution could halve the distribution in one coherent step. This may lead to the new mechanism of *Algorithmic cooling*.

All the experiments will take place in a rubidium magneto-optical trap. In order to create the set of coherent π pulses, we are building a phase controllable Raman laser source, with precise control of the frequency, phase, pulse shape and timing. We shall initially concentrate these experiments on atoms and move to molecules in the near future.

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Cut-Offs and Time Dependent Acceleration at Relativistic Shocks

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We briefly introduce the theory of relativistic shock acceleration and an eigenfunction method used to reduce the computational workload involved. We consider a uniform, isotropic, power-law distribution being swept up by a relativistic shock and compare the results with the non-relativistic theory. This power-law could, for example, have been created by another shock further upstream. The method of extending this to the time dependent system is shown.

A similar approach is then applied to the problem of synchrotron / inverse Compton losses with isotropic momentum independent diffusion and initial results are presented.

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Subsurface Imaging by Polarised Light Rejection for Assessment of Skin Blood Concentration

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A new technique for the investigation of microvascular tissue blood concentration is presented, based on the method of polarisation spectroscopy in superficial skin tissue. Linearly polarised light incident on the skin is partly reflected by the surface layers, and partly backscattered from the dermal tissue. Use of orthogonal polarisation filters over a light source and a CCD suppresses the reflections from the surface, and only the depolarised light backscattered from the dermal matrix reaches the CCD array. By separating the colour planes of an image acquired in this manner and applying a dedicated image processing algorithm, spectroscopic information about the amount of red blood cells (RBCs) in the underlying area of tissue can be discovered.

The algorithm incorporates theory that utilises the differences in light absorption of RBCs and dermal tissue in the red and green wavelength regions. Fluid models compare well to computer simulations in describing a linear relationship between output signal (called $TiVi_{index}$) and RBC concentration in the physiological range of 0-4%. Evaluation of the technique via application of a drug which widens microvascular blood vessels (thus increasing blood concentration in the region) displayed a heterogeneity pattern of the blood concentration, which is typical of the vasoactive agent. Extension of the technique to capture and process continuous real-time data creates a new possibility of online real-time image processing. Application of tissue viability ($TiVi$) imaging include skin care products and drug development, as well as investigations of microvascular vessel growth due to infections, burns, skin grafts, and skin cancers.

Temporal and Spatial Study of Laser-Produced Lithium Plasmas

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Emission imaging and spectroscopy of laser produced plasmas are powerful techniques used to characterize plasma plumes. They have found industrial applications in many areas such as pulsed laser deposition (PLD), where they are used to monitor plasma parameters during the growth of thin films. Recently however, these techniques have been used to study the collision and interpenetration of two counter propagating laser produced plasmas. Spectrally filtered imaging can provide information concerning the dynamics of the collision, such as plume velocities and spatial distributions of emitting species in the plume; whereas spectroscopy provides basic plasma parameters such as electron densities and temperatures. Our initial goal is the detailed characterization of the expansion dynamics of single Lithium plasmas. We will present spectrally filtered images tracking the evolution of neutral and singly charged components of Lithium plasmas; as well as temporally resolved spectroscopic images, from which, we have extracted electron temperatures and densities using relative intensities and the stark broadening of the Lithium lines.

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Multi-Fluid Simulations of Colliding Plasmas

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Single fluid models used to describe colliding plasmas are extensively used in the research community. They can be used to describe the high density stagnation regions where the mean free path is very short and significant stagnation occurs. However, they do not allow interpenetration of the interacting plumes in plume coronal regions, where the mean free path becomes longer allowing interpenetration of the colliding plumes. In these cases, a multi-fluid description becomes necessary to adequately analyse the collision region. Multi-fluid descriptions treat each species as separate fluids and do allow for interpenetration and stagnation where they occur. Here, a multi-fluid description for colliding plasmas is utilised to analyse this region in colliding lithium plumes where interpenetration and stagnation may occur for variant mean free paths arising from differing plume conditions.

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The Evolution of Self-Absorption in the $3p^6 4s$–$3p^6 4p$ Ca^+ Doublet.

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Emission spectroscopy of laser produced plasmas is one of the most important diagnostic tools in use today for measuring fundamental plasma parameters such as electron densities and temperatures. It is often used in applications such as pulsed laser deposition in order to characterize the composition of the plumes used for thin film deposition. The majority of spectroscopic systems currently in use either spatially select small regions of the plume whilst integrating over time or they take a space-averaged spectrum at a specific time. Using spectra acquired in this manner to calculate temperatures and densities can lead to serious errors when using lines from high oscillator strength transitions. Such lines can be subject to significant attenuation and concomitant errors on the determination of basic plasma parameters. We will present time resolved spectroscopic images of Calcium plasmas, which clearly illustrate the effect of self-absorption.

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EUV Aluminum laser plasma studies: Time and Space resolved emission and ionization temperature determination, and enhanced ionization temperature, line and continuum emission via plasma confinement.

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EUV grazing incidence spectroscopy is utilized in studying the emission properties of aluminium and highly charged ions in the regions below 33 nm. Ablation of an aluminium target is achieved via a Nd:Yag glass laser, of energy 0.78 J, 16nsec (FWHM) at the fundamental (1.064 mm).

Firstly laser ablation of a planar aluminium target is studied. The emission profile of various lines in the wavelength range 24 nm to 32.8 nm (51eV-37.8eV) are mapped over a spatial range of 1.8 mm from the target surface and a temporal range of 42nsec after the termination of the laser pulse. Time and space resolved ionization temperatures (Tionz) are calculated for 53 pairs of successively charged ion stages ranging from ALV to ALIX. The peak temperature of each space-time profile is noted, and plotted against the energy difference of the upper level between each ion pair used. A statistical trend of increasing peak ionization temperature with increasing upper level energy difference is presented.

Secondly, emission from a confined laser plasma is achieved via generation of the plasma within a confining rectangular target of dimensions 1.2mm, and depth 3.5mm. The space-time profiles of the ionization temperature (Tionz) are determined from the intensity ratio of ALVII(309 Å)/ALVI(312 Å). In comparison to using a planar target, large increases in the peak ionization temperature, and the area over which the peak exists are observed in the confined laser plasma. The space-time profile of the line width of ALVI(312.237 Å) is also measured for both targets. No increase in the peak line width is observed in the confined plasma, however the space-time profile of the line width was substantially different to that observed in the planar target. Both early phase continuum and late phase line emission are observed to be enhanced in the confined plasma in comparison to plasma undergoing free expansion.

Visible Imaging and diagnostic study of laser plasma plume dynamics with various target configurations.

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Many studies of plasma plume behaviour have been carried out on the effects of electric and magnetic fields, ambient gas pressures, and laser dependent parameters (pulse duration, wavelength and energy). In this work we have investigated plasma generation and evolution under various target configurations. These include planar targets, parallel plates and rectangular cavities. To study the effect of confinement, gated visible ICCD imaging of the expanding plume was utilized to observe the dynamics of the plumes expansion. Using space and time resolved visible emission spectroscopy, space and time resolved N_e, T_{ion} and T_e values were calculated from the emitted spectra for all target geometries employed.

Low-Level Sulphur Detection in Steels using Deep VUV Laser-Induced Plasma Spectroscopy

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Limits of detection for sulphur in steels are investigated using time-integrated Laser-Induced Plasma Spectroscopy (LIPS) in the deep VUV spectral region. Light elements ($Z \leq 20$) have their strongest characteristic emission lines in the VUV, and detection sensitivity may be improved compared to LIPS experiments in the visible or near UV regions. Light elements are industrially important when considering some of the physical and chemical properties of almost all types of steel. Good reproducibility of spectra means that LIPS has the potential to be used as a reliable method for online quality assessment as it can be performed quickly and to a reasonable degree of sensitivity. It has been reported in the literature that heavier elements have been detected at ppm levels [1], light elements have also been detected to the same degree [2].

A novel approach to LIPS used in our laboratory means that we observe spatially-resolved VUV spectra from the plasma, obviating the need for time-resolved detectors since light from the broadband continuum close to the target surface is not captured. This means that a back-illuminated VUV sensitive CCD detector can be used, which provides excellent resolution and sensitivity. Various different ionization stages are detected at different distances from the target surface using this method. A range of experiments has been carried out in order to evaluate the optimum measurement parameters for sulphur in steel plasmas. Performances based on changing parameters such as laser pulse intensity and focus have been studied, in addition to the effects of different ambient gases at various pressures. The results suggest an optimum set of experimental conditions.

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POSTER SESSION P2

Fluorescent and forbidden transitions in Fe III

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The configuration interaction code CIV3 has been used to examine both fluorescent and forbidden lines in doubly ionized iron, which have been highlighted by Johansson et al [1]. We centred our optimisation process on the lower ^7S and $^7P^o$ states, and so our initial investigation involved the allowed transitions $a\,^7S_J - {}^7P^o_{J'}$. Some initial results are given in the table below.

Table 3: f-values and A-values for $a\,^7S_J - {}^7P^o_{J'}$ transitions

g_l	g_u	ΔE (cm^{-1})	f_l	A_l ($\times 10^8\,\mathrm{s}^{-1}$)
$a\,^7S_J - z\,^7P^o_{J'}$				
7	5	51912.89	0.214	5.40
7	7	52245.08	0.302	5.49
7	9	52757.75	0.392	5.66
$a\,^7S_J - y\,^7P^o_{J'}$				
7	5	136055.79	0.0029	0.50
7	7	136163.90	0.0038	0.47
7	9	136332.49	0.0044	0.42

Using the same set of radial functions, this work has been extended to examine both electric dipole transitions and intercombination lines from the a^5D_J ground state to the lowest $^5P^o_{J'}$ and $^7P^o_{J'}$ respectively, and some comparisons have been made with existing atomic data ([2] and [3]). In addition, we include results for the electric quadropole transition $a\,^5D_J - a\,^5S_2$, and once again relevant comparisons have been made.

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Atomic Structure under external confinement: Effect of dense plasma

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Spectroscopic properties of one and two electron ions have been investigated under dense plasma environment. Ion Sphere (IS) model has been adopted to estimate the effect of dense plasma on the structural properties like the ionization potential, low lying excited states, oscillator strengths and transition probabilities of several isoelectronic ions of hydrogen and helium. The ion sphere model assumes the overall charge neutrality inside a sphere called Wigner-Seitz sphere, the radius of which is determined by the plasma electron density. This is an external confinement which produces a potential felt by the valence electrons, different from that experienced by the free ion. The overall effect of the plasma is to reduce the ionization potential, thereby pushing the system to gradual instability with increased plasma coupling. The linear response of the systems leading to the study of their excitation properties have been estimated by using time dependent variation perturbation theory. The response properties have been calculated by using finite basis sets satisfying certain boundary conditions. The number of excited states has become finite and the structural properties change systematically with increased plasma density. Interesting trends are observed along the isoelectronic sequence.

The $5d$ photoabsorption spectra of Pb III and Bi IV

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Investigations of multicharged ions with partially 5d-subshell are of interest owing to the complexity of the 5d spectra caused by intermediate coupling and the large electrostatic interaction between the configurations. Past studies on lead and bismuth showed this to be the case [1-7] with support being sought from isoelectronic regularities to help explain the spectra. Photoionisation data from these studies also provides useful information, for example, in the electronic and magnetic properties of thin films [8-9].

We present the photoabsorption spectra of lead and bismuth ions recorded using the dual laser plasma (DLP) technique [10], in the photon energy range 30 - 65 eV. The experimental observations and theoretical calculations are focused on the 5d-inner shell excitations of the Hg I like ions of lead (Pb III) and bismuth (Bi IV).The lines recorded in the $5d$ photoabsorption spectra of Pb III and Bi IV have been identified with the aid of Hartree-Fock calculations [11] as $4f^{14}5p^{6}5d^{10}6s^{2} \rightarrow 4f^{14}5p^{6}5d^{9}6s^{2}\,np\,,mf$ $(6 \leq n \leq 11)$, $(5 \leq m \leq 15)$.

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The FERRUM project: Experimentally determined metastable lifetimes and transition probabilities for forbidden [TiII] lines observed in η Carinae

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The FERRUM project is an international collaboration aiming to produce reliable oscillator strengths for singly ionized iron group elements of astrophysical interest [1]. A new and very specific branch within the project is to measure lifetimes of metastable states and to determine absolute transition probabilities for parity-forbidden lines, i.e. transitions between levels of same parity.

In the spectrum of an emission line region ejected from the massive star Eta Carinae, called the Strontium filament (SrF), forbidden lines from many elements, in particular [SrII] and [TiII], are observed [2]. These lines are strong in this specific region and valuable for plasma diagnostics. Forbidden lines are not easily produced in laboratory light sources and the atomic parameters for these lines can thus not be measured in a straightforward way.

We have previously reported on measurements of a long lifetime (28 s) of the $3d^2(^3P)4s\ b^4P_{5/2}$ level in [TiII] [3]. In the present paper four additional experimental lifetimes in [TiII] are measured using the laser probing technique (LPT) [4]. We use a combination of laboratory and astrophysical measurements to determine transition probabilities for the [TiII] lines. Branching fractions from some of these levels are derived from Hubble Space Telescope/STIS spectra of the SrF. The astrophysical branching fractions are combined with the experimental lifetimes to determine absolute transition probabilities.

We report lifetimes for the [TiII] levels $b^4P_{3/2}$, $b^2P_{1/2}$, $c^2D_{3/2}$ and $c^2D_{5/2}$, in the range 0.29-17 s, and transition probabilities for eight parity forbidden lines from the levels $c^2D_{3/2}$ and $c^2D_{5/2}$, along with uncertainty estimates.

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Large scale CIV3 calculations of fine-structure energy levels and lifetimes in Mg-like iron, cobalt and nickel

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A large scale configuration-interaction (CI) calculation is performed of excitation energies for 132 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, 3p4p, 3p4d, 3p4f, $3d^2$, 3d4s, 3d4p, 3d4d, and 3d4f configurations of Fe XV, Co XVI, and Ni XVII, using very extensive CI wave functions [1]. In this calculation we considered up to two electron excitations from the valence electrons of the basic configurations and included important correlation effects in the excitation to the 5g orbital. A large number of configurations are used to ensure convergence. These configurations represent all major internal, semi-internal and all-external electron correlation effects [2]. The important relativistic effects in intermediate coupling are incorporated through the Breit-Pauli approximation [3] via spin-orbit, spin-other-orbit, spin-spin, Darwin and mass correction terms. Small adjustments to the diagonal elements of the Hamiltonian matrices have been made so that the energy splittings are as close as possible to the experimental values. These adjustments improve the accuracy of the mixing coefficients which depends in part on the accuracy of the eigenvalues. This is a justifiable fine-tuning technique and is particularly useful for the calculation of intercombination lines [4]. These adjustments also affect the composition of the eigenvectors slightly. In a way, they correct the *ab initio* approach for the neglected core-valence correlation. Our calculated excitation energies, including their ordering, are in excellent agreement with the available experimental results. We predict new data for several levels where no other theoretical and experimental results are available. The mixing among several fine-structure levels is found to be very strong, with most of the strongly mixed levels belonging to the 3s4p, 3p3d, 3p4p, 3p4d, 3p4f, 3d4p, and 3d4d configurations. The enormous mixing among several fine-structure levels makes it very difficult to identify them correctly. Perhaps, that may be the reason for the lack of experimental results for these levels. We believe that our extensive calculated values can guide experimentalists identify the fine-structure levels of these ions. From our radiative decay rates, we have also calculated radiative lifetimes of some fine-structure levels and the results are compared with the experimental data and the other available calculations. Our calculated lifetimes (in ns) of 3s3p($^3P_1$) level in Fe XV (26.60), Co XVI (17.81), and Ni XVII (12.68) are in excellent agreement with the corresponding experimental values (26±2.6; 17.5±1.5; 12±1) of Trabert et al. [5] compared to other available calculations.

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A model approach for calculating alignment and orientation of photoionized open shell atoms.

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The availability of third generation synchrotron beam sources allows for accessing detailed information of the electronic structure of atoms by observing the photoionization products. This can be achieved either by detecting the photoelectron, or, alternatively, by observing the residual ionic state after photoionization of an inner electronic shell, e.g. via subsequent Auger decay or fluorescence emission from the excited ionized state. This yields information in terms of alignment and orientation which are related to deformation and spatial orientation of the electronic charge cloud, and to non-statistical population of the magnetic sublevels, respectively. Most experimental and theoretical investigations, however, have been performed on closed shell atoms.

For open shell atoms, the theoretical description remains principally the same, though, its numerical calculation leaves us with the severe task to deal with more than one open shell for the general case which usually requires non-trivial approaches. This is illustrated by the fact that, to our knowledge, until today numerical photoionization data for alignment and orientation of open shell atoms are sparse.

Berezhko *et al.* calculated the alignment of the $4d$ shell of Cs and of the $3p_{3/2}$ shell of Ge [1]. Numerical open shell data for the orientation are, to our knowledge, not available.

Only in the beginning of the century Yamaoka *et al.* reported on numerical alignment data for the $2p$ shell of Au and Pb[2]. However, all investigations avoided a full open shell approach. Due to this lack of numerical data, the situation is even less advanced for photoionization experiments involving inner shells of open shell atoms. There is one experiment measuring the alignment of the Er $2p_{3/2}$ subshell[3]. The only other experiment has been carried out recently again by Yamaoka *et al.* measuring the $2p_{3/2}$ shell alignment of Au[4].

We are trying to overcome the existing numerical difficulties by proposing a model for calculating alignment and orientation for open shell atoms by relating the dipole matrix elements of the open shell configuration to those of a closed shell system. This allows for determining observable parameters like alignment and orientation of an open shell system though avoiding a complicated and usually non-trivial numerical open shell approach. In order to illustrate the model, Hartree-Fock calculations of alignment and orientation have been performed for the L_3 photoionization of K, Sc and Mn, and for the M_5 and N_7 photoionization of In and Tl, applying different numerical approaches. Dramatic effects have been found for Mn. The model and our results will be presented at the conference.

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Radiative decay of doubly excited helium states

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The decay of doubly excited helium states below the N=2 threshold, cascading radiatively over three steps into the He ground state, were investigated using the photon-induced fluorescence spectroscopy (PIFS) at BESSY II, following a first spectral analysis of the emitted fluorescence radiation [1].

A theoretical description was published [2] from which absolute cross sections can be derived as the product of the resonant excitation cross section of the doubly excited states and their fluorescence rates to decay into the singly excited 1sms(^{1}S) and 1smd(^{1}D) states. Our measurements allow to test the calculated cross sections for the first time on an absolute scale, and branching ratios on a relative scale, which confirm the calculations.

For the three doubly excited singlet states (sp,2n+)(^{1}P), (sp,2n−)(^{1}P) and (pd,2n)(^{1}P) we observe a characteristic decay pattern depending on the radial quantum number A=+1, −1 and 0. We have investigated the n-dependency concerning the strongest decay channels. The (sp,2n+)(^{1}P) states prefer to decay into the 1sns(^{1}S) states, whereas the (sp,2n−)(^{1}P) states prefer to decay into 1s(n−1)d(^{1}D)states and the (pd,2n)(^{1}P) states decay predominantly into the 1snd(^{1}D) states. In addition the angular distribution of the fluorescence radiation was measured. The results are in good agreement with theoretical predictions.

Furthermore, the weakening of the LS coupling scheme and the mixing between singlet and triplet states in helium was confirmed by observation of the 1s6d(^{3}D$_{0,1,2}$) → 1s2p(^{3}P$_{0,1,2}$) transition on a doubly excited singlet state as well as triplet state.

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An anomalous behaviour of cesium atoms orientation in the argon-nitrogen afterglow. Rotational polarization of the nitrogen molecules

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At the investigation of spin-exchange collisions between optically oriented cesium atoms and nitrogen atoms Cs(↑) + N(↓) ↔ Cs(↓) + N(↑) this process is the main relaxation process for Cs oriented atoms in the $Cs - N_2$ gas discharge the very slow (∼ sec) recovery of the cesium atoms spin orientation was observed when the gas discharge has been switched off. The result of such a process is a polarization of the N atoms. At the recombination of the spin-polarized N atoms the polarization can be transmitted to the N_2 molecule. The standard setup for investigating of the optical orientation of alkali atoms has been used.

In order to produce nitrogen atoms the high frequency gas discharge was excited in the extension of the spherical gas-discharge chamber containing the metallic cesium and a mixture of N_2 (2 torr) and Ar (40 torr) at room temperature. The cesium atoms were optically oriented and the signal of magnetic resonance of these atoms was observed. When the discharge is switched off the cesium orientation recovery takes place. At the beginning of the afterglow ($0 < t < 0.5sec$) the cesium spin orientation varies very slow. In the late afterglow ($0{,}75 < t < 1{,}75sec$) the cesium orientation increases linearly. The such behaviour of cesium orientation can be explained by the existence of two processes which take place simultaneously: the brief increasing of the N-atom concentration in the initial moment of the afterglow in the spherical part of the chamber and the decay of the N-atom concentration as a result of the three particle recombination process ($N + N + Ar \rightarrow N_2 + Ar$). The mechanism of the nitrogen atom increasing in the early afterglow is not yet established (for example, it can be caused by the continued diffusion of N- atoms from the discharge zone to the observable zone). From the time dependence of the orientation in the late afterglow we estimated the rate constant of the three body volume recombination K_r. The value $K_r \cong 2 \cdot 10^{-32} cm^6 mol^{-2} sec^{-1}$agrees with the results of previous works (the investigations of the unpolarized particles afterglow) in which the values of the Kr were found in the interval from 0,78 to $3{,}44 \cdot 10^{-32} cm^6 mol^{-2} sec^{-1}$ [1,2]. The mechanism of the N atoms recombination involves nitrogen atom recombination into the $N_2(A^5\Sigma)$ state [2]. At the conservation of angular momentum during the interaction the transfer of angular momentum from atoms to molecule takes place (as for O_2 molecules [3]) leading to the spin-polarization of the N_2 molecule. The redistribution of angular momentum between electron spin system and rotational system in the N_2 molecule results in rotational polarization of the molecule too.

