

PSAS 2002

**Precision Physics
of
Simple Atomic Systems**

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Book of abstracts

Edited by

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Precision Physics of Simple Atomic Systems

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Part I

High resolution spectroscopy of hydrogen and helium

Nonresonant corrections to frequency measurements in the hydrogen atom

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Nonresonant (NR) corrections indicate the limit up to which the concept of energy of an excited atomic state has a physical meaning - that is the resonance approximation. Only within this approximation the line profile can be described by the two parameters: energy and width.

Going beyond this approximation NR corrections arise which define the absolute limit of accuracy of all atomic frequency standards. If the distortion of the Lorentz profile is small the NR corrections reduce to an additional resonance shift that depend on the particular process of the measurement.

We evaluate the NR corrections for the Lyman-alpha transition in neutral hydrogen in case of the photon scattering on the atom. The NR correction to the total cross-section is $\delta = -1,922$ Hz. A part of this correction has been evaluated in [1]. For the differential cross-section the NR correction can be much larger [2] but the correction δ defines the absolute limit for the Lyman-alpha frequency measurements. The evaluation of δ requires the exact expression for the Coulomb Green function and in particular the Sturmian expansion for this function has been employed. The accuracy in the measurement of the Lyman-alpha frequency is far above the value of δ (about 1 MHz [3]).

The NR correction was calculated also for the most accurately measured two-photon resonance $1s - 2s$ in the hydrogen atom [4]. For the measurement process adopted in [4] the NR correction can reach about 10^{-2} Hz [5] while the present experimental accuracy is 46 Hz but the projected accuracy will be two orders of magnitude smaller.

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Contributions of $O(\alpha^7 mc^2)$ to helium fine structure and the fine structure constant

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Measurements of the fine structure splittings in the helium $1s2p\ ^3P_J$ states ($J = 0, 1, 2$) have recently improved to the 30 ppb (parts per billion) level of accuracy [1]. At this level, a comparison with theory is sufficient to determine the fine structure constant α to an accuracy of 15 ppb, provided that all theoretical contributions can be calculated to sufficient accuracy, and to sufficiently high order in powers of α . The purpose of this paper is to summarize the current status of theory, and to give new results for the two-electron QED corrections of order $\alpha^7 mc^2$ a.u.

The theoretical contributions to the fine structure splittings can be expressed as a power series in α involving the lowest-order Breit-Pauli interaction B (including anomalous magnetic moment terms), the second-order Breit interaction, the spin-dependent Douglas and Kroll terms, and finally terms $B^{(5,1)}$ of $O(\alpha^7 \ln \alpha mc^2)$ and $B^{(5,0)}$ of $O(\alpha^7 mc^2)$ first discussed by Zhang [2]. There are also finite nuclear mass and recoil corrections of relative order μ/M to each of these contributions.

With the use of high precision variational wave functions, the leading $\langle B \rangle$ term has been calculated to better than 10 ppb, and similarly for the other terms up to $B^{(5,1)}$ [3]. The final $B^{(5,0)}$ term contains, in addition to one-electron terms [4], a sum of 25 complicated and highly singular two-electron operators. Work on the evaluation of these terms is now essentially complete. They individually contribute at the level of 600 ppb. Once they are fully included, the residual uncertainty from terms of order $\alpha^8 mc^2$ and higher is estimated to be less than 10 ppb [4], thus allowing a determination of α to the full accuracy of the fine structure measurement. Final results will be presented at the conference.

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High-precision measurement of the $n=2$ triplet P intervals in helium: A measurement of the fine-structure constant

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The $n=2$ triplet P $J=1$ -to- $J=2$ and $J=0$ -to- $J=1$ fine-structure intervals in atomic helium have been measured to be 2291174.0(1.4) and 29616950.9(0.9) kHz, respectively. The measurements are made in a thermal beam of metastable $n=2$ triplet S helium atoms which are excited up to the $n=2$ triplet P state using a 1.083-micron diode laser. The fine-structure transitions are driven using microwave fields. The 2.3-GHz $J=1$ -to- $J=2$ measured interval, when compared to highly-precise QED calculations for the interval, provides a strong test of QED, and in particular can be used to verify the accuracy of the 2 triplet P QED calculations. When sufficiently-precise theoretical calculations of the energy interval is available, the measured 29.6-GHz $J=0$ -to- $J=1$ interval will allow for a 15-part-per-billion determination of the fine-structure constant.

Improvements to the experiment (including laser focusing of the metastable helium thermal beam and narrowing of the resonance to a subnatural linewidth) are now being implemented and will lead to a factor of five improvement in the precision of the measurements. These improved measurements, along with improved theory, will allow for a 3-part-per-billion determination of the fine-structure constant, which will be the most accurate determination of this constant.

This work is supported by the Natural Sciences and Engineering Research Council of Canada, by a Premier's Research Excellence Award, by the Canada Research Chair Program, by the Canadian Institute for Photonic Innovations, by the Canadian Foundation for Innovation and by the Ontario Innovation Trust.

Two-Loop Self-Energy Corrections to the Fine-Structure

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The analytic and numerical evaluation of two-loop self-energy corrections has been historically problematic. In the current investigation, we combine analytic methods inspired by a low-energy effective QED hamiltonian (NRQED) with a non-analytic expansion in a scale-separating parameter ϵ , in order to obtain results for the higher-order binding corrections to the two-loop self-energy for P states. Specifically, we are interested in the fine-structure difference in the sixth order of $Z\alpha$, including the non-logarithmic terms.

The two-loop effect for P states is described by the following $Z\alpha$ -expansion:

$$\Delta E_{\text{SE}} = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^4 m}{n^3} H(Z\alpha) \quad (1)$$

where

$$H(Z\alpha) = B_{40} + (Z\alpha)^2 \left[B_{62} \ln^2(Z\alpha)^{-2} + B_{61} \ln(Z\alpha)^{-2} + B_{60} \right] + \mathcal{R}. \quad (2)$$

For the understanding of the fine structure, it is sufficient to calculate the difference of the coefficients for $P_{3/2} - P_{1/2}$ -states. We obtain with the definitions

$$\Delta_{\text{fs}} B_{61} = B_{61}(nP_{3/2}) - B_{61}(nP_{1/2}), \quad (3)$$

$$\Delta_{\text{fs}} B_{60} = B_{60}(nP_{3/2}) - B_{60}(nP_{1/2}), \quad (4)$$

the following results [1]:

$$\Delta_{\text{fs}} B_{61} = \Delta_{\text{fs}} B_{61} = -\frac{n^2 - 1}{3n^2}, \quad (5)$$

$$\Delta_{\text{fs}} B_{60}(2P) = -0.362, \quad \Delta_{\text{fs}} B_{60}(3P) = -0.411, \quad (6)$$

$$\Delta_{\text{fs}} B_{60}(4P) = -0.420, \quad \Delta_{\text{fs}} B_{60}(5P) = -0.420. \quad (7)$$

These results are relevant for the fine structure in hydrogen and as hydrogenlike helium [2], as well as the determination of the fine-structure constant from precise measurements in (atomic) helium [3]. Last, but not least, we would like to mention that the calculational techniques may be useful in a wider context for other unknown non-logarithmic terms of sixth order in $Z\alpha$.

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Towards a Precise Measurement of the He⁺ 2S Lamb Shift

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Recently, corrections at the order of $m\alpha^2(Z\alpha)^5$, the *two-loop binding corrections*, to the Lamb shift were evaluated and found to exhibit very non-perturbative behaviour [1]. Since then, successive numerical calculations of terms at this and higher orders in α have hinted at contradictions between numerical and perturbation theory results [2].

It is now well known that a comparison with Lamb shift measurements in hydrogen is at present unable to comment unambiguously on the correctness of these recent calculations, due to the error introduced by the experimental uncertainty in the size of its nucleus. There are three equally precise but inconsistent measurements of the charge radius of the proton; 0.805(11), 0.862(12) and 0.847(9) fm [3] and the overall spread in these values is as large as the two-loop binding correction itself. The natural choice for probing the two-loop binding corrections is the next simplest system - singly-ionised helium. The error introduced by the experimental uncertainty in the alpha particle radius is relatively much smaller, making Lamb shift measurements in He⁺ potentially sensitive to the recent corrections. This is the motivation for our experiment. We also note that there is presently a small disagreement between the best measured value of the He⁺ 2S Lamb shift [4] and the current theoretical value [5]. Finally, if the He⁺ measurement confirms the theory at the level of the two-loop corrections, then we can combine it with the measurements in hydrogen to extract a new value for the proton size.

We are making the first measurement of the He⁺ 2S-3S interval by Doppler-free two-photon spectroscopy of a slow He⁺ 2S metastable ion beam using continuous-wave UV radiation at 328 nm. A measurement of this transition frequency combined with the value of the Rydberg constant from H experiments allows a determination of the 2S-3S Lamb shift. The two-loop corrections amount to a shift in the theoretical value of around -1.4 MHz, which constitutes roughly 10% of the 2S-3S natural linewidth, making the experiment a potentially very sensitive test of the theory without extensive systematic analysis of the lineshape. The experiment is nearing completion, and we hope to present some data at the conference.

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Precision Spectroscopy of the 1S-2S Transition in Atomic Hydrogen

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The $1S - 2S$ two-photon transition in atomic hydrogen with its natural linewidth of only 1.3 Hz is of particular interest for precision tests of bound-state QED and for the determination of fundamental constants. Moreover, their conceivable variation could be deduced from a comparison of the $1S - 2S$ transition frequency measured with an accuracy of 2×10^{-14} in the year 2000 [1] with the result of a similar measurement to be performed in the near future, providing an alternative approach to astrophysical measurements [2]. In our experiment, a dye laser emitting near 486 nm is locked to an ultra-stable reference cavity. After frequency doubling, the resulting UV radiation near 243 nm is coupled into a linear enhancement cavity inside a vacuum chamber. Cold hydrogen atoms escape collinearly with this cavity from a nozzle cooled to 5–6 K. On their way through the laser field, some atoms are Doppler-free excited via two-photon absorption from the $1S$ ($F = 1, m_F = \pm 1$) ground state to the metastable $2S$ ($F' = 1, m'_F = \pm 1$) state. In the detection region, these atoms are quenched in an electric field and emit L_α -photons which are counted by a photomultiplier. A selection of slow atoms by time resolved spectroscopy reduces the second-order Doppler shift and the time-of-flight broadening. To correct for the AC-stark shift, we measure at different light power levels and extrapolate the transition frequency to zero light power. For an absolute frequency measurement, the $1S - 2S$ transition frequency is phase-coherently compared with a primary frequency standard using a frequency comb technique [1]. The difference $D_{21} = 8E_{\text{hfs}}(2S) - E_{\text{hfs}}(1S)$ of hyperfine intervals in atomic hydrogen can be calculated theoretically, yielding an accurate QED test [3]. Using magnetic shielding around the excitation region, we can determine the $2S$ hyperfine structure by measuring both hyperfine transitions $1S (F = 0) \rightarrow 2S (F' = 0)$ and $1S (F = 1) \rightarrow 2S (F' = 1) \rightarrow 2S (F' = 0, m'_F = 0)$ and $\rightarrow 2S (F' = 1, m'_F = 0, \pm 1)$ transitions. This experiment might yield an accuracy comparable with that of RF measurements of the $2S$ hyperfine structure [4].

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Part II

Precision study of few-electron medium-
and high-Z ions

Virial relations for the Dirac equation and their applications to calculations of H-like atoms

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Virial relations for the Dirac equation in a central field and their application to the case of the Coulomb field are considered. It is demonstrated that using these relations allows one to evaluate various average values for a hydrogenlike atom [1, 2]. An extension of these relations to the case of non-diagonal matrix elements is also considered [2]. This extension provides an effective method for analytical evaluation of infinite sums that appear in calculations based on using the reduced Coulomb-Green function. In particular, this method can be used for calculations of higher-order corrections to the hyperfine splitting and the g factor in hydrogenlike atoms [3, 4].

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Measurement of the $g(J)$ factor of hydrogen like oxygen

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The $g(J)$ factor of hydrogen like ions serves as precision test of bound state quantum electrodynamic calculations. After a first successful experiment on C^{5+} [1] we have now completed a similar experiment on O^{7+} . A single ions is confined in a double Penning trap having two potential minima at two different postions. The magnetic moment was determined via the continuous Stern-Gerlach effect [1] [2]. It results in a splitting of the axial ion oscillation frequency for the two possible spin orientations when the traps magnetic field is inhomogeneous. In the case of O^{7+} the difference in the axial frequency is 0.48 Hz in a total frequency of 360 kHz. The magnetic field was calibrated by measuring the cyclotron frequency of the same in with an uncertainty of less that 10^{-9} . Measuring the spin precession (Larmor) and cyclotron frequencies at the same time eliminates drifts of the magnetic field. A determination of the induced spin flip rate for various ratios of Larmor to cyclotron frequencies gives a resonance curve Fig.1 from which the $g(J)$ factor can be derived. The (preliminary) result of $g(J)=2.000\ 047\ 032\ (6)$ is basically in agreement to the theoretical value $g(J)=2.000\ 047\ 022\ (5)$ [3].

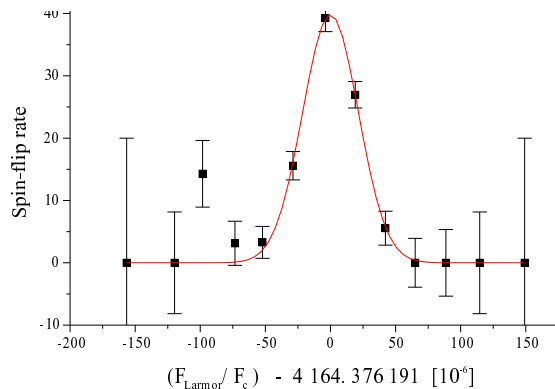


Figure 1: $g(J)$ factor resonance measured in the precision trap

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Recent developments in X-ray tests of QED

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Experimental tests of QED have developed dramatically for simple systems of hydrogen and helium, but there has also been significant progress for medium-Z hydrogenic and helium-like atoms over the last few years. In this area the tests are often based on X-ray spectroscopic measurements, and here we review some of the key developments. Of particular interest is the status of tests of two-electron QED and of np subshell and excited state QED[1].

We discuss some recent secondary tests of the data to confirm the quality, and experimental development to address the dominant systematics in this area.