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Imaging of phase space of trapped ion cloud by observation of spatial distribution of Doppler shift

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The optical-microwave double resonance technique being applied to trapped ions allows for measurements of hyperfine splitting with extremely high precision. This experimental data are indispensable for example in determination of such fundamental properties of nucleus and atomic electronic shell as g_I- or g_J-Lande factors. Since hyperfine interactions lead to superposition of the atomic states with various angular momentum of atomic electronic shells, to couting the breakdown of J as a good quantum number, the appropriate and accurate analysis of experimental data requires the ones on higher laying, mainly metastable, levels. However the investigation of them in radiofrequency trap meets a difficulties when increasing their occupation number. The depletion of metastable levels are caused essentially by collisions which are strongly dependent on spatial distribution of charge and momentum of trapped ions. A lot of work has been done on dynamics, collisions, space-charge effects (see references in [1,2]) for ions trapped in radio-frequency ion trap. Searching for more efficient pumping of the metastable states of Pr^+ and optimizing the detection of the fluorescence light the direct observations with the use of ICCD have been performed for the spatial distribution of the Doppler shift of excitation transition wavelength. The phenomenon has been recorded during the scan of the wavelength of the laser radiation which excites the ions. In similar manner the formation of the ion cloud in the trap has been registered while increasing the pressure of buffer gas. The effects can serve for reconstruction of classical phase space of trapped ions and buffer gas environmental condition.

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Single- and two-photon ionization of Sr

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The investigation of singly charged ions in Paul traps is of strong current interest, since it may become possible to use these ions within trapped-ion qubits. In order to develop these systems, the efficient loading of traps with ions of specific isotopes is a prerequisite. One of the schemes employed at present is isotope-selective two-photon ionization. Absorption of the first photon links the ground state with an excited state, while absorption of the second photon causes ionization. The frequency of the first laser is chosen such that it is tuned to the resonance frequency only for one particular isotope. This scheme has proven to be very successful for loading traps with Ca^+ ions [1,2]. However, this scheme is not only applicable to the generation of Ca^+ ions with specific isotopes, it can be used as well for many other atoms, for example Sr.

The availability of theoretical data on photoionization of excited states would be of signficant benefit to experimentalists in order to estimate beforehand which intermediate state would provide the most efficient scheme. Previously, we have performed single-photon and two-photon ionization studies of the ground state [3] and investigated single-photon ionization of the 4s4p ^{1}P state of Ca to assist the interpretation of trap-loading experiments [2,4]. The same type of approach can be applied to other alkaline-earth atoms such as Sr.

In the present contribution, we investigate single- and two-photon ionization of the ground state of Sr and single-photon ionization of the 5s6p $^1P^o$ state of Sr. The ionization cross sections are obtained using B-spline basis sets and R-matrix Floquet theory. To describe the valence electrons in Sr, we adopt a model-potential description developed by Aymar and co-workers [5]. We find that the single-photon ionization cross sections of Sr show the same characteristics as the cross sections for Ca, but that the similarities disappear for two-photon ionization with final states below the 4d (3d in Ca) threshold. Two-photon ionization with final states between the 4d and 5p thresholds of Sr^+ is dominated by the intermediate 5s6p $^1P^o$ resonance.

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Benchmark results for multiphoton ionization of helium at 390 nm

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We compare single-electron ionization rates of He obtained by the R-matrix Floquet (RMF) approach with those derived from the direct solution of the time-dependent Schrödinger equation. The calculations are performed at 390 nm, a wavelength accessible to Ti:Sapphire lasers via frequency doubling. For intensities between 1×10^{14} and 2.5×10^{14} Wcm^{-2}, we find general agreement between the two approaches within 10% and we believe that this represents a substantial improvement in accuracy and reliability over previous models of intense-field laser-driven two-electron systems.

The time-dependent numerical integration (TDNI) is a finite-difference solution of the full two-electron Schrödinger equation for the helium atom [1]. Like the RMF method, the TDNI method contains no adjustable parameters. The quality of the numerical solutions and of the ionization rates is limited by available computational power rather than by approximations introduced into the model of the helium atom. In the present calculations the maximum measured errors in the energies of bound states, autoionizing states and autoionizing lifetimes are under 0.01%, 0.1%, and 1% respectively. In the TDNI approach, rate calculations are performed by observing the decay of electronic population within a sphere of radius 16 au centred at the nucleus.

The RMF calculations are carried out by combining RMF theory [2] with a B-spline-based inner region description [3,4]. In order to describe the minimum nine-photon ionization entailed, we need a substantial number of Floquet blocks. Hence to limit the size of the calculations, we have chosen to use a single target-state description of He^+: only the 1s state is included. Our Floquet expansion consists of a total of 31 Floquet blocks, of which 22 correspond to absorption and 8 correspond to emission. The maximum angular momentum included is L=13. At the intensities of interest, this corresponds to a total of 217 channels of which 98 are open channels. We obtain the Floquet R-matrix at an inner region boundary of 8 au following a diagonalisation of the inner region Floquet Hamiltonian. The R-matrix is then propagated out to 80 au.

Amongst the complex phenomena observed are several occurrences of channel closing, Rydberg series of intermediate resonances, and overlapping resonances leading to a very complicated spectrum. Despite the complexity, the agreement between results from the two approaches is excellent, and generally well within 10%. We thus believe that the present results can serve as benchmark results for multiphoton ionization of He at 390 nm.

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Metastable Kr^+ Ions in Intense Ultrashort Laser Pulses: Evidence for Recombination of the Field-Ionized Electron

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Perhaps the single most important aspect of intense field studies is the so called 'rescattering' of an ionized electron from its ionic core in a linearly polarized pulse. Elucidated in a seminal paper by [1] the process relies on the ionized electron being decelerated as it is ejected and subsequently re-accelerated towards the core as the polarized field oscillates. Acceleration in the external field, coupled with Coulombic acceleration and focussing leads to an energetic re-collision with the ion core. The narrow momentum distribution of the wavepacket leads to a very high probability of electron-ion interaction during the first few 'passes'. This opens up the fascinating prospect of studying electron-ion scattering phenomena, notoriously difficult to investigate in a conventional beam-beam approach [2], with the added bonus that the electron 'pulse' is on a femtosecond timescale.

Inelastic scattering via the processes of ion excitation and ionization have been widely observed as the non-sequential component of multiple ionization in intense fields. Measurements have been carried out by time-of-flight analysis of the ionized product [3], electron-ion coincidence [4] and COLTRIMS [5]. In the only experiment involving a prepared ion target we have demonstrated suppression of the non-sequential effect in double ionization [6].

For the current measurements an ion target, Kr^+, has again been used but the study has focussed on *metastable excited* ions present in the incident target beam. In this way electrons ionized from an excited state have been observed to recombine to the ground state of the incident ion. This is the first direct observation of recombination, although the process is known to play an important role in high harmonic generation.

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An Electrostatic Ion Trap for Studies of Quantum Molecular Dynamics

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The dissociation of H_2^+ by an intense laser field has been the focus of considerable theoretical and experimental study in recent years. This interest is not only due to the fundamental nature of the molecule, but as it has a vibrational period of 15 fs, the transition from classical (long pulse) to quantum (short pulse) nuclear dissociation dynamics can be studied with current laser technology. A severe limitation of the experimental work is that the H_2^+ is not formed in a well defined vibrational state, but has a population distribution. As the dissociation mechanism is strongly dependent on the vibrational level, it has proven difficult to elucidate a clear picture of the process.

We are developing a compact electrostatic ion trap to undertake the first femtosecond laser studies of a vibrationally cold molecular ion. Using HD^+ ions we will be able to produce ground state ions if they can be trapped for at least 300 ms. By irradiating the ions after this time we will detect the neutral H atoms produced and from their time of flight, the spectrum of the dissociation energy will be derived. We will be presenting the experimental concept and preliminary results of the trap's performance.

Influence of a static electric field on the rubidium D_2 line

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Influence of a static electric field on atomic levels (dc Stark effect) has been studied less extensively than that of a magnetic field (the Zeeman effect). This is because a more complicated technique is required in this case. In this thesis we propose and implement a rather simple technique, which allows one to study the dc Stark effect using a sealed-off cell with internal electrodes. An all-sapphire cell (ASC)[1] (15 mm-long, Ø 15 mm) with titanium electrodes and niobium feedthroughs has been developed, manufactured and filled with natural rubidium. The advantage of the ASC containing highly corrosive atomic vapors of alkali, alkaline-earth and other metals, is that it can operate at high temperatures for a long time without degradation. In the present work, the influence of 10 – 15 kV/cm dc electric field on atomic hyper-fine structure levels of the Rb D_2 line was studied. The experimental setup consisted of two saturation absorption schemes. The first one (assembled with an auxiliary Rb cell) served as a frequency reference for unshifted atomic transitions. The second saturation absorption scheme was based on the ASC with internal electrodes (room temperature). A laser diode with $\lambda = 780$ nm and spectral line-width of 5 MHz was used for resonant excitation of the atomic vapor. It was found that depending on the atomic transition, a decrease of the frequency of the transition in the range of 10 – 20 MHz (3 - 9 MHz) occurs when a dc electric field of $E = 15$ kV/cm ($E = 10$ kV/cm) is applied. The latter indicates that quadratic Stark effect takes place. The implemented technique for studying dc Stark effect is much simpler and more convenient than the atomic beam technique described in [1]. Note that the transparency of the sapphire windows in the UV (down to 170 nm) allows one to study the Stark effect in Rydberg levels (where huge Stark shifts are expected) with the help of an ASC. A theoretical calculation, which takes into account the hyperfine structure of the D_2 line in the case when the frequency shift is of order of the hyperfine splitting is performed. Note, that although the implemented technique based on saturated absorption scheme is simple enough, however the spectral resolution is limited by the natural line-width ~ 6 MHz of Rb D_2 line. The same limitation occurs also when one uses the atomic beam technique. The limited spectral resolution prevents resolving the substructure caused by the Stark effect on different Zeeman sublevels m_F of the hyperfine states. In particular, for $E = 10$ kV/cm the frequency separation between atomic transitions $F_g = 2$, $|m_F| = 2$, $F_e = 3$, $|m_F| = 1$ of ^{87}Rb is ~ 1 MHz. Usage of Coherent Population Trapping (CPT)[3] effect in the cells with internal electrodes can dramatically increase the spectral resolution of Stark spectra, which will allow one to resolve individual transitions between the Zeeman sublevels. Also, this will be helpful for more precise comparison of experimental results with numerical calculations. First results will be presented on the utilization of the CPT scheme for Stark-spectrum registration.

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Two-photon Optogalvanic Spectroscopy of the $5D[7/2]4 \longleftarrow 5S[3/2]2$ Transition of KrI Using a Titanium-Sapphire Ring Laser

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Sub-Doppler spectroscopy of electronic transitions in a discharge cell has usually been done by a method of saturated absorption or laser fluorescence spectroscopy. In an optogalvanic spectroscopy (OGS), the signal is detected as a voltage change at the ballast register when the laser frequency is resonant with the adjacent transition. This method is advantageous because the detection system is simpler and disturbances by the spontaneous emission from the plasma is avoided. We interested in the $5D[7/2]4 \leftarrow 5S[3/2]2$ transition of KrI reported by Cannon and Janik [1], who used a technique of resonance ionization mass spectroscopy. The sub-Doppler two photon OG signal is possibly detected in a good S/N since the virtual state is close to the $5P[5/2]3$ level and be useful as one of the frequency references in the near infrared reagion.

The laser beam from the Ti:Al_2O_3 ring laser (Coherent: 899-21) was focused into a laser galvatron (Hamamatsu Photonics) filled with Kr gas of a natural abundance and was reflected back by a concave mirror. The pumping power used was several 100 mW. An optical chopper was placed in front of the mirror to AM-modulate the counter propagating beam. The OG signal was lock-in detected with a considerable reduction of the Doppler background. The innner diameter of the hollow cathode was 3 mm and its length was 18 mm. The dc discharge current was 0.25 to 1 mA at a gas pressure of 100 to 200 Pa. The optical heterodyne method was adopted for the frequency measurments of line splittings. The second Ti:Al_2O_3 ring laser (Coherent: MBR-110) was frequency-locked to the reference cavity at a stability better than several MHz and was used as a local oscillator. The absolute laser frequency was measured using a wavelength meter (Burleigh: WA1500) calibrated against the Rb D_2 lines [2]. The frequency difference of 0.1 to 5 GHz between the two lasers was detected by a fiber coupled photo mixer (New Focus: 1554) and measured by a MW frequency counter. The frequency of the first laser was swept at a range of 3 GHz with a 1.5 MHz step using a PC system to record the OG signal and the MW frequency.

The OG spectrum was composed of the strong lines of $^{82,\ 84,\ 86}$Kr at the center and the much weaker hyerfine conponents of ^{83}Kr. The spectral resolution was restricted by the Lorentzian line width of 10 MHz. First the line profiles of even mass Kr were fitted and then subtracted to obtain those of ^{83}Kr. The hyperfine coupling constants of A and B and the isotope shift of ^{83}Kr were then determined. Although the results for the ^{83}Kr agreed with those reported within the experimental uncertainty, the isotope shifts for the even mass Kr deviated [1]. We present the specific mass shifts, the field shifts and the differences of the mean square nuclear charge radii determined by using the $5P[5/2]2 \leftarrow 5S[3/2]2$ transition as a reference line [3] combined with those determined for the $5P[K']J' \leftarrow 5S[K'']J''$ transition [4].

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Radiative lifetimes of $3p\,^2P^o_J$ in Boron-like Nitrogen

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The beam-foil installation of the University of Liège has been modified to detect and analyze light with a cooled low noise back illuminated CCD (capacity coupled device) detector which allows the recording of large chunk of spectra with high efficiency. This device has been used to record spectra of nitrogen and measure lifetimes which have been compared with previously measured values. The new setup, which allows simultaneous detection of the two lines of the $3p\,^2P^o$ term of N III (at 409.7, 410.3 nm), confirms some discrepancies in the decay curves of those levels which cannot be explained easily. We will discuss in details the analysis and the accuracy of this experimental work.

On the theoretical side, the rates of all radiative decay channels involving these levels have been evaluated recently by Froese Fischer and Tachiev [1] using the multiconfiguration Hartree-Fock-Breit-Pauli approach. No J-dependency was found by these authors, in line with the investigation of the LS-coupling in light boron-like ions [2], but in contradiction with present observation. We revisit systematically these radiative decay processes for all the allowed and forbidden channels, using the fully relativistic Multiconfiguration Dirac-Fock package [3]. The theoretical results will be compared to each other, hoping to point out some differential effects that could explain the observed J-dependency in the $3p\,^2P^o_J$ lifetimes measured with the improved beam-foil set-up of Liège.

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EUV photoabsorption of laser produced lanthanum plasma: LaV - LaVII

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The photoabsorption spectrum of La V - La VII has been recorded in the 76 - 96 eV region using the dual laser plasma technique [1]. $4d \rightarrow 5p$ transitions from the ground states of La V - LaVII were observed and identified with the aid of multiconfiguration Hartree-Fock calculations [2]. The excited states decay by autoionisation involving $5s$ or $5p$ electrons and rates for the different processes and the resulting linewidths were calculated and compared with experiment. Also observed and identified in the 80 - 91 eV region are transitions from $4d^{10}5s^25p^55d^1$ excited state of La IV and calculations indicate that two electron excitations contribute to the spectrum between 80 - 86 eV.

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Semi-empirical calculations of oscillator strengths in neutral tantalum and comparison with experimental data

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Semi-empirical oscillator strengths for Ta I lines have been obtained by combining theoretical branching fractions with experimental radiative lifetimes.

The calculations were performed using the pseudo-relativistic Hartree-Fock (HFR) method as developed by Cowan [1] in which we have incorporated core-polarization corrections as described in many previous papers (see e.g. [2,3]). These calculations were combined with a well-established least-squares procedure minimizing the discrepancies between the theoretical Hamiltonian eigenvalues and the energy levels determined experimentally by van den Berg *et al.* [4].

The experimental radiative lifetimes were taken from the work due to Salih *et al.* [5] who published values for 35 odd-parity levels between 18505 and 35498 cm^{-1} with the use of time-resolved laser-induced fluorescence on an atomic beam. Additional lifetimes for higher levels situated between 30665 and 45256 cm^{-1} were obtained in the present work by laser spectroscopy using the experimental set-up installed at the Lund Laser Centre (Sweden).

Our results were compared with the absolute transition probabilities reported by Den Hartog *et al.* [6] for 253 Ta I spectral lines.

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Lifetimes along perturbed Rydberg series in neutral thallium

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Thallium atom has been the subject of many lifetime investigations based on the use of a variety of experimental techniques. This includes a laser excited fluorescence technique in an inductively coupled plasma [1], the use of the after-glow of a pulsed r-f discharge [2], the phase-shift approach [3,4], the hook method [5], the double resonance [6], the level crossing [7], the Hanle effect [8] and the beam-foil spectroscopy [9-11].

Most of these investigations however are limited to a few low excitation energy levels (n<8). In view of the technical difficulties involved when measuring long lifetimes, a very limited number of studies have been devoted to the investigation of the behaviour of atomic lifetimes along the Rydberg series up to n-values higher than 8 [9,12,13].

In the present work, radiative lifetimes of 15 Tl I levels belonging to the $6s^2ns\ ^2S_{1/2}$ (n=7-14) and $6s^2nd\ ^2D_{3/2}$ (n=6-12) Rydberg series have been measured using a time-resolved laser-induced fluorescence technique. All the measured levels have been excited from the ground state $6s^26p\ ^2P^\circ_{1/2}$ with a single-step excitation process. The general perturbation of the ns series by the $6s6p^2$ configuration and the corresponding modification of the lifetimes are adequately reproduced by a theoretical model including core-polarization effects combined with a least-squares fit to the observed energy levels. The general behaviour of the lifetime values for the $6s^2np$ odd levels along the Rydberg series is also well reproduced.

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Photoionization using the Dirac R-matrix method

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The non-relativistic and Breit-Pauli R-matrix codes have been extensively used in atomic photoionization. A recent application is to the ions of the nitrogen isoelectronic sequence [1]. For heavier targets the Dirac R-matrix method is appropriate and has been implemented in the DARC code of Norrington and Grant [2,3]. Applications of DARC to photoionization have been few. Some test calculations together with photoionization of Hg are in the 1997 thesis of Bailey [3,4].

In recent years there has been a marked increase in the availablility of experimental cross sections, for example, the photoionization of low-charged ions of I, Xe, Cs and Ba [5]. Exploratory DARC calculations have begun to examine these ions.

The author will review the current capability of DARC for photoionization, summarise the earlier (unpublished) work of Bailey and describe the progress of current work.

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Static Electric Field Effect on Magnetic-field-induced Two-wave Mixing for determining M1/E2 amplitude ratio in Alkali Atoms

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The amplitude $U_B = U_{M1} + U_{E2}$ for the frequency summation, $\omega_1 + \omega_2 = \omega'$, of two laser waves with resonant frequencies ω_1 and ω_2, induced in alkali atoms by a magnetic field $\mathbf{B} = B\mathbf{e}_B$, includes the magnetic dipole M1 and electric quadrupole E2 matrix elements of radiation transition between doublet states $n_1\,{}^2P_{J_1} - n_2\,{}^2P_{J_2}$ and may be written as:

$$U_B = A(a_0\varphi_0 + a_1\varphi_1 + a_2\varphi_2), \tag{1}$$

where the factor A includes magnetic field and ac field amplitudes together with the radial matrix element of quadrupole transition between doublet resonant states $\alpha\omega_2\langle n_2\,{}^2P_{J_2}|r^2|n_1\,{}^2P_{J_1}\rangle$ ($\alpha = 1/137$ is the fine-structure constant) and matrix elements of dipole transitions between the ground state $n\,{}^2S_{1/2}$ and resonant states $n_1\,{}^2P_{J_1}$ of the energy $E_{n_1} - E_n = \omega_1 + \varepsilon$ and $n_2\,{}^2P_{J_2}$ of the energy $E_{n_2} - E_n = \omega' + \varepsilon'$ with complex resonance detuning ε and ε';

$$\varphi_0 = (\mathbf{e}_1\cdot\mathbf{e}_2)\left(\mathbf{e}'^{*}\cdot[\mathbf{n}\times\mathbf{e}_B]\right); \qquad \varphi_{1(2)} = (\mathbf{e}'^{*}\cdot\mathbf{e}_{1(2)})\left(\mathbf{e}_{2(1)}\cdot[\mathbf{n}\times\mathbf{e}_B]\right) \tag{2}$$

are the polarization dependent factors. The factors a_0, a_2 are linear combinations of ten fractions, six of which may include third order resonance singularities corresponding to a product of three detuning factors in denominators and four fractions may have only second order singularities. Eight of the ten fractions depend on the M1/E2 amplitude ratio

$$s = -\frac{5\alpha^2 Z_n\langle n_2P|r^{-3}|n_1P\rangle}{4\omega_2^2\langle n_2P|r^2|n_1P\rangle}. \tag{3}$$

The $a_1\varphi_1$ term in (1) comes from only the M1 interaction, therefore a_1 is directly proportional to s times a linear combination of eight fractions, four of which may include resonance fractions of the third order and four include those of the second order.

The electric field $\mathbf{F}_0 = F_0\mathbf{e}_0$ transforms the dipole forbidden mixing of two waves with frequencies ω_1 and ω_2 into the dipole-allowed one, described by the amplitude

$$U_F = \frac{4F_0}{3B}A(b_0\phi_0 + b_1\phi_1 + b_2\phi_2), \tag{4}$$

where the factors b include fractions with linear combinations of the second-order radial matrix elements for the dc-field induced electric dipole transition at the frequency $\omega_2 = \omega' - \omega_1 \approx E_{n_2} - E_{n_1}$ between resonant states, in numerator, and the E2 radial matrix element $\alpha\omega_2\langle n_2P|r^2|n_1P\rangle$, in denominator, times the combinations of fractions with the second-order resonance singularities determined by the products of two resonance detuning factors in denominators. The factors

$$\phi_0 = (\mathbf{e}_1\cdot\mathbf{e}_2)\left(\mathbf{e}'^{*}\cdot\mathbf{e}_0\right); \qquad \phi_{1(2)} = (\mathbf{e}'^{*}\cdot\mathbf{e}_{1(2)})\left(\mathbf{e}_{2(1)}\cdot\mathbf{e}_0\right) \tag{5}$$

determine dependence on the polarization vectors of ac and dc fields.

Due to interference between the electric-induced and magnetic-induced amplitudes, the polarization asymmetry effects may emerge, unobservable in pure magnetic field. The energy dissipation determined by the imaginary part of resonance detuning (the level widths) may cause the circular dichroism for incident waves and the circular polarization of the sum-frequency wave, generated by mixing linearly polarized incident radiation, $\mathbf{e}_1 = \mathbf{e}_0 = \mathbf{e}_B \perp \mathbf{e}_2 = [\mathbf{n}\times\mathbf{e}_B]$, with the degree of circular polarization directly proportional to the smaller and inversely proportional to the greater of the dc electric and magnetic field amplitudes, both to the real and to the imaginary parts of the resonance detuning, to the fine-structure splitting of the resonance level and to the M1/E2 amplitude ratio (1).

Observation of a Cs^*He_2 and discovery of a Cs^*He_7 exciplex in solid ^4He

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Cesium, the most polarizable of the stable alkali atoms, and helium, the least polarizable element of the periodic table, strongly repel each other in their ground states. This repulsion is due to the Pauli principle and is responsible for a variety of effects, such as the non-wetting of cesium surfaces by superfluid helium (and vice-versa) or the formation of atomic bubbles by alkali atoms embedded in superfluid or solid ^{4}He. However, when the Cs atom is excited to one of the 6^2P states it exerts an attractive force on surrounding helium atoms that leads to bound states, known as exciplexes. The structure of these complexes is determined by the spin-orbit interaction which deforms the shape of the alkali atom's valence electron distribution: helium atoms can be bound in regions in which the electron density and hence the Pauli repulsion are reduced.

Alkali-helium exciplexes have been studied in the past in cold helium gas, on helium nanodroplets, and in superfluid helium. The largest complex observed involving cesium was an apple-shaped Cs^*He_2 exciplex. It was speculated in the literature that complexes with $n > 2$ would not exist.

Here we report on the first observation of Cs^*He_n exciplexes in alkali doped solid ^{4}He matrices. We have observed[1] several new spectral features in the fluorescence from cesium atoms implanted in the hcp and bcc phases of solid helium ($T = 1.5$ K, $p = 26 - 31$ bar) following laser excitation to both the $6^2P_{1/2}$ and $6^2P_{3/2}$ states.

We have calculated the electronic structure of of the Cs^*He_n exciplexes for $n = 1, \ldots, 8$ using adiabatic Cs-He pair potentials and have inferred the emission spectra using the Frank-Condon principle. A spectral feature at 950 nm could thus be assigned to the apple-shaped Cs^*He_2 complex, while emission from the dumbbell-shaped Cs^*He_7 exciplex is the most likely assignment of the strongest emission line observed at 1400 nm. This interpretation is further supported by the fact that the calculation yields the lowest total zero-point energy for the structure with 7 atoms.

Our observations contradict the commonly accepted belief that $Cs^*He_{n>2}$ exciplexes do not exist. The larger Cs-He collision rate due to the higher density in the pressurized solid matrix (compared to gaseous or liquid helium environments) is most probably at the origin of the efficient formation process.

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CO_2 in Intense Ultrashort Laser Pulses: Evidence for NonSequential Dissociation

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One of the most fascinating effects to emerge from strong-field laser interactions with gaseous targets is the observation of enhanced ion yields in the double and multiple ionization at intensities well below the expected threshold. The enhancement over orders of magnitude in signal has been termed 'nonsequential (NS) ionization' as multiple electrons are removed in a single step. It has only been in most recent years, following major advances in laser technology and experimental capabilities, that a more knowledgable understanding of the ionization mechanism has emerged.

Generally accepted as the catalyst for this process is the role of electron rescattering. In a linearly polarized field, following the initial ionization stage, the removed electron is back-propelled by the oscillating laser field to scatter off the parent core. The inelastic scattering event may provide sufficient impact energy for secondary ionization (direct or via excitation followed by field ionization at a lower threshold). The suppression of such an effect with circularly polarized light (electron driven off-axis) is convincing evidence for the rescattering event.

Acknowledged as the driving force behind the phenomena of high-harmonic generation and the observed plateau in above-threshold ionization electron energy spectra, the recollision process has only recently been considered to play a part in molecular dissociation [1]. However the experimental evidence presented is somewhat ambiguous and open to debate. In light of this, we present here for the first time unquestionable evidence for nonsequential dissociation of a molecular ion with CO_2 used as the primary target.

In brief, experimentally we interact intense ($\sim$6x10^{16} Wcm^{-2}), short pulse (55fs), laser light (800nm) with a gaseous CO_2 target. Using a high-resolution time-of-flight spectrometer, we measure the signal from the ionization and dissociation products as a function of the interaction intensity. Intensity variation is achieved by using an Intensity Selective Scan (ISS) technique [2] extracting ions positionally through a finite aperture from precise intensity regions of the focus (along the axial z direction of the laser).

At the conference we give more details on the measurement technique and present strong evidence for the rescattering enhanced dissociation of the $CO_2{}^+$ ion.

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The $a^3\Sigma^+$ state of the NaCs molecule

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The NaCs molecule is one of the prospective objects for photoassociation experiments. Recent success with RbCs [1] and KRb [2] showed the necessity for detailed spectroscopic studies of heteronuclear alkali dimers, especially close to the atomic asymptote. The $X^1\Sigma^+$ ground state of NaCs has been studied in Ref. [3]. Here we present the studies of the first triplet state $a^3\Sigma^+$ of the NaCs molecule.

The method applied is Fourier transform spectroscopy (FTS) of laser induced fluorescence (LIF). A well known technique for reaching the triplet manifold from singlet states consists in employing strong perturbations by mixing singlet and triplet molecular states. In the present experiment excitation of the strongly mixed $B^1\Pi$, $c^3\Sigma^+$ and $b^3\Pi$ states allowed observing transitions to the $a^3\Sigma^+$ state. A single mode CR-599 dye laser (DCM dye) was used for LIF excitation. LIF spectra were recorded by HR120 Fourier transform spectrometer with a typical resolution of 0.015 – 0.03 cm^{-1}. More than 2000 transitions to 800 energy levels of the $a^3\Sigma^+$ state were assigned. The range of vibrational and rotational levels obtained is $v'' = 0 - 18$ and $N'' = 6 - 103$, respectively. The hyperfine structure of triplet lines is partially resolved. The hyperfine splitting turned out to be independent of the vibrational and rotational quantum numbers within the experimental uncertainty.

Differences between the observed $a^3\Sigma^+$ state levels were fitted to the potential energy curve with the IPA method [4]. The preliminary potential reproduces the measured differences with a standard deviation of 0.005 cm^{-1}. The highest vibrational level registered so far ($v'' = 18$, $N'' = 28$) has a classical turning point around 13 Å .

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Strong Orientation Effects in Ionization of H_2^+

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We present three dimensional time-dependent calculations of ionization of arbitrarily spatially oriented H_2^+ by attosecond, intense, high-frequency laser fields. The ionization probability shows a strong dependence on both the internuclear distance and the relative orientation between the laser field and the internuclear axis.

The physical features are explanied in terms of two-center interference effects.

Inelastic scattering of synchrotron radiation on the $1s^{-1}\pi_g^*-$ resonance of N_2^* studied by the N_2^+ (C–X) fluorescence

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Studying the excitation and de-excitation processes in the nitrogen molecule at the $1s^{-1}\pi^*-$ resonance is a long-standing problem since the work of Nakamura *et al* (1969) [1]. In the decay of this resonance two Auger processes are competing: spectator (when the excited π^*- electron remains in the molecule) and participator (when the π^*- electron leaves the molecule). The fluorescence in those states of the N_2 molecule which are resulting from the participator decay, i.e. via the $2\sigma_u^2 1\pi_u^3 3\sigma_g^2 \left(A\ ^2\Pi_u\right) \rightarrow 2\sigma_u^2 1\pi_u^4 3\sigma_g^1 \left(X\ ^2\Sigma_g^+\right)$ and $2\sigma_u^1 1\pi_u^4 3\sigma_g^2 \left(B\ ^2\Sigma_u^+\right) \rightarrow 2\sigma_u^2 1\pi_u^4 3\sigma_g^1 \left(X\ ^2\Sigma_g^+\right)$ transitions have recently been studied in the work [2,3]. In the present work we investigate the fluorescence in the $2\sigma_u^2 1\pi_u^3 3\sigma_g^1 1\pi_g^1 \left(C\ ^2\Sigma_u^+\right) \rightarrow 2\sigma_u^2 1\pi_u^4 3\sigma_g^1 \left(X\ ^2\Sigma_g^+\right)$ process where the excitation of the initial state is mainly due to spectator Auger decay.

In order to measure the $C\ ^2\Sigma_u^+ \rightarrow X\ ^2\Sigma_g^+$ fluorescence at 135 nm $\leq \lambda_{\text{fl}} \leq$ 190 nm we utilize the photon-induced fluorescence spectroscopy (PIFS [4]) exciting by monochromatized synchrotron radiation from the UE 56/2 PGM beam line, BESSY-II, Berlin. Fluorescence band sequences where the difference of vibrational quantum numbers, $\Delta v = v' - v''$, varies in a wide range ($\Delta v = -3 \ldots + 5$) were observed. The intense fluorescence band sequences with $\Delta v \neq 0$ are explained by the large difference between equilibrium distances in the $C\ ^2\Sigma_u^+$ ($r = 1.26$) and $X\ ^2\Sigma_g^+$ ($r = 1.12$) states.

In order to compute the fluorescence distribution within the individual vibrational bands a large scale calculation of the potential curves was performed within the MRSDCI approach. The shapes of computed and measured fluorescence band sequences are in very good agreement.

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Techniques for precision laser spectroscopy of trapped highly charged ions

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We present techniques and intrumentation for precision laser spectroscopy of trapped, highly charged ions nearly at rest. The focus is on a quantitative assessment of forthcoming measurements of the ground state hyperfine (HF) splitting in highly charged ions, within the framework of the HITRAP project. A cloud of identical ions will be confined in a Penning trap, resistively cooled, compressed by use of a 'rotating wall' and irradiated by a cw-laser tuned to the HF transition. The combination of these techniques will ensure a high ion density and therefore high fluorescence rates. At such ion densities, space charge and plasma effects need to be accounted for. Since Doppler broadening of the hyperfine transition is highly suppressed, an unprecedented precision in the wavelength measurement is obtained.

The wavelength of the ground state hyperfine splitting (HFS) in atoms and ions is typically in the microwave domain and thus not accessible with lasers. However, the energy of the $1s$ ground state HFS of hydrogen-like ions scales with the atomic number Z as Z^3 and shifts into the laser-accessible region above $Z \approx 60$ [1]. This allows for accurate measurements of the transition by well-established means of laser spectroscopy and in turn for sensitive tests of corresponding calculations of the transition energy and lifetime [2,3].

A common experimental obstacle in previous measurements has been the Doppler broadening and shift of the transition due to the high velocities of the ions. The measurement scheme outlined here has the advantage that it takes place in cryogenic surroundings with well-localised particles nearly at rest. A bunch of roughly 10^5 ions like for example $^{207}Pb^{81+}$ is captured in flight, resistively cooled to liquid helium temperature and radially compressed by use of a 'rotating wall'. A cw-laser illuminates the ion cloud axially. Based on this combination of techniques we expect ion number densities of order $10^7\,\mathrm{cm}^{-3}$, which, together with the localisation in a nearly spherical cloud of few millimetres in diameter, increases the intensity of detectable fluorescence.

The high charge density of such an ion cloud requires space charge and plasma effects to be taken into account. Calculations as well as simulations show that the cloud density needs to be optimized by appropriate choice of the trapping parameters and the rotating wall frequency. Furthermore, the space charge effect reduces the axial frequency and thus increases the resistive cooling time constant. Energy dissipation into the cloud by accidental excitation of plasma modes needs to be avoided by appropriate choice of the experimental parameters.

From such a measurement of the hyperfine transition, a photon count rate of order $10^3\,\mathrm{s}^{-1}$ at a relative wavelength accuracy of some 10^{-7} can be expected. Thus, the present experiment allows for the precision of HFS measurements to be increased by three orders of magnitude.

This experiment is to take place within the framework of the HITRAP project at the Gesellschaft für Schwerionenforschung (GSI) in Germany where highly charged ions will be produced by the Experimental Storage Ring (ESR), subsequently slowed and cooled, and finally made available at low energies for experiments.

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Photoionization and photo-double ionization of atoms and ions using a quasi two-electron IERM method.

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The intermediate energy R-matrix method (IERM) has proved a successful technique for studying electron scattering by atomic hydrogen and other one-electron ions. Recent developments in our work with the IERM approach have stemmed from the introduction of a core potential which models the effect of a closed inner core of electrons on a single outer valence electron, producing quasi one-electron atoms and ions. Following the success of this method in calculations for electron scattering, the most recent development has been the extension of the quasi one-electron approach to the study of photoionization and photo-double ionization of quasi two-electron atoms and ions.

After implementing the R-matrix theory of photoionization in the core potential modified IERM codes, trial calculations were performed for the photoionization of helium. Finding the cross sections to be in very good agreement with both theoretical and experimental results, we have subsequently undertaken calculations for the photoionization of magnesium and also calcium, results of which will be presented at the conference.

In addition, we have been able to use this method to approximate the photo-double ionization cross sections. This is made possible through the inclusion of large numbers of pseudostates. The approximation is obtained by summing the contribution made by positive energy pseudostates to the photoionization cross section. Preliminary results for helium indicate good agreement with experiment and other recent calculations [1]. We hope to progress to using this method to obtain results for the photo-double ionization of calcium.

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Electron-impact excitation of Fe II

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The spectra of singly ionised iron is extremely important in astronomical observations, and Fe II emission has been observed from nearly every class of astrophysical object at infrared-to-ultraviolet wavelengths. Of critical importance to the interpretation of these spectral lines are the electron impact collision strengths and effective collision strengths. However, the accurate evaluation of this atomic data for the important low-ionised species in the near-neutral iron-peak region has proved impossible until now, due to the complexity of dealing with open d-shell ions. The computational effort for such investigations is formidable, with up to a thousand target states and several thousand coupled channels being involved. These complications are aggravated by the presence of Rydberg resonances located in the low-energy regions. Computational problems arise due to the necessity of including thousands of distinct energies in the scattering calculations, to properly delineate the resonance structures, thereby producing accurate excitation cross sections and ultimately Maxwellian averaged collision rates. To address these problems a parallel R-matrix package, PRMAT [1], has been developed to enable the evaluation of excitation rates of greater accuracy than has been previously possible. This will also provide a greater understanding of the important factors which influence these electron-ion collisions.

An initial calculation [2] for electron-impact excitation of Fe II, involving a 38-state LS-coupled calculation within the three electronic configurations $3d^6 4s$, $3d^7$ and $3d^6 4p$, uncovered large differences in the effective collision strengths amongst low-lying terms when compared with previous works. This calculation has since been extended to include the additional target states which arise from the $3d^5 4s^2$ and $3d^5 4s4p$ configurations, giving 113 LS-coupled levels and a maximum of 350 coupled channels [3]. A detailed study of low-energy electron collisions with Fe II in which configuration interaction effects were systematically included in both the target wavefunction and the collision wavefunction was carried out. It was shown that in order to obtain accurate low-energy partial wave collision strengths, configuration interaction effects in both the target and collision wavefunctions must be carefully balanced. In addition two-electron excitations from the 3p shell to the 3d shell must be included to achieve close to converged low-energy partial wave collision strengths. These calculations have laid the foundation for the approach adopted in the study of electron collisions with other ions, and would have been impossible without the highly sophisticated PRMAT package and the HPCx facility. The optimum model emerging from [3] has now been used to obtain converged effective collision strengths for forbidden transitions in Fe II, some of which will be presented at the conference.

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Multi-state CDW approximation to electron capture during slow p - H collisions

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Collisions between fully stripped ions and atomic hydrogen have long been of interest to both theoretical and experimental physicists. Many studies over a wide range of energies have been performed and a wealth of reliable experimental, as well as theoretical data is available.
This poster will focus on one of the most basic quantum mechanical systems, the collision of a proton and atomic hydrogen, using it to test the viability of a multi-state continuum distorted wave (CDW) based approximation. Previous studies have successfully described resonant electron capture by protons from atomic hydrogen in its ground state. This is relatively easy to model from a theoretical standpoint over almost all impact energies, as the entrance and exit channels are strongly coupled together, and no channels contribute significantly to the appropriate total or differential sections. Hence a simple two state approximation is adequate. A more rigorous test of any theory is provided by comparing estimates for electron capture to the $n = 2$ states of the projectile. Reliable prediction of these quantities is a more demanding test of any theory applied to this particular system. This is because it is necessary to simultaneously include the effects of both resonant, and non-resonant $n = 2$ channels in the calculation. In the present work we will use an orthonormal basis set to construct a trial wavefunction and so the quandary associated with the normalisation of CDW wave descriptions at low energies is automatically remedied. In contrast to other models, such as the atomic orbital expansion proposed by Fritsch and Lin [1] which must include a multitude of target, projectile and pseudostates, it will be shown that a modestly sized basis set, consisting of functions, which simultaneously include the effects of both charge centres, will be sufficient to accurately describe resonant and non-resonant electron capture at both low and intermediate impact velocities.

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A comprehensive study of delayed ionization and photofragmentation of C_{60}

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Owing to its high degree of symmetry and stability, the fullerene molecule C_{60} has been extensively used as a model system for the study of competing decay mechanisms in finite-size systems [1, 2]. Depending on the detailed distribution of the energy deposited in the system, and depending on the duration of the excitation process, a wealth of phenomena may be studied over timescales ranging from ultrashort time in the femtosecond regime, to delayed ionization occurring after tens or hundreds of microseconds. The present contribution reports on detailed measurements of photoelectron and photoion kinetic energy release. Experimental measurements of time-dependent photoelectron spectra observed in thermionic emission of hot C_{60} excited by multiphoton absorption using nanosecond lasers [3] have been supplemented by extensive measurements of the kinetic energy distribution of the photoions. Time resolved velocity-map imaging is used to record photoelectron and photoion spectra and to disentangle fast and slow processes.

The evolution of the kinetic energy distribution of thermal electrons and ions emitted from energy-rich clusters as a function of the delay after multiphoton excitation is described within the general formalism of the detailed balance theory [4]. Combined with relatively standard assumptions regarding dissociation and ionization energies of the various C_{60-2n} species, this formalism has allowed us to simulate the photoion mass spectra and to analyze the details of the kinetic energy distributions of the emitted charged particles under a unified approach.

This complete approach, unifying mass spectrometry and charge particle imaging, represents a unique experimental situation where competing ionization and fragmentation processes could be studied in full details, allowing to refine our understanding of these complex processes.

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Coincidence study of excitation of cadmium atoms by 60 eV electron impact

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Experimental values of the electron impact coherence parameters (EICP) and reduced Stokes parameters are reported for electron impact excitation of the 5^1P_1 state of Cd. The results have been obtained using electron – photon technique for incident electron energy of 60 eV and scattering angles of 10° to 35°. The experimental data are compared with results of theoretical relativistic distorted – wave approximation calculation.

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

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

The atomic beam used in the experiment was obtained by evaporation of a natural mixture of Cd isotopes. As such it contained 75% of atoms with zero nuclear spin I and 25% fraction of ^{111}Cd and ^{113}Cd characterised by I = $^1/_2$. The fluorescence of the latter was partially depolarised due to the hyperfine interaction. However, the experimentally determined Stokes parameters could be easily corrected for the effect, using the well – known formalism of the perturbation coefficients [2, 3]. Theoretical predictions are in a good qualitative agreement with experimental values.

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'Two-particle-one-hole' resonances in electron-impact excitation of Ni V

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Electron-impact collision strengths and corresponding effective collision strengths are of crucial importance in the interpretation of spectra of low-ionisation stages of the iron peak elements Fe, Co and Ni, which occur in numerous laboratory and astrophysical plasmas. However, accurate calculation of these quantities is complicated by the open d-shell structure of these ions, which give rise to many low-lying target states that are strongly coupled. This, in turn, leads to a large number of coupled channels which must be retained in the model, posing a formidable computational challenge. Recently a new parallel R-matrix package, PRMAT [1], has been developed to address this problem, and we are in a position to study successfully much larger collision problems than previously possible. In particular, we have a unique opportunity to gain a deeper insight into the role of configuration interaction effects in both the $(N+1)$-electron collision wavefunction, as well as the N-electron target state wavefunction.