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New value for the mass of the electron

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A new independent value for the electron's mass in units of the atomic mass unit is presented, $m_e = 0.000\,548\,579\,909\,2(4)\text{ u}$ [1]. The value is obtained from our recent measurement of the g factor of the electron in $^{12}\text{C}^{5+}$ [2] in combination with the most recent quantum electrodynamical (QED) predictions for the g factor in hydrogenlike ions. In the QED corrections, terms of order α^2 were included by a perturbation expansion in $Z\alpha$. Our total precision is three times better than that of the accepted value for the electron's mass, $m_e = 0.000\,548\,579\,911\,0(12)\text{ u}$ [3] and agrees with it within 1.5 standard deviations.

In addition, we will also discuss the corresponding result for our recent measurement of the electronic g factor in $^{16}\text{O}^{7+}$ which is not fully evaluated at the time of submitting this abstract but seems to point to a result very close to that obtained from the carbon measurement.

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One-loop self-energy correction to the bound electron g factor

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Spectacular progress in high-precision measurements of the bound-electron g factor for hydrogen-like carbon [1, 2] and the related theoretical investigations provided recently a new independent determination of the electron mass [3]. It yields

$$m_e(g) = 0.000\,548\,579\,909\,24\,(29)(27)\text{ u},$$

where the first and the second error correspond to the experimental and the theoretical uncertainty, respectively. This result agrees with the 1998 CODATA value [4] within 1.5 standard deviations but is three times more precise. Since further progress of experimental investigations is anticipated in the near future, increase of accuracy of the theoretical prediction becomes a problem of particular importance. The leading uncertainty of the theoretical result originates from the one-loop self-energy correction, the most accurate calculation of which was performed in [5].

In the present work, we evaluate the one-loop self-energy correction to the $1s$ g factor with the precision about five times higher than that of [5]. This calculation significantly improves the accuracy of the theoretical prediction for the bound-electron g factor in H-like carbon and oxygen and reduces the total uncertainty of the related electron-mass determination.

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Theory of the g factor of high- Z lithiumlike ions

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Accurate calculations of the g factor of Li-like ions in the range $Z = 6 - 92$ are considered. The interelectronic-interaction, the radiative, the nuclear size, and the nuclear recoil corrections are evaluated to lowest orders in $1/Z$. A special attention is focused on reducing the uncertainty due to the nuclear size effect in a specific difference of the g factors of H- and Li-like ions.

Testing of QED–theory on the Rydberg Series for the He–like Multicharged Ions

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High–resolution spectroscopic measurements on the resonance Rydberg series of two–electrons multicharged ions [1, 2] may be considered as a new impetus for detailed theoretical analysis of relativistic and QED contributions to the binding energies of these ions.

For that purpose the experimentally measured intervals could be expressed as a sum of non-relativistic, relativistic and QED–effects, plus relatively smaller corrections due to size and mass effects. Therefore, if these contributions could be accurately calculated, then an accurate spectroscopic measurements of energy interval can be used to indirect measurement of QED–effects. Evidently, the key point is that it is consistent to use accurate theoretical values for these quantities. In the particular case of Rydberg states QED contribution corresponds approximately to the ionization energy of the ground state of He-like ions, because Lamb shift of the highly excited electron rapidly decrease with increasing a principal quantum number.

In the present work the radiative corrections to the ground state are analyzed and compared with experiments [1, 2] for Al– and Mg–ions. Our theoretical approach based on the use of unified method by combining precise variational methods for non-relativistic energies and the relativistic $1/Z$ –expansion methods for relativistic and QED–effects.

It was demonstrated that the present precise wavelength measurements [1, 2] provide the possibility for the evaluation of the Lamb shift contribution to the ionization energy of the ground state of He–like ions. Thus, these estimated data are rather interesting and appear as independent alternative verifications of QED–contribution to the ionization energy of the ground state of He–like ions for the intermediate Z –lavues.

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Hyperfine quenching of the 2^3P_2 state in He-like ions

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The transition probability of the line $1^1S_0 - 2^3P_2$ in He-like ions with non-zero nuclear spins is calculated. Hyperfine interaction effects which contribute appreciably to the probability under consideration are investigated. The Coulomb and Breit interelectronic interactions are taken into account to first order in $1/Z$ by means of perturbation theory. The calculation is performed for both velocity and length gauges. The transition rates evaluated are in good agreement with previous $1/Z$ and MCDF calculations [1, 2].

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Part III

Study of muonic and exotic atoms

Precision Physics with Light Muonic and Hadronic Atoms

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Recent progress in the theory of atomic cascade in hydrogen-like exotic atoms is reviewed from the viewpoint of precision experiments with μ^-p , π^-p , K^-p , and $\bar{p}p$ atoms. The following problems are discussed in detail.

- The proton charged radius can be determined with an accuracy of 10^{-3} from the energy splitting between the $2S$ and $2P$ states in muonic hydrogen. The feasibility of the μ^-p Lamb shift experiment, presently in progress at PSI [1], depends crucially on the population and the lifetime of the metastable $2S$ state of μ^-p .
- The experiment on precision spectroscopy of pionic hydrogen [2] will determine the πN scattering length with an accuracy better than 1% by measuring the nuclear shifts and widths of the K X-ray lines. To reach this level of precision, the Doppler broadening corrections to the line width must be calculated in a detailed cascade model.
- To improve the measurement of the K^-p scattering length using the spectroscopy of kaonic hydrogen [3], one needs reliable theoretical predictions of the K X-ray yields for different values of the nuclear shifts and widths.
- The $2P$ nuclear widths of antiprotonic hydrogen can be determined from the L X-ray spectra [4], with the Doppler broadening corrections being important for precision measurements.

The latest results of the extended standard cascade model (ESCM) [5], which describes the evolution of the kinetic energy distribution of the hydrogen-like exotic atoms from the very beginning of the cascade, are used to illuminate the problems concerned. Evidences for cascade processes beyond the ESCM and their implications for the precision experiments are discussed.

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Pion-Nucleus Bound-State Spectroscopy as an Indicator of Chiral Symmetry Restoration in Nuclear Medium

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A review is made on the recently developed pion-nucleus bound-state spectroscopy and its implication. Whereas pionic-atom x-ray spectroscopy cannot access to deeply bound π^- states in heavy nuclei (such as the 1s states in Pb), a new type of nuclear spectroscopy, using so called *pion transfer reactions*, was proposed to produce discrete bound states of π^- [1]. Series of successful experiments have been carried out at GSI using the (d, ^3He) reaction at 500-600 MeV deuteron energy on ^{208}Pb [2], ^{208}Pb [3] and $^{116,120,124}\text{Sn}$. They revealed the 1s π^- states in Pb and Sn isotopes, and their binding energies and widths were determined.

Since the π^- binding energies of the 1s π^- states depend on the local (s-wave) part of the pion-nucleus potential, the newly found 1s states in heavy $N > Z$ nuclei are of particular importance in giving the isoscalar interaction parameter (b_0) and the isovector parameter (b_1) separately. It has been emphasized only very recently that the isovector parameter (b_1) in the pion-nucleus potential plays an important role in connection with f_π [4].

The experiment on ^{205}Pb has yielded an isovector parameter b_1 , which is enhanced over the free- πN value, indicating that the squared chiral order parameter (f_π^2) is reduced in the nuclear medium by a significant amount [5]. This is the first clear evidence for a partial restoration of chiral symmetry in the nuclear medium, and is in good agreement with the theoretical expectation by Weise [6].

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First Observation of Microwave-induced Transitions between Hyperfine Levels of Antiprotonic Helium

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Antiprotonic helium is an exotic three-body system consisting of an antiproton, a helium nucleus, and an electron: $\bar{p}\text{-He}^{2+}\text{-e}^- \equiv \bar{p}\text{He}^+$. It has a series of metastable states with lifetimes in the microsecond range, which have been extensively studied by laser spectroscopy at LEAR by the PS205 collaboration and recently at the Antiproton Decelerator of CERN by the ASACUSA collaboration [1].

As a further step ahead in the determination of its structure, we have performed a measurement of the hyperfine splitting of the $(n, L) = (37, 35)$ state of $\bar{p}^4\text{He}^+$ (n = principal quantum number, L = angular momentum quantum number of the antiproton). Due to the large L of \bar{p} in metastable states ($L = 33 \dots 38$), the dominant splitting arises from the interaction of the \bar{p} *angular* momentum with the *electron* spin \vec{S}_e (called *hyperfine (HF)* splitting), while the \bar{p} spin $\vec{S}_{\bar{p}}$ creates a second, much smaller splitting (called *superhyperfine (SHF)* splitting). This leads to a quadruplet structure where each level is characterized by the quantum numbers n , L , $F = L \pm S_e$, and $J = F \pm S_{\bar{p}}$. The hyperfine structure of $\bar{p}\text{He}^+$ has been first calculated by Bakalov and Korobov [2] who predicted a *HF* splitting of 12.91 GHz for the $(37, 35)$ state.

Using a new two-laser microwave triple resonance technique, we could in 2001 for the first time observe two microwave-induced transitions within the $(37, 35)$ state: $(F, J) = (L + 1/2, L + 1) \rightarrow (L - 1/2, L)$ at $\nu_{\text{HF}}^+ = 12.89622 \pm 0.00031$ GHz and $(L + 1/2, L) \rightarrow (L - 1/2, L - 1)$ at $\nu_{\text{HF}}^- = 12.92470 \pm 0.00026$ GHz. The measured frequencies (accuracy $\sim 2 \times 10^{-5}$) agree with recent three-body QED calculations on the level of $< 6 \times 10^{-5}$. The difference corresponds to the precision of the theories which is limited by the omission of terms of order $\alpha^2 \sim 5 \times 10^{-5}$. This measurement provides an important benchmark for the three-body QED calculations, and the higher precision of the experimental value calls for their improvement.

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Theory of the antiprotonic helium atoms. Progress report.

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A progress report on the theory of the antiprotonic helium atoms will be given. The topics to be discussed:

1. Fine and Hyperfine structure of the $(37, 35)$ state of the antiprotonic helium atom and comparison with the latest microwave experiment at CERN.
2. Precise study of the Auger dominant states (essentially resonant states) by the Complex Coordinate Rotation (CCR). Relativistic and radiative corrections to resonant states within CCR approach.
3. Determination of the spin-independent transition energy for the $(36, 35) \rightarrow (34, 33)$ transition which is suggested for the precise two-photon spectroscopy for the current year experiments.

Muonic helium atom. Current status

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Muonic helium isotopes, $({}^{3,4}\text{He}^{2+}\mu^-e^-)^0$, are the three-body bounded systems consisting, respectively, of the ${}^{3,4}\text{He}^{++}$ nucleus and two leptons with the same electrical charge. A comparison of sufficiently accurate theoretical and experimental spectroscopic data for these exotic atoms offers a unique opportunity of refining upon values for the charge radii and polarizabilities of the α^{2+-} and ${}^3\text{He}^{2+-}$ particles, along with QED vacuum polarization. In the talk presented, a current status of theoretical and experimental studies with these fundamental systems is reviewed, particular emphasis being placed on investigations of the hyperfine splitting intervals for lowest muonically- and electronically-excited states. Further implications and potential prospects for future laser spectroscopic studies of these systems are discussed as well.

High-precision laser spectroscopy of antiprotonic helium

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The recent results from laser spectroscopy experiments of antiprotonic helium atoms, carried out at CERN's Antiproton Decelerator are reported. Numerous atomic transition frequencies in both ^3He and ^4He isotopes have been measured to a fractional precision of < 100 ppb. We also describe the latest results of experiments using a newly-commissioned radiofrequency quadrupole decelerator. By developing new sources of ultra-low energy antiprotons, two-photon laser-spectroscopic techniques and advanced laser systems, we ultimately hope to measure the above transition frequencies to a precision of several ppb in the future.

Scalar-QED Effects in Pionium

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Scalar QED is known to be a renormalizable theory, but the evaluation of QED radiative corrections for scalar particles is not very well described in the literature. Here, we investigate a number of QED effects which are of relevance for the bound system of two oppositely charged pions (commonly referred to as “pionium”). This exotic atomic system will be studied in the DIRAC experiment at CERN.

We obtain, as a generalization of the discussion contained in [2], for the generalized Breit hamiltonian [1] of two scalar particles:

$$H_B(\mathbf{r}, \mathbf{p}) = -\frac{\mathbf{p}^4}{4m^3} - \frac{e^2}{8\pi m^2 r} \left[\mathbf{p}^2 + \frac{1}{r^2} \mathbf{r} \cdot (\mathbf{r} \cdot \mathbf{p}) \mathbf{p} \right]. \quad (8)$$

On the basis of this result, the known correction of order $(Z\alpha)^4$ to the spectrum (in the usual convention for the quantum numbers n and l) can easily be verified:

$$\langle \phi | H_B | \phi \rangle = -\frac{\alpha^4 m}{2n^3} \left[\frac{1}{2l+1} - \frac{1}{4} \delta_{l,0} - \frac{11}{32n} \right]. \quad (9)$$

Of particular interest are radiative corrections involving only scalar particles. The self-energy effect (SE) and the relativistic recoil (RR) correction have by now only been studied for spin-1/2 particles. In leading logarithmic approximation, we obtain for a bound system of two oppositely charged, scalar particles of mass m :

$$\Delta E_{\log} = \Delta E_{SE} + \Delta E_{RR} = -\frac{3\alpha^5 m}{4\pi n^3} \ln \alpha^{-1} \delta_{l0}. \quad (10)$$

This result gives a nonvanishing contribution only for S states. Further QED corrections to the spectrum of pionium have been discussed in [3].

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High-Precision Calculation of Energy Levels of the Antiprotonic Helium Atoms

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A few percent of antiprotons stopped in the helium target form antiprotonic helium atoms consisting of an antiproton, an electron and a helium nucleus in metastable states with an extremely long lifetime of the order of a microsecond. Such a long-lived antiprotonic atom has stimulated spectroscopic studies from a viewpoint of antimatter science: CPT invariance and weak equivalence principle, interaction between matter and antimatter, etc. The transition frequencies between the metastable states were measured with precise laser spectroscopy. The data are very challenging to the few-body theory since it is necessary to achieve very high precision in an energy-level calculation managing large interacting angular momenta of $J = 30 \sim 40$. Moreover, agreements between theoretical calculation and experimental results will give precise values of basic property of antiproton.