Urgent need for accurate collisional data for Ni V for interpretation of astrophysical spectra prompted earlier R-matrix calculations by Teng *et al* [2]. It was observed that the collision strength was significantly altered by the presence of 'two-particle-one-hole' resonances arising from the intermediate $(N+1)$-electron states with symmetries $^4\mathrm{G}^o$ and $^4\mathrm{D}^o$ belonging to the $3\mathrm{p}^5 3\mathrm{d}^8$ configuration. However, analysis of Ni IV energy levels indicates that other configurations, e.g. $3\mathrm{p}^5 3\mathrm{d}^7 4\mathrm{s}$ and $3\mathrm{p}^5 3\mathrm{d}^7 4\mathrm{p}$ could give rise to similar resonance features. The aim of this work is to use the PRMAT package to carry out a number of calculations designed to investigate this more fully. Preliminary results demonstrate much larger resonance structure arising from the $^4\mathrm{F}^e$ intermediate $(N+1)$-electron states belonging to the $3\mathrm{p}^5 3\mathrm{d}^7 4\mathrm{p}$ configuration. Latest results will be presented at the conference.

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Dissociative charge exchange of simple molecular ions with a laser excited target

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In most cases, the dissociative charge exchange (DCE) between a molecular ion and an alkali target populates predissociative states [1,2]. Their binding energy is reflected by the kinetic energy released to the atomic fragments. All alkali atoms however have an ionization potential exceeding 3 eV, which limits this kind of dynamical spectroscopy of otherwise non-observable molecular states to those lying somewhat far from the ionization threshold of the transient molecule. In an attempt to bridge this energy gap, we have adapted the set-up dedicated to dissociative charge exchange studies to allow for one- and two-color excitation of the effusive potassium target at the core of the apparatus. Fast molecular ions colliding with laser-excited potassium atoms undergo in-flight dissociation, their fragments being detected by a pair of position-sensitive detectors operating in coincidence. The reconstructed velocity vectors produce high resolution spectra of the total kinetic energy release [3,4].

A preliminary experiment has been performed, in which a single-mode diode laser was used to pump the potassium D2 line, the population of $4P_{3/2}$ atoms being somewhat limited by population and radiation trapping, due to the absence of repumping beam and the large optical thickness of the effusive jet. A fourfold increase of the DCE signal has been found in the case of CO^+ and N_2^+ ions at 2 keV, while no such effect could be seen with H_2^+ and O_2^+. This resonant behavior, together with the average kinetic energy release, permits a reliable assignment of the product quantum states, i.e. $C(^3P)+O(^3P)$ and $N(^4S)+N(^2D)$ respectively. The sharp vibrational series have still to be confronted with spectroscopic data for CO and N_2, keeping in mind that DCE stems from non-radiative decay of the intermediate state, which may be optically forbidden and hence unknown from spectroscopic observations.

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The cold atom micromaser with Λ-type three-level atoms

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The quantum theory of the two-mode micromaser pumped by cold three-level atoms with a Λ-configuration under the two-photon resonance condition is considered. The cold atom micromaser (also referred to as mazer for microwave amplification via z-motion-induced emission of radiation) was first described by Scully *et al.* [1] where it has been shown that a new kind of induced emission occurs when the micromaser is pumped by ultracold atoms, requiring a quantum-mechanical treatment of the center-of-mass motion. We recently extended the description of this system considering detuning effects between the cavity field mode and the atomic transition frequencies [2]. In the present analysis, we consider three-level atoms and extend previous studies related to this case (see e.g. Refs. [3,4] and references therein). For large detunings, the three-level atom reduces to a two-level system described by an effective two-level Hamiltonian [5]. We have shown that this technique may be advantageously applied in the cold atom regime, giving rise to simple physical interpretations of the interaction between the atom and the cavity. Different cavity field modes have been considered in our study. Results of the atomic transition probabilities will be presented. Interesting applications will be discussed, especially the possibility of inhibiting the spontaneous emission of the cold atoms before they interact with the cavity, while preserving the main feature of the cold atom micromaser.

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Quantum entanglement of cold atoms in traps and lattices

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When a group of atoms or ions is cooled to extremely low temperatures and densities, the interatomic interactions and the quantum statistics are critical in determining the collective states of the system. Perhaps the best known examples are Bose-condensed alkali gases and laser-cooled ions in electromagnetic traps. These delicate forms of matter, and their quantum nature, can be exploited as a precise tool for microscopic high-precision measurements, but they also have important applications in interferometry devices and quantum information technology. For example, cold atoms can be manipulated and controlled in optical traps or lattice structures, while ions can be arranged in a crystalline structure in a Paul or Penning ion trap.

The simulation of a many-atom system at very low temperature can be simulated to a high degree of accuracy by solving the Heisenberg field equations. We present the results of our calculations using mean-field theory, quasi-particle models and many-body simulations. The energy spectra and symmetries of the eigenstates are calculated. A detailed study of strongly-entangled atom pairs and quasiparticles is presented for atoms in traps and optical lattices. The nature of quantum entanglement in these systems is studied.

Interference of atomic states with hydrogen-like atoms

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Physical description of the atomic state interference and applications of the atomic interferometer method to precise measuring the Lamb shift in a hydrogen atom are presented in papers[1-2]. In this paper we propose a precise method for measuring the Lamb shift in hydrogen-like atomic systems. In essence it generalizes the method of atomic interferometer which was successfully applied earlier to measure Lamb shift$\delta_{n=2} = 2S_{1/2} - 2P_{1/2}$ in a neutral hydrogen atom to within the 2 ppm error [1]. We study stationary interference of the$2S_{1/2}$ or $2P_{1/2}$ states due to passage of metastable hydrogen-like helium ions $^4He^+$ through static electric fields.Basic theory of atomic state interference is presented and experimental conditions allowing to observing the interference pattern with a beam of $^4He^+$ ions are analyzed. We discuss two schemes that allow us to observe interference of $2S_{1/2}$ or$2P_{1/2}$ states of atoms crossing one of two active zones with electromagnetic fields. The simplest scheme with one active zone is designed rather to observe the interference effect as such and to measure the dependence of its components on both experimental parameters and spectroscopic constants of atomic states. Precision measurements of the Lamb shift can in principle be carried out using the binary interferometer scheme [1]. As a result, we present theoretical interference pattern for two types of atomic interferometers and discuss in detail approaches to precise measuring the Lamb shift $\delta_{n=2}$ in $^4He^+$. The comparative analysis of contributions due to the nuclear structure and QED-corrections in the Lamb shift for $^4He^+$ indicates that the 1-2 ppm accuracy level allows in principle the estimation therms radius of an alpha-particle with an error comparable to the modern experimental accuracy. To evaluate the size of atomic nuclei,it is proposed to assume the validity of QED-equations describing the Lamb shift, and then to directly use the comparison of theoretical and experimental results for the Lamb shift to determine the alpha-particle rms radius.

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Observation of nonlinear resonances for Nd^+ trapped ions by laser induced fluorescence

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The complexity of natural abundance resulting in the overlapping of spectra lines is one of the main difficulties arising when resolving hyperfine spectra of atoms and ions. This problem is particularly serious in neodymium with seven stable isotopes [1]. This issue can be overcome, at least in the case of ions, by trapping them in a quadruple ion trap that can be seen essentially as mass selective filters. Scaning the $a - q$ stability diagram [2] along the line corresponding to a constant ratio of the DC bias the AC radio-frequeny voltages, in so called mass-selective regime, the border of stable motion in the diagram is crossed for certain masses, which therefore can be thrown out. A disadvantage of this method comes from the variation of the trapped ion density which is caused by potential depth variation. Fortunately the physics of ion trap offers a possibility to extract ions selectively, while preserving nearly the same privileged (a, q) position. Following R. Alheit, K. Enders and G. Werth [3] the imperfections of the ion trap electrodes and configuration, being considered as a drawback in typical applications, can be employed to establish suitable conditions (i.e. assuming relevant a end q values), to excite some nonlinear resonance vibrations. Passing the energy via a nonlinear resonance channel to some degree of freedom the magnitude of this motion can dramatically increase causing instabilities. They are of course mass selective and permit to release the unwanted isotopes. The nonlinear resonances comply with a simple, but nevertheless fundamental, linear constraint [4]: $n_r\beta_r + n_z\beta_z = 2\nu$. The parameters β_r and β_z are related to the oscillation frequencies ω_r and ω_z and the frequency Ω of the trapping AC high voltage. They can be expressed also as implicit function of the a and q trapping parameters. The sum $|n_r| + |n_z| = N$ determines the $2N$ order of a perturbing multipole. The main feature of the experimental method applied here is the detection of the nonlinear resonances by observation of the variation in the laser induced fluorescence (LIF) of Nd^+ ions with the excitation: 4f46s $^6I_{7/2}$ 0.000 cm^{-1} $\rightarrow$ 4f46p $^6K_{9/2}$ 23229.99 cm^{-1}. The fluorescence light has been recorded with the photomultiplier and the ICCD camera as the evidence of nonlinear resonances in the motion of the investigated ions. The linear dependence between β_r and β_z parameters described by the mentioned formula allowed us to identify nonlinear resonance lines within the stability diagram resonance i.e. the n_r , n_z modes and the order of nonlinear oscillations .

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Coherent population trapping with femtosecond laser

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Effect of coherent population trapping (CPT) attracts a high interest of spectroscopists in last years. Sensitivity of the effect to external factors (e.g. magnetic field, buffer gas pressure etc.) makes it an attractive object for metrological applications, magnetometry, laser cooling, coherent information storage and control, and some other laser applications [1,2,3].

CPT arises in a three level Λ-system under radiation of bichomatic field. The field components should be phase correlated and there frequency difference should be equal to the energy splitting of the lower levels of the system. Such bichromatic field can be created by frequency modulation of one laser source, but in this case the frequency difference of the field is restricted by the radio frequency region.

Atomic systems a with relatively large splitting of the lower levels of corresponding Λ-system are very attractive objects of study [3,4] due to an expected high Q factor of the CPT resonance. One of the main obstacles for near study is a difficulty of a synthesis of the bichromatic field with large (up to optical) frequency difference of the components. We implemented a new method of synthesis of the bichromatic field with a good phase coherence between its components. The method can be extended to the case of a high frequency difference up to the optical range.

The basic idea of the method is to use coherent properties of spectral modes of a femtosecond laser (FSL). Due to a perfect phase correlation between the modes of FSL, two diode lasers phase locked to different modes become automatically phase locked to each other. The frequency difference between the lasers is restricted only by FSL spectral width. It was shown recently, that the width can be enlarged to the whole optical octave without loss of the coherent properties of the light [5]. In this work we present such bichromatic source and experimental results obtained in rubidium vapour using the source.

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Analysis of nano-sized particles produced in combustion processes by using Infrared and Raman spectroscopy

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Soot formation takes places in combustions processes as a consequence of the incomplete combustion of organic matter as wood, gasoline or diesel fuel. From a chemical point of view, soot is composed by an elemental carbon nucleus, to which are attached, in the growing phase, polycyclic aromatic hydrocarbons [1]. Recently, it was demonstrated that, in particular conditions (slowly sooting flames), soot formations is primed by the presence of some nano-sized particles, which can be really considered precursors for the soot [2]. The study of the chemical-physics proprieties of these particles, possible with different optical techniques, is particularly interesting, and constitutes the essential condition for a deeper understanding of the soot formation process. In this work we present the results of the first investigation of these particles by both Infrared and Raman Spectroscopy. By combining the results of these two techniques, it is possible to get a complete information on the chemical structure of the sample; in particular, it becomes possible to distinguish between the aromatic and the aliphatic character of the investigated particles. The analysis was performed on particles present in aqueous solution and sampled from flames with a different C/O ratio. The main features of the obtained spectra show the presence of both aliphatic and aromatic C-H bonds. The fully interpretations of such result is under study. Future investigation of the same samples by surface-enhanced Raman spectroscopy (SERS) technique are planned.

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Precision laser spectroscopy of hyperfine splittings in highly charged ions

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An accurate measurement of the ground state hyperfine splitting (HFS) in highly charged ions (HCI) is a good test of quantum electrodynamics (QED) in the limit of strong electric fields (10^{15} V/cm) [1]. Such strong fields cannot be produced using conventional laboratory techniques, but naturally exist close to the stripped nuclei of heavy elements like Pb, Bi or U. By detecting the fluorescence from the laser-excited upper hyperfine state of such an ion, the hyperfine splitting can be measured with very high accuracy [2].

A measurement of this magnetic dipole ($M1$) transition wavelength gives information on the QED corrections to the HFS, or on the spatial distribution of the nuclear magnetisation (Bohr-Weisskopf effect)[1]. Its measurement thus allows for critical tests of nuclear models. From a comparison of measurements of the HFS in hydrogen-like and lithium-like HCI, the nuclear effects can be eliminated such that the QED effects can be determined [3,4].

HCI with extremely high charge states, for example $^{207}Pb^{81+}$ or $^{209}Bi^{80+}$, are made available for experiments at the HITRAP facility to be built at GSI in Darmstadt (Germany). The resolution obtained in previous measurements on relativistic HCI at GSI was mainly limited by the Doppler effect [5,6]. A laser spectroscopy measurement of the ground state HFS in cold HCI in a Penning trap should be much more accurate due to the absence of a large Doppler broadening (and shift). Interesting initial candidates for our laser spectroscopy experiments at HITRAP are the $F = 0 \rightarrow F = 1$ transition in hydrogen-like $^{207}Pb^{81+}$ ($\lambda = 1020$ nm, $\tau = 50$ ms [5]), and the $F = 4 \rightarrow F = 5$ transition in lithium-like $^{209}Bi^{80+}$ ($\lambda = 1554$ nm, $\tau = 83$ ms [6]).

In order to reach the necessary accuracy, the HCI will first be loaded and confined in a Penning trap. Electron capture (neutralisation) by collisions is strongly reduced by operating the trap at cryogenic temperatures under UHV conditions. Once trapped, the HCI will be cooled by resistive cooling and radially compressed using a 'rotating wall' technique. A spectrum of the ground state hyperfine transition can be obtained by scanning the laser wavelength across the resonance, while recording the fluorescence from the trapped excited HCI. Laser excitation along the trap axis, on an ion cloud smaller than the laser beam, will help to ensure that the transition is fully saturated. Repeated measurements on a single cloud of ions can be made, as detection is not destructive. We expect fluorescence rates of several thousand counts/sec, on a background of several hundred counts/sec.

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Isotope Shift Measurements of Fe I

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Doppler-free saturation absorption laser spectroscopy was applied to measure the isotope shifts of eight spectral lines of Fe I in the wavelength range from 619 to 668 nm, using a cw ring-dye laser. The measurements were performed in a see-through hollow-cathode discharge [1], where the cathode material is efficiently sputtered and all energy levels of the neutral atom and also ionisation states are populated. The hollow cathode was filled with a Fe foil in its natural isotopic composition in all our experiments. The gas discharge was run at a current of around 100 mA in an Ar atmosphere of 1.6 mbar.

The spectral lines investigated for the isotope shifts were transitions between levels of the configurations $3d^6 4s^2$ and $3d^7 4s$ to $3d^7 4p$. The experimental results will be presented.

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The double photoionization cross section of helium near threshold

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The emission of two electrons following the absorption of just one photon by a target atom or ion cannot occur in the absence of electron-electron correlations due to the single-particle nature of the dipole interaction. The near threshold region for the escape of two electrons is of particular interest as both electrons move slowly and, therefore, have much time to interact.

Two different theories have been developed which model the energy dependence of the double photoionization cross section near threshold. The earliest classical dynamics analysis, carried out by Wannier [1], derived a power-law dependence of the double photoionization cross section. In contrast to the Wannier power law, the Coulomb-dipole theory [2] predicts an oscillating but still monotonically increasing double photoionization cross section near threshold. Here, the idea is, that the faster leaving electron is subject not only to a Coulomb field but also to a dipole field caused by the residual ion and the slower leaving electron.

Recent extensive experimental studies of the double photoionization cross sections of atomic Li [3] and Be [4] near threshold have brought oscillations in these cross sections to light. The oscillations, which are much more pronounced for Be than for Li, are supposed to be connected with both atoms featuring at least one loosely bound electron [4].

According to this hypothesis, the oscillations in the double photoionization cross section of He, which is the simplest two-electron atom, can be expected to be extremely small if the incident photon is absorbed by the ground state $1s^2\ ^1S$. An early experiment by Kossmann et al. [5] does not provide any indication of an oscillating double photoionization cross section. For the excited states $1s2s\ ^{1,3}S$ of He, however, the respective double photoionization cross sections could show oscillations near threshold.

To find out more, we started with a time-dependent model calculation on the double photoionization of He from the ground state and the excited state $1s2s\ ^1S$ where the electron-electron correlations are described in the lineland model, i.e. $V(r_1, r_2) = 1/(r_1 + r_2)$. For excess photon energies up to 1 eV the agreement with the Wannier power law is good but no oscillations have been observed.

As this may indicate the necessity for a full quantal description, we have started carrying out time-dependent close-coupling calculations on the double photoionization of He. The six-dimensional total wavefunction is propagated in time using a numerical lattice for the two radial coordinates and coupled channel expansions for the four angular coordinates. The two dimensional non-uniform lattice is partitioned in both radial coordinates to speed up the calculations as, due to the very low energies of the escaping electrons near threshold, the radial extent of the lattice has to be extremely large demanding a huge amount of running time.

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Stark effect studies in low-lying $^1\Pi$ states of NaCs: experiment and theory.

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We report the Stark effect studies in $G(3)^1\Pi$ state of NaCs molecule aimed to obtain permanent electric dipole moments and Λ-doubling constants, as well as *ab initio* calculations of the respective values in low-lying $^1\Pi$ states of NaCs.

The procedure of experimental determining of permanent electric dipole moment values $d(v', J')$ was as follows [1,2]. After selecting and identifying a definite Ar^+ laser induced fluorescence (LIF) $^1\Pi \rightarrow X^1\Sigma^+$ progression consisting of either singlets or doublets, the dc electric field has been applied causing $e - f$ parity mixing between Λ-doubling components of $^1\Pi$ state. As a result, extra ("forbidden") lines appear in LIF spectra when Starks splitting energy becomes comparable to the Λ-splitting Δ_{ef}. The ratio of "forbidden" line intensity over the "allowed" line intensity is governed by the parameter d/Δ_{ef}, thus fitting the intensity ratio as dependent on the electric field strength yields the d/Δ_{ef} ratio value.

The Λ-splitting value was measured directly by electric radio frequency - optical double resonance [3]. This means that we applied with radio frequency (1-500 MHz) changing electric field to the NaCs molecules and observed changes in the LIF spectra. When electric field frequency was in resonance with Λ-splitting, "forbidden" lines appeared. Known values of Λ-splitting allowed us to pass from the d/Δ_{ef} ratio to the permanent electric dipole moment value $d(v', J')$. Permanent electric dipole moment and Λ-splitting have been measured for 13 different rovibrational levels of $G(3)^1\Pi$ state, spanning $v' = 0 - 32, J' = 19 - 75$ range of vibrational and rotational quantum numbers. Measured values of $d(v', J')$ fall within the range $4.5 \div 8.5$ D, and q-factors decreasing from $7.8 \times 10^{-6}\text{cm}^{-1}$ to $0.7 \times 10^{-6}\text{cm}^{-1}$ as v' increases from 0 to 32.

The *ab initio* electronic structure, Λ-doubling constant and permanent electric dipole moment functions on the internuclear distance of NaCs were performed by means of many-body multipartitioning perturbation theory (MPPT) [4] for explicit treatment of core-valence correlation generally similar to that used in [3]. The calculations are in good agreement with experimentally obtained values.

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Hyperfine Structure Measurements in LaII Utilizing Laser and RF Double Resonance Technique

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A fast ion beam laser spectroscopy (FIBLAS) method to measure hyperfine separations is to combine FIBLAS and rf excitation in a technique called Laser and Radio Frequency Double Resonance (LRDR) spectroscopy [1].

The hyperfine structure of the 5d 6s b^1D_2 level in LaII has been measured utilizing LRDR in a collinear geometry. The magnetic dipole and electric quadrupole hyperfine constant has been extracted. The results are in good agreement with previous FIBLAS measurements done by Maosheng et. al. [2] and Hohle et. al. [3], but the accuracy of the present experiment is 100 times higher.

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Autoionizing and highly lying levels in the Sn IV and Sn V spectra

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The spectrum of tin excited in a vacuum spark (C =7500 μF, L = 7 - 25 μH, U = 220 V) has been studied in the 200 - 600 Å wavelength region. A 3 m grazing incidence spectrograph with a 3600 l/mm grating was used for the 200 - 350 Å region (plate factor respectively 0.36 - 0.45 Å/mm). In longer region the spectrum was recorded on a 6.65 m normal incidence spectrograph with a plate factor 1.25 Å/mm. New identifications were made in the Sn IV and Sn V spectra.

The Sn IV spectrum with a $4d^{10}5s$ ground configuration belongs to the Ag I isoelectronic sequence. Lower energy levels with the excitation of the outer 5s electron as well as the levels of the $4d^95s^2$ configuration are listed in Ch.Moore's tables[1]. Later the $4d^95s5p$ configuration was added[2, 3]. We studied the $4d^{10}5s$ - $4d^95snp$ (n = 5,6), $4d^{10}5s$ - $4d^95snf$ (n = 5-9) and $4d^{10}5p$ - $4d^95p^2$ transitions from the configurations with excited electron from the $4d^{10}$ subshell. Most of the levels of these configurations are located above the Sn IV ionization limit. The value of the limit was improved due to observation of the transitions from the $4d^{10}ns$ (n = 8-10) levels. The $4d^{10}7d$ configuration was also found. Six levels were located in the $4d^95p^2$ configuration, four of them are above the ionization limit. As expected, the largest autoionization width 0.52 Å has the $4d^{10}5p$ - $4d^95p^2$ $(^3P)^2D_{5/2}$ transition. All the levels of the $4d^95snp$ ($n > 5$) and $4d^95snf$ configurations lie above the ionization limit. We identified 12 most intense lines of the $4d^{10}5s$ - $4d^95s6p$ and $4d^{10}5s$ - $4d^95snf$ (n up to 9) transitions and measured their autoionization widths.