Non-relativistic energies and widths are calculated by means of the complex-scaling method, because the metastable states concerned here are not true bound states but Feshbach-type resonant states. This method improved the accuracy of the calculated energy up to the few ppb (10^{-9}), i.e. by one order of magnitude as compared to our previous calculations [1] based on the real-scaling method. The relativistic corrections derived from the Bright-Pauli Hamiltonian are calculated in the first order perturbation theory. We also consider the Lamb shift of one loop corrections. The results obtained are in good agreement with the experimental values [2] within 30 ppb. When a more accurate value of the charge-to-mass ratio of antiproton is considered, the uncertainty of antiproton charge is estimated at 70 ppb.

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Calculation of resonant states in $\text{He}^{2+} + \text{e}^+ + \text{e}^-$ three-body system

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The three-body system consisting of a helium nucleus, an electron and a positron has no bound state but has resonant states. For this three-body system, the existence of broad resonant states has been a controversial question [1, 2, 3]. Recently, Igarashi and Shimamura performed hyperspherical close-coupling (HSCC) calculations, but did not find such resonances. We calculate the energies and widths of resonant states using the coupled rearrangement channel (CRC) method and the complex coordinate rotation (CCR) method. The results are shown in Table 1 together with literature values. We confirm the existence of broad resonances, because the resonant states fulfill the extended virial theorem and the convergences of energies on complex energy diagrams are obtained with the CCR calculation. We also obtain narrow resonances. Our results of calculations for the narrow resonances are in good agreement with those of the HSCC calculation. Since the widths of the broad resonances are in the same order of magnitude as the energy spacing of the three-body system, channel functions used in the HSCC calculation must be inappropriate for the broad resonances.

Table 1: S-wave resonances in $\text{He}^{2+} + \text{e}^+ + \text{e}^-$ three-body system. Each resonances is expressed as (E_r, Γ) , where E_r is the resonance energy and Γ is the width.

Bhatia et al. [1]	Ho [2]	Igarashi et al. [3]	This work
(-0.365, —)	(-0.37050, 0.1294)		(-0.3704, 0.1292)
(-0.195, —)	(-0.1856, 0.0393)		(-0.185, 0.040)
		(-0.250012, 7.7×10^{-6})	(-0.250014, 7.4×10^{-6})
		(-0.075595, 1×10^{-13})	(-0.07544, 5.0×10^{-4})
		(-0.06742, 6.8×10^{-4})	(-0.0675, 7.6×10^{-4})
		(-0.06432, 3.6×10^{-4})	(-0.0642, 4.6×10^{-4})

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Field-induced enhancement of annihilation rate for determining $2p - 2s$ level splitting in $(\pi^+ - \pi^-)$ -atom

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The $ns - np$ level splitting in a hadron atom — a fundamental constant determined mainly by the strong π - π interaction and vacuum polarization — may be used in crucial testing precise predictions of low energy QCD. A method for measuring the $2s - 2p$ splitting in $(\pi^+ - \pi^-)$ atoms ($A_{2\pi}$), based on dc-field-induced mixing of rapidly annihilating $2s$ state to long-living $2p$ state, thus enhancing the annihilation rate, was recently worked out in [1]. The sensitivity of the method may increase essentially if a time-dependent field is used, oscillating in resonance with the $2p - 2s$ transition frequency $\Omega = E_{2p} - E_{2s}$.

In this paper the field dependence for the probability of annihilation is calculated for relativistic $A_{2\pi}$ in nl -states with $l \neq 0$ in a space with an oscillating electromagnetic field. Numerical analysis demonstrates that the field-induced annihilation probability for atoms with "resonant" velocity v , such that $\gamma\omega_0 \approx \text{Re}\Omega = \Omega_1$, may be enhanced significantly; here $\gamma = 1/\sqrt{1 - v^2/c^2}$, ω_0 is the field frequency in a laboratory reference frame (*lrf*). The position of the resonance on the γ -axis determines Ω_1 . The width of the resonance depends on the $2s$ -state life-time and is proportional to the amplitude of field $F \approx B_0\gamma$ seen by atom in its center-of-mass reference frame (*cmrf*); B_0 is the field amplitude in the *lrf*. The field B_0 may be electric or magnetic, as for $\gamma \gg 1$ the electric and magnetic field of one and the same amplitude B_0 transform into one and the same (in magnitude) electric field F of the *cmrf*. The field-dependent decay probability $P_d(\gamma; B_0, \omega_0)$, for three different values of B_0 and three values of ω_0 , is presented with resonance curves based on the field-free exponential curve $P_d(\gamma; 0, \omega_0)$ of fig.2 (a). The net field effect is given by relative decay probability $D(\gamma) = (P_d(\gamma; B_0, \omega_0) - P_d(\gamma; 0, \omega_0))/P_d(\gamma; 0, \omega_0)$ of fig.2 (b).

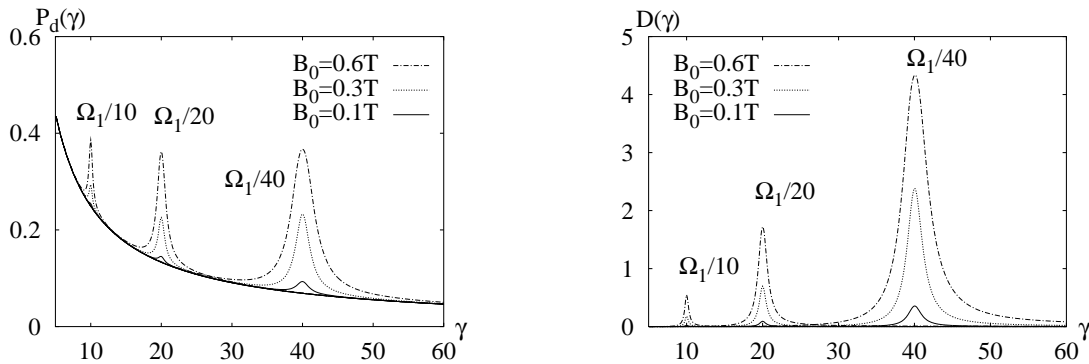


Figure 2: $P(\gamma)$ (a) and $D(\gamma)$ (b) for $(A_{2\pi})$ -atoms traveled a 1cm path in a magnetic field of *lrf* amplitude $B_0 = 0.1, 0.3$ and 0.6 T and *lrf* frequency $\omega_0 = \Omega_1/10, \Omega_1/20$ and $\Omega_1/40$.

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Trapping Atomic Hydrogen with Buffer Gas

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We report on progress towards the magnetic trapping of atomic hydrogen using the buffer gas loading technique[1]. The equipment for trapping, cooling and performing laser spectroscopy will be described. The trap consist of a simple ^4He pumped 1 kelvin cryostat with an antihelmholtz superconducting magnetic bottle. The laser system is based on a Ti:saphire laser which has its frequency doubled twice. In the first doubling stage we implemented a new technique for frequency locking the cavity resonance to the laser frequency[2]. The plans and simulation tools for the sympathetic cooling of H and other species are discussed. These developments have connection to the ATHENA[3] experiment at CERN and to frequency metrology, as we discuss.

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A Continuous Coherent Lyman-alpha Source for Antihydrogen Experiments

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Laser radiation at Lyman-alpha (121.6 nm) will be essential for experiments with cold antihydrogen atoms. The strong Lyman-alpha transition (1S–2P) is the only transition which is practical for laser cooling. The highest cooling-efficiency, lowest temperature, and best magnetic sub-level selectivity is expected for *continuous* coherent radiation. In addition to laser cooling, radiation at Lyman-alpha also makes the non-destructive optical detection of antihydrogen atoms in a magnetic trap feasible. The first source of continuous coherent radiation at Lyman-alpha and natural-linewidth 1S–2P spectroscopy of ordinary hydrogen will be reviewed. The prospects for laser-stimulated recombination, laser detection, laser spectroscopy, and laser cooling of antihydrogen in the ATRAP experiment will be discussed.