Palladium - like Sn V has the ground state $4d^{10}\ ^1S_0$. The energies of the $4d^95s$, $4d^96s$, $4d^95p$, $4d^95d$ and $4d^85s^2$ configurations are well known[1,4]. Also 15 lines of the transitions to the ground state from J = 1 levels of the $4d^9np$ (n = 6-7) and $4d^9nf$ (n = 4-9) were observed[5]. We identified more than 200 new spectral lines of the $4d^95s$ - $4d^96p$, $4d^95s$ - $4d^85s5p$, $4d^95p$ - $4d^97s$ and $4d^95p$ - $4d^96d$ transitions and found 80 levels of the $4d^97s$, $4d^96p$, $4d^96d$ and $4d^85s5p$ configurations. The number of known Sn V lines and levels was increased by a factor of 2. In the 200 - 209 Å region 12 lines with measurable autoionization widths were observed. They were identified as the $4d^95s$ - ($4d^85s6p$ + $4d^85s4f$) transitions.

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Interpretation of M- and N-shell x-ray satellites of Pd $L_{\alpha 1,2}$ transition by using MCDF calculations

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The X-rays emitted from multiply ionized atoms exhibit pronounced satellite structure reflecting the distribution of spectator vacancies at the moment of the x-ray emission. Fine details of such x-ray satellite spectra can be studied with the high resolution diffraction spectrometry. In the present experiment, which was performed at the Paul Scherrer Institute (PSI), the ion beams of O^{7+} and Ne^{6+} of energy 279 MeV and 178 MeV, respectively were used. The excited x-ray spectra of the $L_{\alpha 1,2}$ ($L_3M_{4,5}$) and $L_{\beta 1}$ (L_2M_4) transitions in Zr, Mo and Pd have been measured using Von Hamos crystal spectrometer [1] with energy resolution of about 0.6 eV for the energy range studied. As a result, complicated x-ray spectra of M- and N-shell satellites as well as L-shell hypersatellites for the studied elements were measured with high resolution.

In order to interpret the measured spectra the multi-configuration Dirac-Fock (MCDF) calculations were performed [2] for excited multivacancy configurations $M^{-m}N^{-n}$, with the maximum number of vacancies for the M-shell m=4 and for the N-shell n=1 taking into account s, p and d states. The calculated MCDF x-ray multiplet structures were convoluted with the Lorenzian profiles described by the natural single vacancy (diagram) width [3,4] broadened due to a presence of a given number (m,n) of additional vacancies, and the instrumental (Gaussian) resolution of the spectrometer measured in the separated experiment for calibration Sc $K_{\alpha 1,2}$, V $K_{\alpha 1,2}$ and Fe $K_{\alpha 1,2}$ lines. The measured x-ray satellites spectra were reproduced by the linear combination of calculated MCDF multiplets by using the least-square method to find the individual weights for considered multi-vacancy configurations $M^{-m}N^{-n}$. The theoretical MCDF reproduce resonably well the measured satellite structure for Pd $L_{\alpha 1,2}$ ($L_3M_{4,5}$) transition. We find that further progress can be obtained by including in calculations the configurations with higher number of spectator vacancies in the N-shell. In near future we plan to extend this calculations for Zr and Mo in order to interpret the spectra measured for these elements.

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Resonances in few-body systems

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Doubly or multiply excited states in atoms or ions are frequently encountered in atomic processes such as ionization, charge transfer or electron-ion recombination. Their signature is a resonance, i.e. a dramatic change of the probability for a process for e.g. specific photon energies. Since resonances can change the probability for a process with orders of magnitude there is an obvious interest to be able to describe them and make quantitative predictions of their effects. The requirements on the computational approaches are high since the excited states are highly correlated systems embedded in the continuum. Few-body systems are here important test-beds since they permit an ab initio treatment and still exhibit strong collective effects.

We will show examples from three different systems;

• In negative ions there is no long range Coulomb force and as a consequence the number of bound states is generally small. The ions show, however, still rich resonance spectra. During recent years the photodetachment studies of doubly excited states have been extended to photon energies where triply excited states can form. The simplest negative ion that can be triply excited is the pure four-body system He-, where 40 eV is needed to reach the triply excited states[1,2]. These states are above the threshold for ejection of two-electrons and the dominating decay mode is in two steps; first autodetachment to a doubly excited state in the parent atom and then this state decay through a second Auger process.

• Muonic molecular ions in excited states have been predicted to form, with high probability, in collisions between excited muonic atoms and hydrogen molecules. Their presence and decay properties will have significant impact on the analysis of the muon catalysed fusion cycle as well as on the interpretation of exotic hydrogen spectroscopy. The muonic molecular ion ($pp\mu$) is more "atomic" than ordinary molecules and has similarities both with the hydrogen molecular ion (H_2^+ or ppe) and the hydrogen negative ion (H^- or pee)[3].

• It has been predicted by several authors, see e.g. Ref. [4] that positrons can form resonances with He^+, but the nature of these resonances has never been clarified. Qualitatively, such quasibound states exist because the electron and positron can form positronium (Ps), thus "hiding" the positron from the nuclear repulsion. Neutral Ps in its ground state ($n = 1$) is attracted to the $Z = 2$ charge by a polarization potential, $\sim -Z^2/2R^4$. Excited-state Ps can have a permanent dipole moment leading to a $-dZ/R^2$ attraction. Such potential supports in principal infinite series of resonances.

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Investigation of Fine and the Hyperfine Structure of the Odd Configurations $3d4s4p$, $4s^24p$ and $3d^24p$ of Neutral Scandium

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In the past few years the effect of hyperfine structure also became increasingly important in astrophysics [1,2]. Scandium (Sc) is apparently a much more abundant element in the sun and certain stars than on earth. It is one of the elements with only one stable isotope. This isotope has the mass number 45 and nuclear spin I =7/2. A parametric analysis of the fine and hyperfine structure of the configuration of even parity has already be done [3]. Here we present the results of a parametric analysis of the three odd-parity configurations $3d4s4p$, $4s^24p$ and $3d^24p$.

For the parametric fine structure calculations using the program code of Cowan [4], 26 parameters are required, eight for $3d4s4p$, two for $4s^24p$ and ten for $3d^24p$ as well as six configuration interaction parameters. The three configurations $3d4s4p$, $4s^24p$ and $3d^24p$ are comprised of 23, 2 and 45 theoretical fine structure levels, respectively. Using the 62 experimental energy levels in a least squares fit with 19 free parameters, an average deviation of 95 cm^{-1} was achieved.

The parametric investigation of the hyperfine structure is based on the experimental data from our Sc paper [3] and from the literature. For the three configurations of odd parity, 26 experimental A constants were available. Based on the results of the fine structure calculation and the experimental hyperfine structure data, the magnetic dipole hyperfine structure was analysed using our HFSAC and HFSFIT programs [5,6]. Theoretical predictions for the magnetic dipole hyperfine structure constants A for all levels of the configurations $3d4s4p$, $4s^24p$ and $3d^24p$ are given.

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Annihilation of antiprotonic hydrogen $\bar{p}p$ induced by ion collisions

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Antiprotonic hydrogen $\bar{p}p$ is an exotic hydrogenic atom composed of a proton p and its antiparticle, namely an antiproton $\bar{p}$. Since the pair of $\bar{p}$ and p promptly annihilate by strong interactions once they come sufficiently close to each other, the antiprotonic hydrogen is strictly an unstable atom. The level width Γ due to the annihilation is ~ 1 keV for the $1s$ state, and is still large for ns states unless the principal quantum number n is extremely high [1]. However, the $\bar{p}p$ atoms, having $\ell \geq 1$, can be considered to be practically stable (e.g., $\Gamma \sim 50$ meV for the $2p$ state [1]).

Recently, the $\bar{p}p$ formation process has been well investigated theoretically in collisions of antiprotons with atoms or molecules; i.e, $\bar{p} + H \rightarrow \bar{p}p + e$ [2], $\bar{p} + H_2 \rightarrow \bar{p}p + H + e$ [3], and $\bar{p} + H_2^+ \rightarrow \bar{p}p + H$ [4,5]. In these processes, the $\bar{p}p$ atoms are produced mostly in very high orbitals $n, \ell \gg 1$. Therefore, the produced $\bar{p}p$ atoms is expected to be generally very stable. However, the ℓ mixing is induced by electric fields (the Stark effect) or by ion collisions, and can lead to the transition to the ns state. If such a process occurs very effectively, the $\bar{p}p$ atoms, though initially having high ℓ, will soon annihilate, as first demonstrated by Day *et al.* [6].

The present report theoretically investigates the annihilation of $\bar{p}p$ atoms induced by ion collisions. The condition that the $n\ell(\geq 1) \rightarrow ns$ transition occurs most frequently is given by the so-called Massey's criterion, i.e., $\Delta E_{ns}\tau \sim 1$ (in atomic units), with ΔE_{ns} being the energy shift from the hydrogenic degenerate level and τ the collision time. Since the width Γ_{ns} is roughly equal to ΔE_{ns} for the $\bar{p}p$ atoms [1], we find $\tau \sim 1/\Gamma_{ns}$. This suggests that the annihilation likely occurs during a course of collisions. In such a case, we cannot treat the ℓ-mixing collision and annihilation problems separately in a theoretical calculation.

In the present report, I carry out an accurate collision calculation for the ℓ mixing within the same n manifold, simultaneously taking account of the ns annihilation channel with use of an optical potential model. Because of $\Gamma_{ns} \sim \Delta E_{ns}$, the $np \rightarrow ns$ transition can occur at impact parameters much larger than the related ones in the collisions for $\Gamma_{ns} = 0$. The annihilation cross sections will be reported as functions of the collision energy and the initial state (n, ℓ).

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Molecular Properties of Benzylazide, Ortho-, Meta- and Para- Methylbenzylazide

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Organic azides are industrially important in seismic explosives, propellants and photo-resistors [1]. Their ability in the formation of highly reactive nitrene intermediates makes them useful as important reagents in semiconductor technology for inserting into stable chemical bonds. The thermal decomposition of organic azides is responsible for more uniform doping and for the preparation of single-crystal gallium and silicon nitride epitaxial layers on semiconductors substrates at relatively low temperature [2].

Up to now, very little is known about aromatic azides and only some theoretical ab initio calculations focused on the prediction of the photo-chemistry of aromatic azide behavior have been performed [3].

In this work ab initio and density functional calculations of the molecular properties of benzylazide and its ortho-, meta- and para- methyl isomers were performed. We report detailed analysis of several molecular properties of these molecules, such as conformational equilibrium structure, ionization energies and vibrational spectrum.

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On the electron-impact broadening of the nitrogen (^{1}D)3s^{2}D - (^{1}D)3p^{2}P^o 7904.5 $\AA$ line

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Recently Bartecka et al. [1] have determined experimentally Stark widths (line widths due to collisions with charged particles) for N I 3s'^{2}D-3p'^{2}P^o multiplet and have found very large values. Obtained widths are 1.4 to 2.9 Å for electron densities (1.2-2.1) x 10^{16}cm^{-3} and temperatures 9200-13600 K. With the standard semiclassical theory [2] we obtain one order of magnitude smaller values.

Table 4: This table shows electron−impact broadening parameters (full width at half intensity maximum W, shift d, the quasistatic ion broadening parameter A, the total width due to elecron- and ion-impacts W$_{e+i}$(Å), and the coefficient of the ion-dynamic contribution D for N I 3s'^{2}D-3p'^{2}P^o multiplet, for perturber density of 10^{16}cm^{-3} and temperatures from 2500 up to 50,000 K. Transition and averaged wavelength for the multiplet (in Å) are also given in the Table. By dividing C by the corresponding full width at half maximum, we obtain an estimate for the maximum perturber density for which the line may be treated as isolated and tabulated data may be used.

TRANSITION	T(K)	WIDTH(A)	SHIFT(A)	A	W$_{e+i}$(Å)	D
3s'^{2}D-3p'^{2}P^o	2500.	0.682E-01	0.359E-01	0.1345E-02	0.6822E-01	0.3600E-01
	5000.	0.736E-01	0.462E-01	0.1269E-02	0.7371E-01	0.4628E-01
7906.7 A	10000.	0.845E-01	0.430E-01	0.1145E-02	0.8457E-01	0.4312E-01
C = 0.43E+20	20000.	0.108	0.400E-01	0.9531E-03	0.1080	0.4013E-01
	30000.	0.127	0.334E-01	0.8427E-03	0.1273	0.3358E-01
	50000.	0.156	0.270E-01	0.7218E-03	0.1564	0.2716E-01

All details on the theory and calculation procedure are given in [2,3]. Needed atomic energy levels are taken from [4]. Here are provided all data for Stark broadening, needed for discussion and different considerations. Further experimental and theoretical investigations of this interesting multiplet are needed.

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EUV photoabsorption of a Te plasma

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EUV photoabsorption spectra of the tellurium isonuclear sequence Te I - Te IV have been recorded. Photoexcitation from the 4d subshell is the dominant process in the 50-150 eV energy region. Above the 4d ionisation threshold the spectra of Te I - Te III were found to be dominated by a 4d-ϵf shape resonance, which peaks at 88 eV in each case. With increasing ionisation, inroads are made into the resonance as the available oscillator strength in the ϵf channel is redistributed amongst transitions to nf discrete states. In the Te IV spectrum discrete structure dominates the spectrum, the strongest features arise due to transitions of the type $4d^{10}5s^25p \rightarrow 4d^95s^25p4f$.

Hartee-Fock with configuration interaction was used to identify the strongest discrete features in the experimental spectra [1]. The relativistic TDLDA (time dependent local density approximation) code of Zangwill and Liberman [2] was used to account for the 4d-ϵf absorption profile. There is good agreement between predicted and observed profiles for Te I - Te IV, both for discrete and continuum absorption.

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Reanalysis of the fine structure of even configuration system of scandium atom

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We report the fine structure analysis of the even configurations system of Sc atom in a large multiconfiguration basis. The complete energy scheme in the energy region up to 49000 cm^{-1} has been established.

We have tried to take into account first- and second-order effects in the fine structure of scandium as comprehensively as possible with all experimental energy level available at present [1,2]. The calculations were beginning with the basis of three configurations model space $(3d+4s)^3$ and further have extended this system up to 58 configurations. We have observed that gradual expansion of the configurations basis (through direct inclusion of the interactions with configurations, which originate from one- or two-electron excitations from the configurations $3d^3$, $3d^2$ 4s and 3d $4s^2$), leads to a decrease of the values of the two- and three-body radial parameters. With the most extended basis of 58 configurations we can put zero values for α and β parameters for $3d^3$ configuration. However, the three-body parameter Ts(3d,3d,4s), in spite of the extension of the basis has retained a significant value. In fine structure of even configurations of scandium atom very strong interactions between the configurations has been observed, particularly with the configurations originating from the excitation of two electrons from the $(3d+4s)^3$ system to configurations including a $4p^2$ core. The strength of these interactions is most clearly manifested in the energy positions of the levels $3d(4s4d)^1$D;SLJ and $3d(4s5d)^1$D;SLJ which lie below the levels $3d(4s4d)^3$D;SLJ and $3d(4s5d)^3$D;SLJ respectively. In the absence of this interaction, the relative positions of these levels would be reversed. Furthermore, the value of radial integral R^1(4s4d,4p4p) is about 50% greater than the value predicted from Hartree-Fock calculations. We must point out, that the good agreement between calculated and experimental energy for the levels of 3d4s5d configuration was obtained only if the value of the R^1(4s5d,4p4p) integral was almost three times as large as the value obtained from Hartree-Fock calculations.

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Hyperfine structure analysis of the even configuration system of scandium atom

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The hyperfine structure analysis of the even configuration of Sc I has been performed in approximate basis of 22 configurations ($3d^3$, $3d^24s$, $3d^25s$, $3d^24d$, $3d4s^2$, 3d4sn′s(n′=5-9), 3d4sn″d(n″=4-7), 3d4sn‴g(n‴=5,6), $3d4p^2$, 3d4p5p, $4s4p^2$, $4s^25s$, $4s^24d$, $4s4f^2$). The configurations selected for the basis have to satisfy the following conditions: they should contribute to eigenvector composition of the levels with experimentally determined hfs constants and they should extend in the energy region up to 49000 cm^{-1}. For all the levels belonging to the selected configuration basis the predicted hfs A constants have been calculated within this work. We have tried to determine not only the total value of the configuration interaction effects in the hyperfine structure, but to estimate the particular contributions as well, both from the core polarization effects and far-configuration-mixing effects. This could inspire similar theoretical calculations and thus enable comparison of experimental and theoretical values. In order to include the J-off-diagonal effects in the hyperfine structure, direct diagonalization of the matrix containing J-diagonal as well as J-off-diagonal elements was performed. It is the first application of the diagonalization of hfs energy matrix (in the basis of $\Psi(configuration, vSLJF)$ states) in the many configurations approximation. It requires the precision up to 16 significant digits. In spite of scarcity of experimental data it has been possible to estimate for the first time in Sc atom the values of magnetic octupole hyperfine structure constants C_{corr} for the levels investigated with the methods of atomic beam magnetic resonance (ABMR) or laser-rf double resonance on an atomic beam (ABMR-LIRF)[1-3].

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Investigation of metal clusters and fullerenes in a Penning ion trap

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Atomic clusters are systems containing between very few (two, three, four,..) to several thousand atoms. They can be classified according to their interatomic bonding. For example, metal-cluster atoms are bound together via metallic bonding and carbon-cluster atoms are connected via covalent bonds. The physics of atomic clusters is itself an interesting area of study, due to the fact that these independent systems have their own properties that are found to be strongly dependent on the number and type of atoms that they contain. Furthermore, atomic clusters 'bridge' the gap between atomic physics and solid-state physics, that is, the more atoms that a cluster contains, the more the properties of the cluster approaches that of bulk matter.

In the case of small atomic clusters, it has been observed that many of their properties do not vary monotonically with size, for example, properties such as electron affinity, ionisation energy and binding energy. There are two major aspects that govern these properties: The spatial positions of the atoms within the cluster and the electronic structure, in particular, the behaviour of the atomic valence electrons. By comparison of different charge states the influence of electronic and geometric effects can be distinguished. Thus, in the last decade, multiply-charged clusters have received much attention as a research topic.

The ClusterTrap apparatus in Greifswald was originally developed in order to facilitate the study of metal-cluster ions of various charge states [1,2]. Recently, the apparatus has been further adapted and a new ion source has been implemented in order to extend research into a different area of atomic cluster physics - that of fullerenes [3].

The ClusterTrap setup is centered around a Penning ion trap. The carbon-cluster source allows production of either singly- and multiply-charged cations by electron bombardment of neutral fullerenes evaporated from an oven, or, singly-charged negative fullerene ions by electron attachment to neutral fullerenes. Multiply-charged carbon-cluster anions are subsequently created by exposure of trapped fullerene mono-anions to an electron bath, a technique originally used to produce multiply-charged metal-cluster anions [3,4]. The Penning trap enables the storage of ions for long periods of time such that their properties can be further investigated. Experimental techniques applied include collisional activation of trapped ions which may result in fragmentation (in the case of cations) or electron emission (in the case of anions), and the use of laser excitation which allows time-resolved investigations of the same processes.

The first part of this contribution provides a comprehensive overview of the recently developed fullerene ion source and the ion-trapping techniques used both in the creation of dianionic carbon clusters and in the manipulation of the motion of the stored atomic clusters. The second part summarises new results of experiments on the decay processes of trapped fullerene ions by use of collisional and laser excitation.

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Tin based laser produced plasma source development for EUV lithography.

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The source of extreme ultraviolet (EUV) radiation for the next generation of lithography tools is one of the key questions facing the semiconductor processing industry. The choice of wavelength for extreme ultraviolet lithography (EUVL) is based on the availability of Mo/Si multilayer mirrors with ∼70% reflectivity at 13.5 nm, with a reflectance bandwidth ∼0.5 nm. The required conversion efficiency of the source for EUVL will be close to 3%, in a 2% bandwidth around 13.5 nm, allowing the exposure tool to achieve a throughput of 100 wafers per hour [1]. However, xenon, one of the most studied possible sources, was measured to have a maximum conversion efficiency of ∼1% [2]. Hence, it is unlikely that the required conversion efficiencies will be achievable with xenon based sources, whereas tin has been identified as a potentially brighter emitter at 13.5 nm. The transitions responsible in tin arise from $4p^6 4d^n$ — $4p^5 4d^{n+1}$+$4d^{n-1}4f$ lines in a number of adjacent ion stages (Sn^{5+}–Sn^{13+}), which merge to form an unresolved transition array (UTA) [3].

In order to maximise the in-band emission from tin a number of parameters must first be optimised, e.g. the laser power density required to obtain the ion stages forming the UTA in tin, and the opacity of the plasma, to prevent reabsorption of the produced light. With respect to the latter, when tin is present as a low percentage impurity in a target of low Z elements the emission from the UTA is found to be increased in some cases. Previous studies [4] have also shown that emission from targets doped with cerium can be increased 7-fold by use of a prepulse-main pulse system to generate more favourable initial conditions for plasma formation.

Here at UCD laser produced plasmas formed from ceramic targets, doped with various concentrations of tin, are studied in order to determine the optimum plasma conditions and concentration of tin for the production of radiation in the 2% bandwidth centred at 13.5 nm. The plasmas are created with a 1 J, 15 ns Nd:YAG laser pulse, with the spectrum in the 9–17 nm region and in-band energy recorded with a 0.25 m grazing incidence absolutely calibrated flat field spectrometer. Comparisons with a steady state, collisional-radiative model [5] and atomic structure calculations using the Cowan suite of codes [6] show good agreement for the laser power density predicted to optimise the in-band EUV radiation. To date the maximum conversion efficiency of laser energy into the 2% bandwidth is ∼2.9%. This was obtained for laser power densities between 1×10^{11} and 2×10^{11} W cm^{-2}, with targets containing 4.5–6.5% tin by number. Furthermore, initial prepulse experiments, using an electronic delay system, have yielded a 75% increase in the intensity of the UTA.

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Methods of atomic spectroscopy for addressing diversity.

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For the first time, this year, EGAS does not mean European Group for Atomic Spectroscopy any more, in the title of the annual Conference. The fact that atomic systems are taken into consideration is quite positive, but is elimination of the word 'Spectroscopy' favourable? It seems, at least, an opportunity for recalling some specificities which remain essential in many cases, and have been at the origins of many developments, including quantum mechanics. Methods used by spectroscopists, when dealing with very complex systems, seem to lack in some other fields of science, where diversity is involved too, but rather treated as something to be eliminated, with probabilistic statisticals tools, without much efforts for classification and multiscale observation. Could a general description of spectroscopic methods become a wider concern, for those who demonstrate, in their daily research, how details and globality are taken into account, for the understanding of new features and mechanisms in atomic system?

I will try to show how introducing a 'spectroscopic paradigm' can be beneficial in some major fields outside physics, including medicine, with the hope of some help for improving the description. The word paradigm could be taken here according to its simplest definition, namely, of a template for grammatical purposes, e.g. conjugation of verbs, where the radical can be changed, but the form remains the same. According to hyperfine structure studies in very complex atomic spectra, coincidences of structured details are important in the understanding of mechanisms which are hidden by the complexity of effects; many more features are of interest.

I will discuss some examples where the acceptation of spectroscopic methods could help securing some results of major societal importance, not yet well accepted because significative probabilistic statistical studies are found too scarce, in the absence of clearly understood mechanisms.

- Electromagnetic pollution and chemical pollution, do already use some spectroscopic tools, but prevention could learn from our methods of analysis, when facing human diversity, and the complexity of mechanisms.

- Homeopathy, which I consider a major question for physics, is pointed out by observations of enormous amounts of correlated details observed on patients, including animals; data are, nowadays, treated in a way similar to spectral data, including databanks, and computer search for coincidences; but also, spectroscopic details of Raman enhancement were already observed, and reported by C.Luu in her thesis of Pharmacy, some 30 years ago. It could be a preliminary for new advances in the study of chemical reactions in solution, to understand how the potentization effect observed occur when shaking solutions. It means also a revolution as concerns the role of concentrations in toxicology.

- Analysis of daily observation of weather, according to empirical rules given in proverbs, to be compared to the Landé rule, provides some hints towards an interpretation in terms of coupled effects. Dust from the solar system impinging on the atmosphere, with water circulation related to oceanic tides, seem at the origin of a diversity where pure effects are rare, but help deciphering intermediate cases. This puts some questions to astrophysicists, who are currently aware of spectroscopic methods; could the link proposed here help give a higher priority to spectra analysis, for their own benefit?

Energy-resolved spectra of double-electron ATI at 390 nm

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Recently it has been shown [1] that in helium the process of simultaneous double-ionization generates two-electron wavepackets that absorb excess energy (above the minimum required for double-ionization) in integer multiples of $\hbar\omega$. This process, which we call double-electron above-threshold ionization (DATI), can be distinguished from the ATI of sequential double-ionization in several respects. DATI is a two-electron dynamical process in which the two electrons absorb energy in a correlated fashion: the individual electrons themselves will not absorb energy in discrete units, but instead the sum of their final-state energies will be found to be constrained to integer multiples of the photon energy above the (ponderomotive shifted) ground state energy. By contrast, if two singly-ionizing electrons are ejected from the atom and undergo ATI then each will absorb energy independently of the other and each will escape at energies that are restricted to a discrete number of photons above their respective ionization potentials.

We will report calculations of DATI in helium at optical wavelengths (390 nm) and at intensities in the 4×10^{14} to 12×10^{14} Wcm^{-2} range. Double-ionization at this wavelength and intensity range is a poorly understood process since it falls outside the domain in which classical rescattering arguments are fully applicable. The accepted explanation of simultaneous double-ionization due to rescattering assumes that a singly ionizing electron absorbs energy from the field and returns to the atom with sufficient excess energy to eject the remaining electron. The threshold intensity at which this can occur at 390 nm is 12×10^{14} Wcm^{-2}. Below about 9×10^{14} Wcm^{-2} the returning electron cannot even excite the remaining bound electron to the lowest energy excited state of the residual ion. The physics of simultaneous double-ionization below this intensity remains an open question. Double-ionization of helium at 390 nm therefore opens up a relatively unexplored domain in the physics of atom-laser interactions. This wavelength and intensity range is readily obtainable from frequency doubled Ti:Sapphire lasers. Experimental studies of intense-field double-ionization of helium at 390 nm have recently been reported [2].

DATI energy spectra are obtained by calculation of the momentum-space joint probability distribution of the ejected two-electron wavepackets, which in turn are obtained from the numerical integration of the full-dimensional time-dependent helium Schrödinger equation. Given that DATI is a highly correlated two-electron process in the intense-field non-perturbative limit, it is evident that a high-accuracy theoretical investigation of the process requires a rigorous treatment of the two-electron laser-driven Schrödinger equation. Although this approach is computationally demanding, high-accuracy calculations have great practical application in, for example, the determination of peak laser intensities in the short-pulse intense-field limit [3]. In theoretical problems, they provide crucial support in the design and calibration of simplified models of multi-electron atom-laser interactions [4]. We discuss some of the computational challenges of full-dimensional calculations at optical wavelengths.

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Selective Excitation of Aluminium Ion Lines in Helium and Neon Hollow Cathode Discharge: Possibilities of UV Laser Oscillation

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Hollow cathode glow discharges have been widely used as an excitation medium for a large number of metal vapour laser lines with wavelengths extending from the near infrared to the deep UV spectral range. Nowadays the hollow cathode metal vapour lasers are the only continuously oscillating direct laser source in the deep UV. Laser oscillation bellow 300 nm is achieved on ion lines of only three metals: copper, gold and silver [1]. Cathode sputtering is used to produce the required metal atom density in the hollow cathode discharge.

We have made an analysis of the general energy level structure of the singly ionised Al. It is found that in the UV spectra of Al II there are many intensive lines originating from levels which can be populated selectively via charge transfer collisions with either helium or neon ions. Some of these levels are known to be the upper levels of already obtained Al ion laser transitions, excited in a hollow cathode discharge [2,3].

The emission spectra of aluminium in the 200-400 nm spectral range is measured in a cylindrical Al hollow cathode at discharge conditions typical for laser oscillation. The hollow cathode is a cylinder with 4 mm inner diameter and 30 cm in length, made of aluminium. The Al atom density is produced by cathode sputtering. As compered to copper, gold and silver, aluminium sputters poorly but, as shown in [2,3], it is possible to create sufficient for lasing aluminium atom density. The discharge is operated in either He or Ne as buffer gas at discharge current density 0.5 A/cm^2. An enhancement of the spontaneous emission intensity on some of the Al ion lines in the UV spectral range in Ne (He) compared to He (Ne) discharges is observed, indicating that the excitation of the corresponding levels by charge transfer is much higher in Ne (He) than in He (Ne) discharge. All these lines originate from levels, which presumably are excited by charge transfer collisions with Ne or He ground state ions, respectively. It is very likely to establish population inversion on some of these Al ion transitions and to obtain laser oscillation. Using the available data for the transition probabilities, we have evaluated the possibility to obtain laser gain on a number of Al ion lines in the UV spectral range.

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Effective cross sections of the positive and negative ions formation of thymine molecules

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In our previous investigations [1,2], which were carried out with molecules of the nucleic acid components (cytosine, thymine e.a.), we have observed the different physical processes (excitation, ionization, dissociative excitation and dissociative ionization) under electron impact. Objective data for ionization absolute cross sections of molecules can be obtained only in a precision physical experiment when the medium influence is practically absent. Such approach with applying of the modern technique of normally crossed molecular and electron beams was realized at present work.

In this research the molecular beam was formed by a thermal effusion source. The molecules concentration was determined directly in experiment and was equal to $6 \cdot 10^{10}$ cm^{-3}. The electron beam was obtained by means of a five-electrode gun. The electron beam current was about $1 \cdot 10^{-6}$ A with an energy spread of $\Delta E_{1/2} \sim 0.3$ eV (FWHM). The electron gun was located in lengthwise magnetic field with induction $1.2 \cdot 10^{-2}$ Tl. The energy was calibrated using SF_6^- anions recorded in the same experimental conditions. The connecting collector [3] was installed for total collection of the molecular ions formed in crossed electron and molecular beam region. The absolute value of the cross sections negative ions formation of the nucleic acid bases – thymine - was found in the direct experiment for the first time using our original technique. The ionization cross section has maximum at 95 eV energy and is $1.4 \cdot 10^{-15}$ cm^2. The threshold of the positive ion formation is 9.2 ± 0.1 eV. The energy dependence of the effective cross sections for thymine negative ions formation has the distinct resonance at 1.1 eV electron energy. Maximal ionization cross section is $8.4 \cdot 10^{-18}$ cm^2. It is important, that the absolute ionization cross sections are the total cross section factly because it include the cross sections of the ion formation both for the whole molecules and their fragments.

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Two-photon double electron ejection from He^-

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We report here on our recent work concerning the two-photon double electron ejection of He^- ions between 2.9 and 3.3 eV in intense laser fields. Complementary experiments are carried out to investigate the simultaneous nature of electron ejection both in the total ionization yield and the ejected electron spectra.

The total ion yield is measured with the same apparatus as described in [1], where a 4 keV beam of He^- ions, produced by double charge exchange in a Cs vapor cell, is illuminated at right angle by laser pulses around 400 nm. The 1s3s4s ^{4}S resonance, located below the 1s3s ^{3}S photodetachment threshold, exhibits a complicated peak-and-dip structure in the He^+ ion yield. The dip is interpreted as a result of the loss of excited ions by spontaneous detachment at the entrance of the gaussian laser profile, which is possible as the interaction time ($\sim$ 90 ps) is much longer than the lifetime of the 1s3s4s ^{4}S state [2]. This interpretation is supported by the observation of the neutral signal which shows a peak at the exact position of the dip in the ionization signal, with similar width.

The origin of the peak-and-dip structure may be further clarified by reducing the interaction time. This may be achieved by operating the ion beam at higher velocities and/or by reducing further the laser spot size. We expect the dip to disappear gradually as the time of flight of the ions through the laser spot is reduced, since ions will have less time to detach before reaching the center of the laser beam where double ionization takes place. Such measurements will be presented at the conference.

The simultaneous character of the two-electron ejection can be unambiguously demonstrated by recording the correlated angular and energetic distributions. While sequential ejection is characterized by discrete electron energies ensuring energy conservation for a single photon absorption, the collective ejection allows for energy sharing between electrons. Additionally, a strong angular correlation is expected for equal energy sharing. This is currently investigated by means of the fast beam photofragment spectrometer developed by Pedersen *et al.* [3]. As slow electrons are to be detected, one makes use of the large velocity of the target ions (up to 50 keV), combined with an axial electric field, to map the electron velocities onto a MCP detector with a hole and a phosphor screen imaged by a CCD camera. Triple coincidence is needed to clear the signal from uncorrelated single electron events.

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Spectroscopy of the G(3)$^1\Pi$ state of NaCs

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Till recent time experimental information about electronic states of the NaCs molecule was limited to the ground singlet state $X^1\Sigma^+$ and low vibrational levels for the excited $D(2)^1\Pi$ state [1]. NaCs *ab initio* calculations are presented in Ref. [2]. In Ref. [3] laser induced fluorescence (LIF) transitions $G(3)^1\Pi$ - $X^1\Sigma^+$, $E(4)^1\Sigma^+$ - $X^1\Sigma^+$ and $D(2)^1\Pi$ - $X^1\Sigma^+$ were studied by the Fourier transform spectroscopy yielding an accurate ground state potential. These experiments provided rich spectroscopic information also on the excited states, particularly the $G(3)^1\Pi$ state. Here we present the $G(3)^1\Pi$ state analysis based on these data, as well as on additional experiments performed in order to include a new data set of low vibrational levels.

At the first stage of the experiment NaCs molecules were formed in a specially designed metal cell [3]. Further experimental studies were performed in a heat pipe oven. The $G(3)^1\Pi$ - $X^1\Sigma^+$ LIF was excited by an Ar^+ laser and a single-mode frequency cw Nd:YAG laser. Due to the presence of the argon buffer gas we were able to observe rich rotational relaxation spectra. These allowed us to enlarge the data set for the $G(3)^1\Pi$ state significantly, as well as to obtain information about the Λ-splitting in the $G(3)^1\Pi$ state. The latter lead to derivation of Λ-doubling parameters, so called q-factors, in a wide range of rotational and vibrational quantum numbers.

The data field for the $G(3)^1\Pi$ state includes about 720 energy levels and covers the range of rotational quantum numbers from J'=3 to 190 and the range of vibrational quantum numbers from v'=1 to 31, which coresponds to 85 % of the potential well depth. Direct fit of the potential energy curve to the level energies is realized using the IPA method [4].

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Dynamic effects in autoionizing resonance forming

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The new *ab initio* results for autoionizing profiles in photoionization cross section of outer p electrons in various species are calculated. Our theoretical approach combines non-relativistic Hartree-Fock approximation to obtain the initial wave functions basis and the Many-Body Perturbation Theory (MBPT). Energies of single-electron states are corrected by the means of Dyson Equation Method to include the *dynamic polarization* of electronic core. Then the Random Phase Approximation with Exchange (RPAE) procedure as the first order approximation is built. It takes into account the *dynamic polarizability* of an atomic system interacting with a weak electromagnetic field. Within the RPAE frames only the processes with one excited electron at each moment are considered. However, this first order approach is not enough describing autoionizing resonances in np electrons photoionization cross section associated with weak $ns \rightarrow (n{+}1,2,...)p$ transitions. Since the RPAE terms for phototransitions from inner ns shell are small comparing to strong $np \rightarrow \epsilon d(s)$ transitions, the next order for amplitudes cannot be neglected. These second order terms correspond to processes with two excited electron-hole pairs at each moment [1]. The second excited pair screens the direct Coulomb interaction between the excited quasi-bound $(n{+}1,2,...)p$ electron and ns hole (*dynamic screening*). So that the new photoexcitation amplitudes and matrix elements of effective inter-electron interaction with "two particles — two holes" processes taken into account differ from the RPAE values a lot. It leads to changing of calculated resonance shapes.

Thus, for krypton and krypton-like ions (Rb^+, Sr^{2+}) the resonance profiles obtained within the RPAE frames have asymmetric peak shapes. However, a window-type structure was observed experimentally [2] for the most of resonances. With dynamic screening taken into account the calculated results agree with the experiment. For resonances in neutral Kr^0 atom, Rb^+ ion and the first $(4s^{-1}4p^65p)$ resonance in Sr^{2+} ion window-type profiles have been obtained. The second $(4s^{-1}4p^66p)$ resonance in Sr^{2+} has a small maximum following the deep. In Y^{3+} ion the $4s^{-1}4p^65p$ energy lies under the $4p$ ionization threshold and higher resonances have well pronounced peak shapes. These results are in good agreement with previous multi-configurational calculations of A.Neogi et al [2].

The second part of our work is devoted to the autoionizing resonances in alkali atoms series (K^0, Rb^0, Cs^0). The theoretical treatment of these objects is much more complicated due to different behaviour of electrons with opposite spin projections. Two well resolved Rydberg series (one for each spin projections of $4s$ electron) appear. The RPAE approach overestimates the cross section in resonance again: peaks instead of windows are obtained. Dynamic screening taken into account improves resonance parameters, so the experimental data [3] are described fairly [4].

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Decay rates of doubly excited multi-charged ions

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The new results of radiative and Auger decay rates for double excited $4l4l'$ states in ionic series O^{**6+} – O^{**5+} – O^{**4+} and C^{**6+} – C^{**5+} – C^{**4+} are calculated. The problem of decay rates determination for highly charged and multiple excited positive ions is related to the general interests and many applications [1]. In particular, the information about these processes in the series of positive ions is needed for analysis of X-ray spectra obtained from the comets and other astrophysical objects. The basic mechanism of cometary X-rays production is radiative stabilization of electrons captured from comet atmosphere by highly charged projectiles ($O^{8(7,6)+}$, $C^{6(5,4)+}$) contained in the solar wind [2,3]. The double capture to $4l4l'$ state occured to be the most probable. This double excited state can decay emitting either Auger electron or soft X-ray quant. We have done the calculations of decay rates for these competitory processes in oxygen and carbon ions.

The calculations have been completed both for partial and total decay rates within the single configuration Hartree-Fock approximation and with account for many body effects. The results have shown that Auger branch is more probable for O^{**6+} and O^{**5+} ions, but for carbon ions and for O^{**4+} the probability becomes smaller. However, talking about cometary radiation, the X-ray spectra only can be measured. We have obtained radiative spectra of ions stabilization for the wide band of outcoming photon energy calculating probabilities of all possible transitions from all initial $4l4l'$ configurations. The main contribution to total decay rates is from $4p^2$ configuration. The most stable state is $4f^2$ since only triple cascade relaxation is allowed.

The obtained results for O^{**6+} are in good agreement with previous calculations [4].

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Spectroscopic studies of wide bandgap semiconductor materials

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ZnO, a semiconductor with a direct band-gap of 3.4 eV and an exciton binding energy of 60 meV, is a leading candidate material for the production of blue/UV emitting LEDs and laser diodes. First studied in the 1960s, it was subsequently neglected, but re-emerged recently with the development of growth techniques for large area single crystals and thin films. Producing p-type material has been a major challenge, since as-grown ZnO contains significant concentrations of n-type defects and impurities whose identities remain controversial. Our research is focussed on establishing the chemical identity of the dominant n-type impurities and on exploring new strategies for successful p-type doping. Here we report on experiments aimed at correlating the sharp line band edge photoluminescence features, long associated with donor bound exciton recombination, with particular n-type dopants.

In the photoluminescence of ZnO there have been previous assignations of donor bound excitons to gallium. In order to check this assignment we used samples implanted with low doses of selected radioactive isotopes. Using the characteristic decay of a radioactive isotope, a particular optical feature can be shown to be due to a particular element if photoluminescence intensity changes can be correlated to the half-life of the implanted isotope. Radioactive ^{72}Zn, which decays to ^{72}Ga, and thence to ^{72}Ge, was implanted into ZnO at the ISOLDE facility in CERN. Photoluminescence measurements are taken at the on-site Apparatus for Photoluminescence Investigations with Radioactive Isotopes off-Line (APRIL). Photoluminescence (PL) measurements were recorded over 5 half-lives of the ^{72}Zn isotope. The intensity of a near band-edge feature, a line commonly labelled I_8at 3.36 eV, was found to match the concentration of gallium. In that first experiment, the ^{72}Zn beam had unfortunately about 40 % ^{72}Ga contamination and this complicated the analysis somewhat. In order to obtain cleaner data we repeated the experiment using ^{73}Ga which decays to ^{73}Ge with a half-life of 4.9 hours. Any possible contaminants in the beam had short lifetimes of the order of seconds; therefore this beam was much cleaner than the previous one. We again saw the I_8 line decay and also found some evidence of photoluminescence due to stable ^{73}Ge atoms, the product of the radioactive decay process, which will be followed up in future experiments.

Performance Evaluation of FEC Codes in Highly Spectrally Efficient 42.6 Gbit/s Coherent WDM Optical Transmission System

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Over the last number of years, the capacity of long haul digital transmission systems has increased as a result of advancement in a number of different technical areas, such as forward error correction (FEC) codes and modulation formats [1]. The ITU G.975 Reed Solomon code with 7% overhead for FEC in optical communication systems provides a net coding gain (NCG) of around 5 dB. This may be increased by use of enhanced FEC codes, such as Low-Density Parity Check (LDPC) and Turbo codes, with a NCG of 10.2 dB, for a noise limited channel with modest overhead [2], and a maximum of 15 dB [1]. Moreover, transmission systems are now capable of operating at bit rates over 40 Gbit/s, where spectral efficiencies of up to 2.5 b/s/Hz were reported [3], and even higher efficiencies are theoretically possible [4].

However, at such efficient systems, the bit error rate of the transmitted channels is limited not only by optical signal-to-noise ratio, but also by linear and nonlinear crosstalk. The consequent change in the error statistics means that it may no longer be accurate to assume the same performance from FEC codes. In this poster, we report the implementation of a technique to directly assess the performance of FEC codes operating at 42.6 Gbit/s, without the use of bitwise demultiplexing or lower bit rate decoders. We also present the experimental system setup used to generate the highly spectrally efficient wavelength division multiplexed (WDM) transmission system used. Furthermore, we demonstrate the actual performance of selected RS codes, in this transmission system.

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Compact System for Soft X-ray Point Projection Absorption Spectroscopy and Imaging of Laser Produced Plasmas

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We report the development and construction of a compact soft X-ray (SXR) spectrometer designed to study freely expanding plasmas as well as plasma-plasma and plasma-wall collisions. The light source is a laser produced plasma, operating at 5 Hz, yielding intense SXR emission from a selection of targets of varying Z from Mg to rare earth and neighbouring element targets covering the 1 – 2.5 keV photon energy range. The dispersive element is a flat crystal (usually KAP or ADP) afixed to a rotary mount to permit wavelength range selection. X-rays, dispersed by the flat crystal are recorded on an in-vacuum, back illuminated CCD (Andor DX420-BN). Apart from emission spectroscopy, the system may also be used for X-ray point projection absorption spectroscopy [1,2,3] in the future. We report instrumental performance measures and illustrative preliminary results from this new setup.