Part IV

Study of muonium and positronium

Search for an exotic 3–body decay of orthopositronium

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Abstract

The long-standing 5σ discrepancy between the measured and predicted orthopositronium ($o - Ps$) decay rate in vacuum has been recently confirmed by more precise calculation including corrections of the order α^2 .

We report the results on search for an exotic 3–body orthopositronium decay into a photon and two weakly interacting penetrating particles ($X_{1,2}$). Our preliminary result excludes this decay mode as the origin of the discrepancy. The limit on the branching ratio $Br(o - Ps \rightarrow \gamma + X_1 + X_2) \leq 3 \times 10^{-5}$ at 90% CL is set.

A Detector with High-Detection Efficiency in 4- and 5-Photon-Positronium Annihilations

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We had measured 4- and 5-photon-positronium annihilations at first time in refs. [1, 2], respectively. We had got the annihilation rates and limits of annihilation rates to new particles, e.g. axions, in ref. [3] and a charge-conjugation violating process [4]. Relations with the lifetime problem are also discussed [5,6].

We used a multi-gamma ray spectrometer (UNI) which consists of 32 NaI(Tl) scintillation counters (3 inch phi x 4 inch long) with lead shields, each being located on a surface of an icosidodecahedron. The front face of each scintillator is placed at a distance of $L=262\text{mm}$ from the center of UNI. At this set up, the detection efficiency of 4- and 5-photon-annihilation processes are too small to get the enough number of events to analyze in physics. In order to get larger detection efficiency, we should set the NaI(Tl) scintillators closer to the target while the positrons are transferred from outside of UNI [7].

The old principle of designing UNI was that we suppressed backgrounds (BG) as low as possible allowing modest efficiencies for 4- and 5-photon-annihilation events, i.e., to get the highest S/N . The new concept is to get the highest S/σ where σ is an error of one standard deviation of the signal including BG effect. Higher S/σ means larger number of events with smaller BG taking into a statistical effect. The detection efficiencies with BG effects are studied with respect to L using a detector simulator based on EGS4 using from 2 to 5 photon annihilation events generated by QED processes. As a result, the detection efficiency and S/σ of 5-photon annihilations at $L=136\text{mm}$ increase 529 and 17 times larger than those at $L=262\text{mm}$, respectively.

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Two-loop contributions to radiative-recoil corrections to hyperfine splitting in Muonium

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We have calculated single-logarithmic and nonlogarithmic radiative-recoil corrections generated by the electron and muon one-loop polarization insertions in the exchanged photons [1]

$$\begin{aligned} \Delta E = & \left\{ - \left[6\zeta(3) + \frac{33}{4} \right] \ln \frac{M}{m} - \frac{97}{8} \zeta(3) - 16\text{Li}_4\left(\frac{1}{2}\right) + \frac{2\pi^2}{3} \ln^2 2 - \frac{2}{3} \ln^4 2 \right. \\ & \left. + \frac{5\pi^4}{36} - \frac{13\pi^2}{36} - \frac{4495}{432} \right\} \frac{\alpha^2(Z\alpha) m}{\pi^3 M} \tilde{E}_F. \end{aligned}$$

The new contributions improve the theory of hyperfine splitting, and affect the value of the electron-muon mass ratio extracted from the experimental data on the muonium hyperfine splitting.

This work was supported by the NSF grant PHY-0049059. Work of V. A. Shelyuto was also supported in part by the RFBR grant # 00-02-16718.

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Effects of strong interaction in the energy spectra of hydrogenic atoms

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We consider the proton polarizability contribution δ^P to the hyperfine splitting (HFS) in electronic and muonic hydrogen [1]. Preserving exact dependence on the lepton mass m_1 we can present δ^P in the form [2]:

$$\Delta E_{\text{HFS}}^P = \frac{Z\alpha m_1}{2\pi m_2(1+\kappa)} E_F(\Delta_1 + \Delta_2) = \delta^P E_F, E_F = \frac{8}{3} \frac{\mu_P m_1^2 m_2^2 (Z\alpha)^4}{(m_1 + m_2)^3}. \quad (11)$$

$$\Delta_1 = \int_0^\infty \frac{dQ^2}{Q^2} \left\{ \frac{9}{4} F_2^2(Q^2) \beta_0(\sigma) - 4m_2^3 \int_{\nu_{\text{th}}}^\infty \frac{d\nu}{\nu} \beta_1(\sigma, \theta) G_1(\nu, Q^2) \right\}, \quad (12)$$

$$\Delta_2 = -12m_2^2 \int_0^\infty \frac{dQ^2}{Q^2} \int_{\nu_{\text{th}}}^\infty d\nu \beta_2(\sigma, \theta) G_2(\nu, Q^2), \quad (13)$$

where ν_{th} determines the pion-nucleon threshold and the functions $\beta_{0,1,2}$ have the form:

$$\beta_0(\sigma) = 2 \frac{\sqrt{1+\sigma} - 1}{\sigma}, \quad \sigma = \frac{4m_1^2}{Q^2}, \quad (14)$$

$$\beta_1(\sigma, \theta) = \frac{\theta}{\sigma(-1+\sigma\theta)} \left[\frac{-2\sqrt{1+\sigma} + 2 - 4\sigma^2 - 2\sigma}{\sqrt{1+\sigma}} + \frac{2\sigma(-\theta^2 + \theta^{3/2}\sqrt{1+\theta} + \theta + 2)}{\sqrt{\theta(1+\theta)}} \right], \quad (15)$$

$$\beta_2(\sigma, \theta) = \frac{2}{\sigma(-1+\sigma\theta)} \left[1 - \sqrt{1+\sigma} + \sigma \left(-\theta + \sqrt{\theta(1+\theta)} \right) \right], \quad \theta = \frac{\nu^2}{Q^2}. \quad (16)$$

The calculation of δ^P was based on three main ingredients:

- the evolution equations for the polarized structure functions $G_{1,2}(\nu, Q^2)$ of the deep inelastic $e(\mu)p$ scattering in the nonresonance region;
- the phenomenological hadron-quark model in the resonance region;
- the experimental data for the nucleon polarized structure functions obtained at SLAC, DESY, CERN.

The values of proton polarizability contributions obtained for electronic and muonic hydrogen are equal respectively: $\delta^P(\text{ep}) = 1.4\text{ppm}$, $\delta^P(\mu\text{p}) = 4.6 \times 10^{-4}$.

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Hadronic Effects in Leptonic Systems

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The accuracy of QED calculations for a hydrogen atom and heavier atomic systems is essentially limited by the uncertainty related to the nuclear structure. There are a few QED quantities belonging to purely leptonic physics, among them muonium hyperfine structure and anomalous magnetic moment. However, even in the case of the purely leptonic QED calculation one has to take into account the hadronic contributions. The leading hadronic effect is due to hadronic vacuum polarization.

Here we consider the leading hadronic contribution [1] to the muonium hyperfine interval and estimate higher order corrections [2]. We also discuss the hadronic correction to the muon anomalous magnetic moment [3].