A key motivation for the development of this system is the study of freely expanding, collisional, and surface collisional plasmas in the soft X-ray regime. The latter, often referred to as laser plasma-wall interaction (LPWI) was first observed in 1982 by Presnyakov [4] and is set to become an important concern in the new Extreme-UV lithographic (EUVL) process currently under development in the semiconductor industry. Preliminary Soft X-ray emission spectra from freely expanding plasmas and (hopefully) from plasma - surface collisions will be presented. This system, under development in DCU is versatile and gives the ability to probe various plasma expansion scenarios on a routine basis.

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Space resolved measurements of plasma parameters using x-ray spectroscopy of He-like argon

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Measurement of line radiation in the soft X-ray region is a promising tool for the diagnostics of high-temperature plasmas. In particular, x-ray spectroscopy of the He-like lines provides the information on the balance of the impurities and the main plasma characteristics.

The Bragg spectrometer / polarimeter of Johann type at the tokamak TEXTOR has been upgraded for spatial resolution. The spectrometer consists of a spherically bent quartz crystal with radius of 3.85m, cut 11(2)0 and a 2-dimensional multi wire proportional counter. For He-like spectra the Bragg angle is around 54 deg, the plasma is located between the meridional and the sagittal focus of the crystal. The system allows to observe the plasma in vertical direction of about $\pm$12 cm from the plasma center, i. e. $\pm$26 % of the minor radius of the tokamak. The vertical resolution in the plasma is about 2 cm and the spectral resolution λ / $\Delta\lambda$ is about 5000.

In the experiments, the argon has been injected to the plasma at the end of the discharge, when the plasma current is ramped down and the plasma temperature profile shrinks. The spectra provided the ion temperature and the plasma motion via Doppler broadening and shift of the He-like lines. The electron temperature has been obtained from the intensity of the Li-like dielectronic satellites. The charge state distribution has been calulated from the doubly excited Li-like satellites, populated by inner shell excitation, and a detailed analyses of the triplet lines of He-like argon.

A recently developed optimization model has been applied to the measured spectra. It is based on a non-linear least-squares fit of the theoretical spectrum to the experimental data. It incorporates the atomic processes for the He-like spectra as well as the information on the radial distribution of the plasma parameters. The atomic data are based on level calculations with the ATOM and MZ codes, excitation and dielectronic recombination rates by R-MATRIX and AUTOSTRUCTURE calculations, respectively. At the final stage, a collisional radiative modelling of H-, He- and Li- like stages elaborates the different processes which contribute to the intensity of the lines.

During normal operation, the variation of the plasma parameters over the range of the measurement is small, and only for low plasma currents and hence narrow temperature profiles, a considerable change in the x-ray emission and the plasma parameters has been seen. In the future, a compact x-ray spectrometer, which observes about 2/3 of the plasma radius, will be installed at TEXTOR.

Do positrons measure atomic diameters?

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Albert Einstein in his paper on Brown's motion [1] in May 1905 asked if "any exact dimensions of atoms" (eine exakte Bestimmung der wahren Atomgröße möglich) can be determined from classical thermodynamics. Nowadays, methods like, Röntgen-ray diffraction, viscosity studies, van der Waals gas-state yield molecular radii with high precision; unfortunately, they show quite a spread: for Ar the viscosity yields 1.83Å and van der Waals 1.24Å ; for He one expects a lower radius but the values obtained are 1.09Å and 1.33Å respectively [2].

Recently, a new apparatus for total cross sections for positron scattering in gas phase has been constructed at Trento University [3]. The measurements for Ar, N_2, H_2 [4] showed that, from energy of a few eV up to the positronium formation threshold, the cross sections are *constant*. Only classical mechanics for hard-sphere scattering gives cross sections independent on energy. Applying the geometrical formula πR^2 we obtain from this and also other experiments following radii: 0.34Å for He, 0.63Å for H_2, 1.0Å for Ar, 1.6Å for CO_2 [5], 1.9Å for SF_6 [5], showing quite a "reasonable" scaling.

Atomic static potential is repulsive for positrons, so the hard-sphere hypothesis is plausible. However the classical mechanics gives differential cross sections uniform in angle, in disagreemnt with experiment for Ar or N_2 [6]. Applying quantum mechanics for hard-sphere scattering, the shape of the experimental differential cross sections can be qualitatively reproduced but integral cross sections are too high. The ab-initio quantum calculations [7] agree well with the experiment but the theoretical total cross section is not constant and *slowly falls* with energy. For totally absorbing sphere (black body-like) quantum mechanics predicts integral cross section of πR^2 for absorption and πR^2 for elastic scattering, independently on energy and only for a "grey"-sphere, partially absorbing and partially reflecting, the total cross section can be exactly πR^2. Does any absorption process exist in positron scattering on atoms *below* thresholds for electronic excitation and Ps formation?

Gribakin and King [8], in helium, postulated the formation of virtual positronium. We have observed such a process experimentally, appearing as Feshbach resonances at 1.4 and 2.2 eV [5]. If this process is present also in complex atoms, does it balance the falling part of elastic scattering in a way that slow positrons see atoms as classical grey spheres?

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The recent progress on the cesium fountain VNIIFTRI

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Russian State Time and Frequency Service relies on a group of H-masers and classical Cs-beam primary -frequency standard. H-masers are used as time keeper with a long-term stability near $\sim 2 \times 10^{-15}$ uncertainty.We started our Cs fountain project in the spring 1999, hoping to get an uncertainty at least on order less.In this paper, we report the main results of the development of a laser cooled cesium fountain VNIIFTRI. We describe the mechanical constructions of the fountain, laser system, microwave-field synthesizer, and analyze in detail the results of the recent measurements. They are in the following:

1. To increase the light intensity the horizontal beams were returned to the setup by means of additional mirror reflectors. The experimental observations showed that the number of cooled atoms was approximately doubled when these mirrors were used.
2. We have theoretically and experimentally investigated the different approaches for substantial increasing the population of the $F = 3, M = 0$ state in Cs atom by applying an additional pumping laser source on $F = 3 - F' = 2$ and $F = 3 - F' = 3$ transitions.
3. The preliminary results are obtained on the observation of Ramsey oscillations in the atomic fountain with the width of the central resonance ~ 1 Hz upon cooling cesium atom down $\sim 2\mu K$.

We intend to use the acquired experience and methods [1-3] for the development of a fountain frequency reference with the systematic uncertainty $\simeq 10^{-15}$, which will be used in the State primary time and frequency standard of the Russian Federation.

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Calculation of atomic properties using the non-linear coupled-cluster method

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One high-precision method to calculate atomic properties of one- electron systems and to study parity nonconservation (PNC) in heavy atoms is the relativistic linearized coupled-cluster method that sums infinite sets of many-body perturbation theory terms. In the present formulation of this method, single and double (SD) excitations are included completely and certain classes of triple excitations are partially added. The properties of alkali-metal atoms calculated using this method have generally been found to agree very well with experiments. However, further progress in the study of fundamental symmetries in heavy atoms calls for the improvement of the current methodology. This work is aimed at the complete restoration of the non-linear coupled-cluster terms at the SD level. Among the numerous types of non-linear coupled- cluster terms, only six will contribute to the single or double all-order equations. We have derived expressions for all six of those terms, conducted the angular reduction, and modified the single and double all-order equations accordingly. Special care has been taken to ensure proper symmetry of the double excitation coefficients. Numerical evaluation of these terms is in progress.

Carbon I transitions observed in χ LUPI

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The quality of atomic data needed for the analysis of the observed spectra has never been greater due to the launch of several space telescopes. However this analysis is been hampered greatly by the relative inaccuracy of much existing atomic data (particularly oscillator strengths).

The chemically peculiar star χ Lupi was the target of the "Pathfinder Project", a mapping of the UV spectrum of the star. At present there is substantial disagreement between the synthetic and observed spectra of χ Lupi for a number of C I transitions. Hence high quality atomic data is urgently required. The following transitions have been examined to meet this need.

		Calculated Transitions		
$2p^2\ {}^1D_2$	–	$2pns$	${}^1P^o$, ${}^3P^o$	n: 4-5
$2p^2\ {}^1D_2$	–	$2pnd$	${}^1P^o$, ${}^1D^o$, ${}^1F^o$, ${}^3D^o$, ${}^3F^o$	n: 3-5
$2p^2\ {}^1S_0$	–	$2pns$	${}^1P^o$, ${}^3P^o$	n: 6-7
$2p^2\ {}^1S_0$	–	$2pnd$	${}^1P^o$, ${}^3P^o$, ${}^3D^o$	n: 5-7

Large scale systematic calculations were undertaken to find accurate oscillator strengths of several weak Carbon I transitions. The CIV3 [1] code was used. These calculations involved finding extensive configuration interaction wave functions for the states of the transitions. Relativistic effects were included.

The agreement between calculated energies and experiment can be improved by making small adjustments to the diagonal Hamiltonian matrix elements. This process is known as fine tuning (Brage and Hibbert [2]). Oscillator strengths are calculated using energy differences rather than actual energies, so improving these energy separations should provide for a more accurate calculation of the oscillator strengths. By using the CIV3 code these minor adjustments were made to produce the required energy separations.

The results are then compared with those of A.Hibbert *et al* [3], and lead to significant improvement in the accuracy of the oscillator strengths.

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K-shell photoionization of the C^{2+} ion

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Photoionization cross-section data on carbon ions are required for the modelling of stellar evolution [1]. Absolute photoionization (PI) cross-section measurements for K-shell photoionization of Be-like C^{2+} ions have been determined in the photon energy range 292 eV - 325 eV. Absolute measurements compared with theoretical results from the R-matrix method indicate that the primary C^{2+} ion beam consisted of 62 % ground-state ($1s^22s^2\ ^1S$) and (38 $\pm$ 10)% metastable state ($1s^22s2p\ ^3P^\circ$) ions. A combined experimental and theory approach in the photon energy range 292.5 eV - 325 eV indicate the present of several autoionizing states for this complex resulting from 1s $\rightarrow$ 2p and 1s $\rightarrow$ 3p inner-shell promotions. Suitable agreement is seen between theory and experiment for absolute photoionization cross sections.

The measurements reported here were performed on undulator beamline 10.0.1.2 at the Advanced Light Source (ALS) using the ion-photon-beam (IPB) endstation [2]. Absolute PI cross sections for a beam of C^{2+} ions ionized by synchrotron radiation have been determined. The magnitude of absolute experimental PI cross sections, resonance energies, and autoionization linewidths of K-shell-vacancy Auger states show suitable agreement when compared with theoretical estimates.

Further details will be presented at this conference along with a comprehensive set of results.

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Coherence Resonances in Rubidium Irradiated by Frequency-modulated Light

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It was recently demonstrated that irradiating alkali atoms in constant magnetic field (MF) by linearly-polarized frequency-modulated light, narrow resonances appear centered at Larmor frequency that is integer multiple of the modulation frequency. These resonances have been registered as non-linear magneto-optical rotation [1] or directly in the transmitted through the atomic sample light [2].

In this communication we present results of experimental and theoretical study of coherent resonances of Rb (D_1 line) atoms irradiated by circularly-polarized frequency-modulated light. With this approach the resonance contrast is significantly increased and hf-optical pumping is reduced compared to the case of linear polarization. Experimental study is performed in the laboratory magnetic field with orthogonal to the laser beam geometry. Few kHz-width resonances are observed in the fluorescence dependence on modulation frequency. We propose a simple model for theoretical analysis of the resonances based on the density matrix approach. In the frame of atoms, the laser frequency modulation (with frequency deviation larger than atomic line width) is considered as intensity modulation of the radiation. Therefore we can assume that the atom is subject to light pulses with duration much shorter than its Larmor period. If the period of precession of the atomic angular momentum in the MF coincides with light pulse period, the atom would be into a non-absorbing state after each rotation of the momentum, thus it will not interact with any of the subsequent light pulses. If the two periods are different the atom absorption will increase significantly.

The obtained results are applied for Earth MF measurement with nT sensitivity, and are of importance for measurement of atom energy levels splitting.

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The binomial potential of electron-proton interaction and the solution of some problems of quantum mechanics with its help

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In the given work some problems of the quantum mechanics are submitted as result of our incomplete representation about character of forces existing in interaction of electron with a proton.

So if to present interaction of electron with a proton as the binomial potential:

$$V = -(e^2/r) + \Gamma/r^2 \tag{1}$$

where in the right part the first member represents a Coulomb attraction of electron with a proton, and second - hypothetical pushing away of these particles, the simple and convincing answers can be given on many questions of the quantum mechanics.

First of all, the answer to the most phenomenal question of the quantum mechanics is found: why in the theory of Schrödinger it is possible without sufficient representation about character of interaction of particles in system and without an explanation of oscillatory process to receive in the good consent with experiment discrete levels of energy.

Further in work on the basis of potential (1) is shown the basic opportunity of the decision of a classical task of movement of electron in a field of a proton for atom of hydrogen, with an explanation of postulates of Bohr, a constant of Plank and other ratio, which could not be explained within the framework of the classical mechanics earlier. In the theory of Schrödinger with the help of potential (1) the opportunity has appeared to understand and to explain a number of its internal contradictions, including, for the first time in a task of atom of hydrogen it was possible to receive stable in time a wave package and to explain in classical interpretation the mechanism of birth of quantum. And in generally, potential (1) is submitted as a link between the classical and quantum theories.

Thus, in the given work the attempt is undertaken to show, that potential of interaction of electron with a proton actually represents of two-members formula (1), instead of Coulomb's, as it is accepted now.

Collisional Self-Broadening of Lithium $2p - 2s$ Line Core

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This study aims at the quantum-mechanical computation of the width Γ and the shift Δ of the resonance line $2p - 2s$ of lithium, ^{7}Li, atoms evolving in their parent monatomic gas. In the frame of the impact approximation, the method developed by Baranger [1,2] shows that these two spectral parameters are expressed in terms of the phase shifts caused by the ground $\mathrm{Li}(2s) + \mathrm{Li}(2s)$ and excited $\mathrm{Li}(2p) + \mathrm{Li}(2s)$ collisions.

The upper and lower phase shifts needed in the width $Q^{(w)}$ and shift $Q^{(s)}$ cross sections are calculated by solving numerically the corresponding Schrödinger equation for which we have constructed the singlet and triplet potential energy curves from recent and reliable RKR and/or *ab initio* data points calculated in the present work [3,4]. The long- and short-range forms, $\sim 1/R^n$ and $\sim a\exp(-bR)$, with n, a, and b being some constants, are smoothly connected to these data points.

Our theoretical results show that the cross sections, effective in linewidth and shift, vary with energy E like $Q^{(w)} \sim +8320.73/\sqrt{E}$ and $Q^{(s)} \sim -916.97/\sqrt{E}$ (in atomic units). They further show that Γ and Δ do not depend on temperature and may be reproduced by simple formulas, $\Gamma \sim 8.78 \times 10^{-7} N$ and $\Delta \sim 0.90 \times 10^{-7} N$, where N is in cm^{-3} and both Γ and Δ in s^{-1}.

Moreover, since large angular-momentum values are involved, we have tried to apply to this problem a semi-classical procedure as outlined in Mott and Massey [5]. From the application of this procedure, it appears that the influence of the long-range R^{-3} forces are prominent and that the values of $Q^{(w)}$ and $Q^{(s)}$ agree quite well with the quantal calculations. The discrepancies do not exceed 11 % in the first case and 2 % in the second.

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Diffusion Property of Excited and Ground Monatomic Lithium in a Gas of Helium

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The diffusion property may correctly characterize and be a good tool to diagnose the light-induced drifting phenomena. The case of ground and excited alkali-metal atoms in noble gases is particularly of great interest [1-4].

We report in this work our theoretical calculations of the diffusion coefficients and their variation with temperature of Li($2s$) and Li($2p$) in He buffer gas. We have first constructed from reliable and accurate *ab initio* data points the potential curves of the molecular dimers that dissociate into Li($2s$) + He and Li($2p$) + He [5]. Then, using the Chapman-Enskog model [6], we have calculated the cross sections effective in diffusion of the ground $X^2\Sigma^+$ and the excited $B^2\Sigma^+$ and $A^2\Pi$ states for energies ranging from about 10^{-8} to 10^{-2} hartrees. The calculation of the diffusion coefficients has been performed for several temperatures up to 2000 K.

When compared to the experimental results of Atutov *et al.* [4], who measured at 600 K and a pressure of 1 atm the relative difference between the ground and excited diffusion coefficients $(D_g - D_e)/D_g \simeq 0.13 \pm 0.02$, our theoretical results show that they agree very well and lead in the same conditions to $(D_g - D_e)/D_g \simeq 0.08$. The comparison has also been made with some theoretical data of D_g and D_e from Hamel *et al.* [1], Redko [2], and Parkhomenko [3]. In all cases, the agreement with the different results is also found and the discrepancies do not exceed 10 %.

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The use of magnetic-field-induced frequency mixing for determining M1/E2 amplitude ratio in alkali atoms

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Three-photon spectroscopy with polarized laser beams is a worthwhile method for detecting the ratio of M1 and E2 amplitudes of the dipole-forbidden radiative transitions between doublet states $n_1\,{}^2P_{J_1} - n_2\,{}^2P_{J_2}$ of alkali atoms. Static magnetic field $\mathbf{B} = B\mathbf{e}_B$ in this case may provide conditions for coherent mixing of two resonant laser waves with frequencies $\omega_1 = E_{n_1P_{J_1}} - E_{nS} - \varepsilon_{J_1}$, $|\varepsilon_{J_1}| \ll \omega_1$ and $\omega_2 \approx E_{n_2P_{J_2}} - E_{n_1P_{J_1}}$ and generation of a sum-frequency wave $\omega' = \omega_1 + \omega_2 = E_{n_2P_{J_2}} - E_{nS} - \varepsilon'_{J_2}$, $|\varepsilon'_{J_2}| \ll \omega'$ on atoms in their ground state $|nS\rangle$. Complex quantities $\varepsilon_{J_1} = \Delta_{J_1} - i\Gamma_{J_1}/2$ and $\varepsilon'_{J_2} = \Delta'_{J_2} - i\Gamma'_{J_2}/2$ include both resonance detunings Δ_{J_1}, Δ'_{J_2} for real parts and resonance level widths Γ_{J_1}, Γ'_{J_2} for imaginary parts.

The M1/E2 amplitude ratio, arising from inter-shell spin-orbit mixing,

$$s = -\frac{5\alpha^2 Z_n \langle n_2P|r^{-3}|n_1P\rangle}{4\omega_2^2\langle n_2P|r^2|n_1P\rangle} \tag{1}$$

(Z_n is the charge of the atomic nucleus, $\alpha = 1/137$ is the fine-structure constant) appears explicitly in the magnetic-dipole part U_{M1} of the total amplitude $U = U_{E2} + U_{M1}$, which may be written as

$$U_{E2} = A(u_0\varphi_0 + u_2\varphi_2); \quad U_{M1} = -As(v_0\varphi_0 + v_1\varphi_1 + v_2\varphi_2). \tag{2}$$

The factor A includes the field amplitudes together with the dipole and quadrupole transition matrix elements. The polarization-dependent factors are

$$\varphi_0 = (\mathbf{e}_1\cdot\mathbf{e}_2)\left(\mathbf{e}'^{*}\cdot[\mathbf{n}\times\mathbf{e}_B]\right); \qquad \varphi_{1(2)} = (\mathbf{e}'^{*}\cdot\mathbf{e}_{1(2)})\left(\mathbf{e}_{2(1)}[\mathbf{n}\times\mathbf{e}_B]\right). \tag{3}$$

The factors u and v include nine and eight fractions correspondingly, with resonance denominators, involving complex quantities ε_{J_1}, ε'_{J_2}. Five fractions in u and four fractions in v exhibit third-order singularities. E.g. (with account of only triple-resonant terms)

$$u_0 = \frac{2}{(\varepsilon_{3/2})^2\varepsilon'_{1/2}} - \frac{4}{\varepsilon_{1/2}(\varepsilon'_{3/2})^2} - \frac{2}{(\varepsilon_{3/2})^2\varepsilon'_{3/2}} - \frac{6}{\varepsilon_{3/2}(\varepsilon'_{3/2})^2} - \frac{1}{\varepsilon_{3/2}(\varepsilon'_{1/2})^2}, \tag{4}$$

with the symmetric transposition relation $u_0(\varepsilon \leftrightarrow \varepsilon') \leftrightarrow -u_2$, $v_0(\varepsilon \leftrightarrow \varepsilon') \leftrightarrow -v_2$ and $v_1(\varepsilon \leftrightarrow \varepsilon') = -v_1$. Instead of two $3/2 - 3/2$ triple resonance fractions (terms 3 and 4 in the r.h.s. of eq. (4)), the M1 amplitudes v_0 and v_2 include additional fractions with $1/2 - 3/2$ third-order singularities, $2/((\varepsilon_{1/2})^2\varepsilon'_{3/2})$ and $-2/((\varepsilon'_{1/2})^2\varepsilon_{3/2})$, respectively.

The polarization asymmetry which appears in equations (2) – (3) evidently depends on the M1/E2 ratio (1) which thus may be determined with the use of polarized incident radiation. The absence of the term with φ_1 in the E2 amplitude may be used to cancel out U_{E2} for $\mathbf{e}_1 = \mathbf{e}_B \perp \mathbf{e}_2 = [\mathbf{n}\times\mathbf{e}_B]$ when $U_{E2} = 0$ and only the magnetic dipole amplitude $U = U_{M1} = -Asu_1\varphi_1 \neq 0$ determines completely the process' cross section. In addition, the difference between resonance structures of v and u amplitudes in (2) may also be used to distinguish between the contributions of the M1 and E2 terms.

Numerical data for M1/E2 ratio s, for linear polarization and circular dichroism degree in Cs, Rb and K atoms demonstrate feasibility for determining experimentally non-diagonal matrix elements of the spin-orbit interaction.

Proposal for a solid-state laser system for precision spectroscopy of atomic hydrogen

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We present first results of the performance evaluation of a diode-laser system generating 243 nm UV radiation necessary to excite two-photon 1S-2S transition in hydrogen atoms.

The two-photon precision spectroscopy of the 1S-2S transition in atomic hydrogen has recently reached the precision of a few parts in 10^{-14} being one of the most precisely measured atomic transitions [1]. In so far a dye-laser based system has been used. Laser frequency has been measured using a femtosecond laser frequency comb locked to a Cs atomic fountain clock [2].

We are now developing a portable diode-laser based system that will replace the dye laser system and will bring the set-up one step closer to a practical optical atomic hydrogen clock.

Our new diode laser system is based on a commercial laser (Toptica TA-SHG) consisting of a grating stabilized diode laser at 972 nm followed by a 1 W tapered amplifier and a bow-tie type doubling stage that yields 200 mW at 486 nm. The blue light is doubled in a second doubling stage (Laser Physics Wavetrain delta-shape cavity). We measured at most 20 mW at 243 nm that is comparable to the UV output power from the dye-laser based system.

We stabilise the diode laser on an external Fabry-Perot cavity with a finesse of 100,000 in order to reduce the laser line width and we measure the optical beatnote signal with the dye laser system. The measured beatnote line width is below 1 kHz FWHM in 3 s averaging time. We believe that it will be possible to reach a line width below 50 Hz after some improvements on the reference cavity.

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Ultrafast Effects in Semiconductors and their Exploitation for All-Optical Logic

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In todays telecommunications industry, the emphasis is on higher speed and higher capacity photonic systems. The speed at which data is currently transferred in commercial networks is as high as 10 Gbit/s, having been increased from a maximum of 2.5 Gbit/s recently in an attempt to reduce the overall cost per bit of information transfer. Most of the point-to-point transmissions in these networks are carried out in the optical domain, with light signals being sent from laser sources, along optical fibres. However the majority of the signal processing operations (including switching and signal regeneration) is done in the electrical domain. The light signals are first converted to electric signals, then electronic devices are used to perform the processing task and finally the signal is reconverted to the optical domain. This scheme works well at 10 Gbit/s. However, when the line rate is increased to 40 Gbit/s or higher, electronics becomes expensive and power and space consumption become an issue. At such high speeds it may become advantageous to keep the signal in the optical domain and increase the use of all-optical devices and techniques. This project is concerned with the study of semiconductor devices and their exploitation for facilitating all-optical logic and signal processing at high bit rates. Non-linear optical properties arise when these devices are illuminated with optical signals; for example, the refractive index or optical gain is changed momentarily when the device is illuminated with an intense light pulse. These properties can be used to modify the behaviour of one light signal in the presence of another, for example by cross-gain and cross-phase modulation. These effects are assessed for their suitability for controlling optical signals, for use in ultrafast optical logic. The project addresses the physics of spectral hole burning, carrier heating and other ultrafast effects, which occur following the optical excitation of semiconductor devices. These effects occur on very short timescales, of the order of tens to hundreds of femtoseconds. However, such fast features are not yet fully understood, and certainly not yet exploited, in the context of optical processing. The effect of these processes on the refractive index of semiconductor materials is investigated so that the semiconductor devices performances in an interferometric arrangement can be better understood and exploited. This is important as most optical processing operations are realised in asymmetric interferometers. With better understanding of these operations the implications of the ultrafast effects on all-optical processing at high line rates can be explored, along with the viability of a future all-optical based telecommunications system.

Influence of the stray magnetic field on the high order coherence resonances

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This work presents a theoretical consideration on the influence of an arbitrary oriented (stray) magnetic field on the high-order coherent resonances [1, 2] created in an atomic system irradiated by a single-frequency strong laser field. Our interest in the problem was provoked by the latest works of Budker et al [3] and Auzinsh et al [4].

We obtain exact numerical solutions for the population (ρ_0^0), the quadrupole (ρ_0^2) and/or the hexadecapole (ρ_0^4) longitudinal alignment of the resonant levels (f) with quantum numbers $F_f = 1$, 2 exited from the ground state (φ) with corresponding quantum numbers Fφ =1, 2 by a single frequency laser.

A model was developed for the case of perturbation of the scanned magnetic field H_0 by an additional one, which is arbitrary oriented, whereas the laser field E is linearly polarized and orthogonal to H_0. Numerical simulations were used to obtain the amplitudes and width dependencies of the nonlinear resonances related to different ranks of the tensor components ρ_q^κ. A special attention was devoted to the effect of small stray magnetic fields on the scalar and tensor hexadecapole ($k = 4$) components and their influence on the observed fluorescence and/or absorption signals. The obtained solutions show that in a strong laser field both components of the parasitic magnetic field distort the signal formed by the driven magnetic field. The simultaneous influence of the two stray magnetic field components results in the appearance of orientational tensor components, which are a consequence of the interaction through the optical coherences.

The corresponding signal contrast and broadening with respect to a parallel and a perpendicular to E laboratory magnetic field agree qualitatively with the recent experiments [3, 5]. The present results could be of importance for the application of the nonlinear magneto-optical resonances for precise magnetic field measurements.

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Lifetime studies in the C(2)$^1\Sigma^+$ state of NaRb molecule

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We present results of the lifetime (τ) studies in the C $^1\Sigma^+$ state of NaRb molecule. The study included theoretical calculations and measurements of the τ - dependencies on the C $^1\Sigma^+$ state vibrational and rotational quantum numbers v', J'. Theoretical radiative lifetimes were calculated from the *ab initio* dependencies of the C $^1\Sigma^+$ - X $^1\Sigma^+$ and C $^1\Sigma^+$ - A $^1\Sigma^+$ transition dipole moment on internuclear distance [1]. The τ - dependencies calculated in the v'- range from v'=0 to v'=49 show noticeable continuous decrease of the radiative lifetime from about 60 ns to 35 ns with increasing v'.

The experiment was performed in alkali resistant glass cells containing a mixture of natural Na and Rb (natural abundance of ^{85}Rb and ^{87}Rb). The Ar^+ laser lines 514.5 nm and 528.6 nm were used to excite selectively v', J' levels in the v - range from 24 to 44. In order to reach lower vibrational levels the CR-699-21 ring dye laser with Rhodamin 6G dye was used. The assignment of C $^1\Sigma^+$ - X $^1\Sigma^+$ transitions was based on the X $^1\Sigma^+$ [2] and C $^1\Sigma^+$ [3] potentials, as well as on the direct Fourier Transform spectroscopy data [3]. The effective lifetimes τ_{eff} of the particular (v', J') C $^1\Sigma^+$ levels were determined directly from the fluorescence decay after pulsed excitation employing time-amplitude conversion and one-photon statistical analysis technique. The spontaneous lifetime values were obtained by varying the temperature within 180 to 280 °C range and extrapolating τ_{eff}^{-1} to zero pressure. Overall we have obtained 14 spontaneous lifetime values for v', J' levels within $v'-$range from v'=2 to 44 and $J'-$range from J'=8 to 96. Good agreement between the theoretical calculations and the experimental data is obtained.

The work has been supported by the NATO SfP 978029 - Optical Field Mapping grant and by EC 5^{th} Frame "Competitive and Sustainable Growth" grant G1MA-CT-2002-04063, as well as by the Latvian Council of Science (grant No 04.1308) and the Russian Foundation for Basic Researches (grant No 03-03-32857 and No 03-03-32805). The authors are indebted to M. Auzinsh for numerous useful discussions and to O. Martinsons and E. Gevelis for assistance in the experiments.

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The electronic spectrum and molecular constants of the HfO molecule

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The new laser intracavity method was developed to obtain electronic spectra of diatomic molecules that consist of complex system of narrow and partly overlapped lines [1]. This method has been applied to investigate spectrum of the HfO molecule in gas phase. The molecules of HfO were produced by the pulsed electric discharge (0.1 μF, 10 kV) in the mixture of hafnium tetrachloride ($HfCl_4$, 99.98% of purity) with oxygen and argon (pressure 1-2 Torr). The discharge reactor was heated up to 150^{o}C to maintain the necessary vapour pressure 0.1 Torr of $HfCl_4$.

Spectra of the HfO were obtained by 4 meter's spectrograph (the operating orders of grating are 24-27, linear dispersion 0.1 nm/mm). The time delay of probing laser flash related to discharge flash started the HfO molecule formation was about 50-70 μs.

New 11 bands assigned to A-X and 5 bands assigned to B-X transitions were obtained. These bands are red shading; rotational lines with quantum number J>150 were discovered for the R-branches.

For the first time the vibrational bands with $\upsilon' = \upsilon'' = 7$ and new band progressives with $\Delta\upsilon = \pm 1$, 2 were identified. This new data provided assistance to calculate the most reliable vibrational constants for coupled electronic states. The calculated values are: $\omega_e(X^1\Sigma) = 974.74$ cm^{-1}, $\omega_e\chi_e$=3.31 cm^{-1}; $\omega_e(A^1\Sigma) = 914.26$ cm^{-1}, $\omega_e\chi_e$=3.28 cm^{-1}; $\omega_e(B^1\Pi) = 907.05$ cm^{-1}, $\omega_e\chi_e$=3.39 cm^{-1}.

The rotational analysis of some bands of A-X and B-X transitions was carried out. The calculated rotational constants are: $B_e(X^1\Sigma) = 0.386306$ cm^{-1}, $B_e(A^1\Sigma) = 0.378031$ cm^{-1}, $B_e(B^1\Pi) = 0.377821$ cm^{-1}. By comparing calculated values with literature ones [2], we drew a conclusion that A-X and B-X band systems assigned to $A^1\Sigma$-$X^1\Sigma$ and $B^1\Pi$-$X^1\Sigma$ transitions before should be assigned to $b^3\Pi_0$-$X^1\Sigma$ and $b^3\Pi_1$- $X^1\Sigma$ transitions.

The new band system of HfO was observed in the region of 16581.4 - 16273.2 cm^{-1}. This band system was partly analysed and tentative assigned to transition between the ground $X^1\Sigma$ and the triplet $c^3\Sigma$ states. According to [3] the energy of $c^3\Sigma$ state should be around 14000-18000 cm^{-1} above the ground state.

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A new apparatus for the study of electron-impact fragmentation of clusters

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A new experiment has been set up for the study of electron and photon impact fragmentation of clusters. Van der Waals clusters are generated in a supersonic expansion. The clusters are probed with energy-resolved electron impact and fragmentation into ions and long-lived neutral metastable species will be investigated. Alternatively an excimer-dye laser can be used to excite or fragment the clusters.

A reflectron time-of-flight mass spectrometer is used for mass-selective detection of ionized fragments. A neutral metastable particle detector is used for time-of-flight detection of neutral metastable fragments, yielding kinetic energy distributions of these fragments. Detection of neutral metastable fragments has been applied extensively to study electron and photon impact dissociation of many different molecules, but has only recently been applied in fragmentation studies of rare-gas clusters.

The intial focus will be on van der Waals clusters such as rare-gas clusters and clusters of alcohol. Plans are to extend the study to metal-embedded rare-gas clusters (MR_n clusters with M = Hg, Na, K, and R = Ar, Kr, Xe) and to water clusters with biomolecules in solution. An overview will be given of the apparatus, the data acquisition, and plans for the future.

Ionization of sodium Rydberg atoms in collisions and by blackbody radiation in single and crossed atomic beams

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The results of the experimental and theoretical study on associative ionization (AI) of Na(nL) Rydberg atoms in collisions with Na(3S) ground-state atoms and on thermal ionization (TI) of Rydberg atoms by blackbody radiation (BBR) at the ambient temperature of 300 K in single and two crossed at the right angle effusive atomic beams are reported.

The experiments were performed in a vacuum chamber with effusive thermal atomic beams at the 2×10^{10} cm^{-3} density of Na(3S) and 630 K temperature of the atomic beam sources. The Rydberg nS and nD states with n=8-20 were excited in two steps by tunable pulsed lasers at 5 kHz repetition rate. Molecular Na_2^+ and atomic Na^+ ions were detected by a time-of-flight mass-spectrometer. It has been found that atomic and molecular ions were produced by the BBR induced photoionization and the AI, respectively. The AI rate constants of the nS and nD states with n=8-20 have been measured for the first time using a novel method based on the measurement of a ratio of molecular and atomic ions signals. This method eliminates the need to determine the absolute number of Rydberg atoms, the excitation volume, and the effective lifetimes of Rydberg states. Instead, it requires to calculate or measure the absolute values of BBR ionization rates, W_{BBR}, taking into account the population mixing and L-mixing processes. The new experimental and theoretical data on W_{BBR} have been obtained and discussed.

In order to compare the measured AI rate constants with theory, a stochastic model of associative ionization in collisions of Rydberg atoms with ground state atoms has been developed. It is based on the Duman-Shmatov-Mihajlov-Janev (DSMJ) theory [1] and takes additionally into account the redistribution of population over a range of Rydberg states prior to ionization, which is caused by non-adiabatic processes in overlapping multiple level crossings of quasi-molecular Rydberg states. The redistribution is modeled as diffusion of electrons in the Rydberg energy spectrum using a Fokker-Planck type equation. The theoretical associative ionization rates have been calculated for Na(nL)+Na(3S) collisions with n=5-25 and L=0, 1, 2 and compared with the available experimental data and with calculations performed with DSMJ model. The stochastic model demonstrates substantially better agreement with experiments than DSMJ model for lower n.

Experimental and theoretical results have been published and submitted in [2] and [3], respectively. This work was supported by INTAS (Grant No. 2001-155), Russian Foundation for Basic Research (Grant No. 02-02-16332) and Deutsche Forschungsgemeinschaft.

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M1-E2 interference in Zeeman effect of 461.5 nm line of Bi I.

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The $6s^2 6p^3$ ground configuration of bismuth gives rise to five levels $^4S_{3/2}$, $^2P_{3/2,1/2}$ and $^2D_{5/2,3/2}$. Since electric - dipole transitions between states of the same parity are forbidden, all levels of the $6s^2 6p^3$ configuration are metastable. Weak magnetic - dipole (M1) and electric - quadrupole (E2) transitions between these levels are permitted in the second - order radiation theory. The 461.5 nm line ($^2P_{1/2} \rightarrow ^4S_{3/2}$) is of mixed M1+E2 type. In the Zeeman effect of mixed multipole line the intensity of pattern is not a simple sum of two contributions for M1 and E2 radiations taken in proportion to their transition probabilities, but should be modified by an interference term.

The spontaneous transition probability for a single photon emission in the presence of magnetic field can be expressed, according to

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

where D is percentage admixture of E2 radiation, a_{ab}^{M1} and a_{ab}^{E2} are pure magnetic-dipole and electric-quadrupole components, respectively, and the cross a_{ab}^{M1-E2} term describes the interference effect.

The M1-E2 interference was observed experimentally, for the first time, by Jenkins and Mrozowski [1] for the line 733.0 nm of ^{208}Pb I. The interference effect in emission spectra causes the difference between the intensities of $\Delta M = \pm 1$ Zeeman patterns observed in longitudinal and transverse directions of observation. This phenomenon, in a series of experiments, was used for precise determination of the electric-quadrupole admixture in forbidden lines.

We report studies of the interference effect in 461.5 nm line. A special computer program considering the M1-E2 interference was designed to obtain the predicted contour of the Zeeman structure of the line. By variation of free parameters, describing the line shape and the electric-quadrupole admixture calculated profiles were fitted to the recorded spectra. The E2 admixture was found to be $(7.4 \pm 0.4)\%$. Our result was compared with recent theory and other experiments.

Acknowledgments

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Effects of bound state wave functions on the (e, 3e) process on He

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Electron impact double ionization process of atoms is very important for investigation of electron-electron correlation in the bound as well as in the continuum states. We present in this communication the results of our calculation of five-fold differential cross section for the (e, 3e) process on He in first Born approximation using various bound state wave functions (one parameter, Byron and Joachain, Bonham and Khol and Le Sech wave functions) of He to study the electron-electron correlation in the bound state. We perform the calculation of FDCS in the 3 Coulomb wave approach [1-3] in theta variable and constant theta-12 modes and vary different kinematical variables to investigate effects of various bound state wave functions of He on the angular profile of FDCS. We observe that with the decrement of ejected electrons energy, the angular profile of FDCS gets similar. We further observe that it becomes almost identical at very low ejected electrons energy. We also compare our results with the recently performed (e, 3e) experiment of Lahmam-Bennani et al [4] at incident electron energy 601 eV.

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Relativistic (e, 2e) processes on Cu, Ag, Au and U atoms in non-coplanar geometry

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The ionization of atoms, ions and molecules by electron impact are basic processes of atomic and molecular physics, with fundamental applications in different areas as astrophysics, condensed matter physics, plasma physics, fusion physics, surface science etc. Electron coincidence experiments in which an incoming electron knocks out a bound electron in a collision with target and the two outgoing electrons are then detected in coincidence with defined kinematics are known as (e, 2e) experiments. Such types of investigations have been done to study the momentum distribution of valence electrons in atoms and molecules [1]. Recently, Sud et al (2004) [2] and Sud and Purohit (2003) [3] have theoretically demonstrated electron dichroism effect in the relativistic (e, 2e) processes for the K-shell ionization of atoms in non-coplanar asymmetric geometry. They observed that the longitudinal spin asymmetry is measurable and has a sensitive dependence on the interference between transition charge and component of the transverse transition current.

We present in this communication the results of our calculation of longitudinal spin asymmetry for the K-shell ionization of Cu, Ag, Au and U atoms at incident electron energies 300 and 500 KeV using plane wave Born approximation in one photon exchange. In the present study we keep the post collisional kinematics of the ejected electron constant and vary the recoil momentum of the ion. We will discuss the dependence of longitudinal spin asymmetry on the incident electron energy and kinematical conditions used in the present investigation.

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Formation of Excited Strontium Ions at the Electron Collisions with Metastable Atoms

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The values of the cross sections for the formation of the excited strontium ions are known to be the interaction constants. In addition, such data complement the results of the studies on the metastable atoms ionization by electron impact and allow some mechanisms of the above process to be clarified. Up to date no data are found in literature on the cross sections of electron interactions with metastable strontium atoms resulting in their ionization with simultaneous excitation.

The experiments were carried out by an optical method with the use of a crossed metastable atomic and electron beam technique. The experimental parameters were as follows: electron beam current was $\sim 20\mu$A at the energy spread of $\sim$0.5 eV (FWHM); the triplet metastable Sr atom concentration at the beam interaction region determined by an absorption technique was $5{\cdot}10^{-9}$ cm^{-3}. The relative accuracy of determination of the absolute excitation cross sections for ionic lines was $\sim$50%.

As a result of the experimental studies, we have determined the absolute excitation cross sections for the most intense SrII spectral lines (at the 15 eV incident electron energy). For the resonance ion doublet (the $5^2S_{1/2}$–$5^2P_{3/2}$ transition) the cross section for the excitation from the triplet metastable states reaches $5{\cdot}10^{-20}$ m^2, while that for the excitation of the same doublet from the ground state at 15 eV is $\sim 6{\cdot}10^{-21}$ m^2. Thus, in the case of excitation out of the metastable states the cross section almost by order of magnitude exceeds that for the excitation from the ground state.

Compare now the obtained data on the electron-impact excitation cross sections for the SrII spectral lines with the total SrI ionization cross section out of the metastable states. The sum of the excitation cross sections for the measured spectral lines at 15 eV energy provides $8.5{\cdot}10^{-20}$ m^2, whereas the total cross section of SrI ionization from the metastable states is $\sim 23{\cdot}10^{-20}$ m^2 (at the same energy) [1]. This means that more than 35% of the Sr^+ ions resulted from ionization out of the metastable states are produced in the excited states.

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High-energy X-Ray satellites spectra in the Lα_2 region.

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The X-ray satellite spectra arising due to $\overline{2p_{3/2}3x}$-$\overline{3x3d}(x \equiv s, p, d)$ transition array, in elements with Z = 73 to 90, have been calculated. While the energies of various transitions of the array have been determined by using available HFS data on $\overline{1s}$ - $\overline{2p3x}$ and $\overline{2p_{3/2}}$ - $\overline{(3x, 3x')}$ Auger transition energies, their relative intensities have been estimated by considering cross sections of singly ionized $\overline{2x}(x \equiv s, p)$ states and then of subsequent Coster Kronig and shake off processes. The calculated spectra have been compared with the measured satellite energies in Lα_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 one satellite observed in the Lα_2 region of the x-ray spectra of various elements and named α_s in order of increasing energy are mainly emitted by $\overline{2p_{3/2}3d}$ - $\overline{3d^2}$ transitions. It is observed that the satellite α_s in all these spectra can be assigned to the superposition of three intense transitions namely $^3P_1$ - $^3D_1$, $^3D_2$ - $^3D_3$ and $^3D_2$ - $^3D_1$. The three remaining satellites in $_{80}$Hg namely Lα_{13}, Lα_{14} and Lα_{17} are found to have different origin in different elements. The possible contribution of other transitions of the $\overline{2p_{3/2}3x}$ - $\overline{3x3d}(x \equiv s, p, d)$ array having intensities comparable with the above transitions, and the corresponding lines which have not yet been observed, have also been discussed.

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