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g-factor in a light two body atomic system

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Energy levels of a two-body atomic system in an external homogenous magnetic field can be presented in terms of magnetic moments of its composites, however, those magnetic moments being related to bound particles differ from their free values.

Study of bound g factors in simple atomic systems are now of interest because of a recent progress in experiments on medium Z ions (see e.g. [1]) and of a new generation of muonium experiments possible with coming intensive muon sources.

We consider bound corrections to the g factors in several atomic systems experimental data for which are available in literature:

- hydrogen, muonium, helium-3 ion;
- muonium;
- hydrogen-like ions with spinless nuclei at medium Z ;
- muonic atoms.

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Development of the new method of the positronium generation. Abilities and future trends.

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Presently the positron ring dedicated to the positronium generation and called Low Energy Positron Toroidal Accumulator (LEPTA) is under construction at the JINR (Dubna). The main application of such a ring is the generation of monoenergetic and directed flux of positronium atoms positronium-in-flight and the performance of experiment with this flux. The positronium is generated in interactions of positrons, circulating inside the storage ring-accumulator, with free electrons of the cooling electron beam that have velocities very close to the positron velocities. This permits obtaining a high positronium flux with small angular and velocity spreads of the atoms and provides a significant advantage for proposed arrangements of experiments, so called positronium-in-flight set-ups, as compared with traditional approaches in which positronium is generated in targets. In particular, the precision in measuring positronium parameters (life time, the probability of decays with momentum conservation and charge invariant violation (CPT violation), fine structure of the positronium spectrum, Lamb shift measurements) can be enhanced by several orders of magnitude. Moreover, some experiments, that are unrealistic within traditional schemes, becomes feasible with the proposed facility.

Part V

Precision frequency metrology

The $^{199}\text{Hg}^+$ Optical Frequency Standard

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We have previously constructed and operated an all-optical atomic clock based on the $^2S_{1/2} - ^2D_{5/2}$ electric-quadrupole transition at 1.06 PHz (10^{15} Hz) in a single, laser-cooled $^{199}\text{Hg}^+$ ion and a femtosecond-laser/microstructure-fiber optical comb generator [1]. Additionally, absolute frequency measurements of the Hg^+ clock transition have been made against the NIST atomic-fountain primary frequency standard [2]. The dominant systematic error in the Hg^+ optical clock arises from the interaction between the D-state electric-quadrupole moment and a static electric-field gradient (caused for example, by patch charges on the trap electrodes). Theoretical estimates place an upper limit for the plausible frequency shift in our trap of about one part in 10^{15} and show that the shift will average to zero over any three orthogonal, equal-amplitude, magnetic field directions [3]. In order to investigate the quadrupole shift, as well as other systematic effects, we have constructed a second Hg^+ frequency standard. Differential measurements between the two standards will allow us to measure fractional frequency shifts below 10^{-16} in measurement times of a few minutes. By careful attention to magnetic fields in the new traps as well as to stray charges on the electrodes, we hope to demonstrate a fractional frequency uncertainty less than one part in 10^{16} .

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Optical Frequency Standards with Trapped Ions

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A single laser-cooled ion in a Paul trap can serve as a reference in an optical frequency standard of very high accuracy. We investigate the electric quadrupole transition $^2S_{1/2}(F=0) \rightarrow ^2D_{3/2}(F=2)$ of $^{171}\text{Yb}^+$ at 436 nm (688 THz). This transition is attractive because the natural linewidth is only 3.1 Hz and the $m_F = 0$ component does not show a linear Zeeman effect in small magnetic fields. So far the transition has been observed with a Fourier-limited linewidth of 30 Hz. Using a femtosecond optical comb generator and a Cs fountain clock, the transition frequency has been measured with a 1σ uncertainty of 6 Hz only [1]. With a relative uncertainty of $1 \cdot 10^{-14}$ this is now one of the most precisely known optical atomic transition frequencies. We are preparing experiments with two independent traps to make optical frequency comparisons with an accuracy beyond that of the Cs clock. A comparison of transition frequencies in different ions like Hg^+ , In^+ or Yb^+ over a period of about one year may lead to an improved limit on the present value for a possible temporal change of the fine structure constant. We are also studying the 3.5 eV *nuclear* transition in the $^{229}\text{Th}^{3+}$ ion as a unique candidate for an optical frequency standard and as a high precision system to probe the strong interaction.

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Interference of atomic states method: on limits of an accuracy for atomic characteristics

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We have considered a comprehensive comparison between radiospectroscopic method and atomic interferometer method to confirm the absolute uncertainties in precise measurements of atomic characteristics.

In the series of measurements by Pipkin et al. [1, 2] used the rf–spectroscopy technique known as the “separated–oscillatory method” proposed by Ramsey [3]. This method permits to obtain the line of the $(2S_{1/2}, F = 0) \longleftrightarrow 2(P_{1/2}, F = 1)$ transition whose width is one–third the natural linewidth. This method gives a line with a width which, because of the Ramsey interference, is determined by the distance between the rf fields rather than by the natural transition width. On the other hand, another reason for the line narrowing is that the lifetimes of the atoms passing through the system prove to be longer than their lifetime in the 2P state.

The key property of the atomic interferometer method [4, 5], independence on the natural linewidth of atomic transition 2P-1S, is analysed in some details.

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An Optical Clock/Frequency Standard at 657 nm Based On Laser-Cooled Neutral Calcium Atoms.

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Optical atomic clocks are receiving increased attention due to their enormous potential for high stability and accuracy, and because of the revolution in optical metrology that resulted from the development of fs-laser-based optical clockwork [1]. We have constructed a high performance diode-laser-based optical frequency reference that uses the $^1S_0 - ^3P_1$ transition (400 Hz natural linewidth) in laser-cooled neutral Ca at 657 nm. Absolute frequency measurements against the Cs-based NIST time ensemble via fs-laser metrology have led to a determination of the clock frequency (~ 456 THz) with 26 Hz uncertainty [2]. Measurements of the short-term fractional frequency instability against the Hg^+ ion clock system via the fs-laser comb [1] yielded an upper limit of $6 \cdot 10^{-15}$ @ 1s. In order to improve these results by an order of magnitude or more, we are currently developing a second-stage cooling scheme for Ca. This approach uses quenched cooling with the narrow clock transition and can reduce the atomic temperature by nearly three orders of magnitude.

In addition to its importance in the frequency standards community, this work could be used in tests of fundamental physics. In particular, transition frequency comparisons between Ca and Cs clocks could serve to check for drifts in fundamental constants over time. The history of frequency measurements of the Ca clock transition relative to the primary Cs microwave standard over the past eight years will be presented. These measurements constrain the relative fractional drift to $< 2(\pm 8) \cdot 10^{-14} \text{ yr}^{-1}$.

The authors thank S. Diddams, J. Bergquist, K. Vogel, and Th. Udem for their important contributions to this work.

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VNIIFTRI Cesium Fountain

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Russian State Time and Frequency Service relies on a group of H-masers and the classical Cs-beam primary frequency standard. H-masers are used as time keeper with a long term stability near 10^{-15} , while Cs standard is used for H-maser calibration and it has $(2 - 3) \times 10^{-14}$ uncertainty.

We started our Cs fountain project in the spring 1999, minding to get uncertainty at list one order less. We have developed a titanium vacuum system, consisting of two ion pumps, vacuum gauge and vacuum sleeve. The vacuum sleeve is used for a baking-up the system with a powerful external vacuum pump. There are molasses and detection zones in (0,0,1) configuration. They are changeable and very similar in design, but molasses zone section has an additional vacuum flange for Cs reservoir. The microwave cavity section and free flight section finish the vacuum chamber. The final vacuum in the pumping region is evaluated as 10^{-9} Torr. The vacuum system is surrounded by C-field coil, a permalloy screen, thermostat coil and another two magnetic screens.

An optical mounting is placed around the whole system. The optical beams about 10 mm in diameter can be balanced and adjusted in polarization. A laser system consists of the master and repumping laser and two injection ones. Master laser is frequency locked to an inverted pick in F4-F5 transition and the repumping one is locked to the inverted pick in F3-F2 transition [1]. The inverted picks simplify the operation of an AFC and increase reliability. To probe the microwave transition the specially designed H-maser is under development.

To check operation in molasses mode we have put on one layer of the magnetic shield and we have got a molasses operation. Then we have made some experiments with measuring the temperature of the Cs cloud. Time of flight and pulse width was measured and the width of the pulse is the same for molasses and for the MOT. The temperature in the MOT is evaluated as 6 K and in the molasses the temperature is about 2 K. We have got cold atoms, all systems operate satisfactory and we hope to see microwave fringes in the near future.

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Part VI

Fundamental constants

Single Ion Mass Spectrometry at 100 Parts per Trillion and Beyond

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To date our group has measured a total of 14 neutral masses ranging from the masses of the proton and neutron to the mass of ^{133}Cs , all with relative accuracies of typically a part in 10^{10} — one to three orders of magnitude better than the previously accepted values [1, 2]. This precision was achieved by comparing the cyclotron frequencies of two single atomic or molecular ions alternately confined in a Penning trap. The magnetic field fluctuations during the 5-10 minutes required for switching from one ion type to the other limited the precision of the mass ratio to a few parts in 10^{10} for a 4 hour night data set during which the Boston electric subway (our biggest source of magnetic field noise) was not operating.

We have now virtually eliminated the effect of magnetic field fluctuations by simultaneously trapping both ions of interest and measuring their cyclotron frequencies *simultaneously*. Using that technique, the statistical uncertainty on the ratio of the frequencies approaches a few parts in 10^{11} after only a few hours of measurement, even during the day when the magnetic field is very noisy. Since we exploit the magnetron modes of motion to maintain a separation distance of ~ 1 mm between the ions, we expect that systematic perturbations of the cyclotron frequency ratio from Coulomb interactions should be below 10^{-11} . However, applying this technique to measure the ratio N_2^+/CO^+ , we observe sudden large and bistable changes of the cyclotron frequency ratio. To understand these changes, we developed many techniques to probe (and control) the dynamics of the two ions in the trap and have experimentally confirmed the predicted behavior. We currently attribute the sudden jumps in the ratio to quantum transitions between rotational levels of the CO^+ molecule which has a big dipole moment. We are now working towards experimentally confirming this model.

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Simple atoms, Quantum electrodynamics and fundamental constants

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We present a brief overview of applications of precision study of simple atoms to test bound state QED and to accurately determine values of fundamental physical constants. In particular, we consider

- Precision spectroscopy of the hydrogen atom and tests of theory of the Lamb shift and determination of the Rydberg constant;
- Study of the hyperfine structure in light two-body atoms (hydrogen, deuterium, helium-3 ion, muonium, positronium);
- g-factor of electron and nucleus in a two-body atomic system;
- Determination of the fine structure constant α by means of QED and atomic physics.

We discuss uncertainties of QED calculations related to the nuclear structure effects and pay a special attention to QED tests, which are free of such a problem. In particular we consider the $2s$ hyperfine structure in the hydrogen atom and helium-3 ion [1].

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Do the fundamental constants vary in the course of the cosmological evolution?

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Contemporary theories of fundamental interactions (SUSY GUT, Superstrings/M-theory and others) predict that fundamental physical constants change in the course of the Universe evolution. In multidimensional theories (Kaluza-Klein, “p-brane” models and others) variations of fundamental physical constants are a direct result of the cosmological evolution of extra-dimensional sub-spaces. In some theories (e.g. Superstrings) variations of the constants are a consequence of evolution of the vacuum state (a vacuum condensate of some scalar field or “Quintessence”).

Clearly, experimental detection of such variations of the constants would be a great step forward in our description of Nature.

We estimate the cosmological variation of the proton-to-electron mass ratio $\mu = m_p/m_e$ by measuring the wavelengths of molecular hydrogen transitions in the early Universe. The analysis is performed using high spectral resolution observations (UVES/VLT, $FWHM \approx 7$ km/s) of two damped Lyman- α systems at $z_{abs} = 2.3377$ and 3.0249 observed along the lines of sight to the quasars Q 1232+082 and Q 0347–382 respectively.

The most conservative result of the analysis is a possible variation of μ over the last ~ 10 Gyrs, with an amplitude (cf. [1])

$$\Delta\mu/\mu = (5.7 \pm 3.8) \times 10^{-5}.$$

The result is significant at the 1.5σ level only and should be confirmed by further observations. This is the most stringent estimate of a possible cosmological variation of μ obtained up to now.

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Part VII

Structure of proton and nuclei

The Structure of Light Nuclei and its Effect on Precise Atomic Measurements

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My talk will consist of three parts: (a) what every atomic physicist needs to know about the physics of light nuclei [and no more]; (b) what nuclear physicists can do for atomic physics; (c) what atomic physicists can do for nuclear physics. A brief qualitative overview of the nuclear force and calculation techniques for light nuclei will be presented, with an emphasis on debunking myths and on recent progress in the field. Nuclear quantities that affect precise atomic measurements will be discussed, together with their current theoretical and experimental status. Finally, a discussion of those atomic measurements that would be useful to nuclear physics will be presented.

Systematic Model Calculations of HFS in Light and Heavy Ions

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Systematic model calculations are presented for the magnetization distributions and the HFS for light and heavy ions with mass close to $A \sim 6, 208, 235$, in order to test the interplay of nuclear and atomic structure. A high precision measurement of lithium isotope shifts (IS) for suitable transition, combined with an accurate theoretical evaluation of the mass-shift contribution in the respective transition, can be used to determine the root-mean-square (rms) nuclear charge radius of Li isotopes, particularly of the halo nucleus ${}^{11}\text{Li}$ [1]. Concerning the mass shift evaluation, the QED terms for light atoms are comparable in size to the nuclear size corrections so that the nuclear radius could be determined independent of QED uncertainties. An experiment of this type is currently underway at GSI and ISOLDE, CERN [2]. However, the field shift contributions between the different isotopes calculated in [1] can be reevaluated using the results obtained for the charge radii in Ref. [3], thus casting, with knowledge of the ratio of the HFS constants to the magnetic moments, new light on the (IS) theory. For heavy charged ions theoretical results presented in Ref. [4], demonstrate that the n -body magnetization distributions reproduce quite well the HFS of hydrogen-like ions. In Ref. [5] ab-initio calculations of the HFS of ${}^{209}\text{Bi}^{80+}$ were performed to explain the role played by the QED contributions on the HFS of heavy ions. Here, the positive continuum gives an important contribution to the HFS, thus modifying the theoretical results obtained in other models. [6]. The present results have initiated a detailed investigation of the structure of lithium-like ions heavier than bismuth, in order to analyze the new experiments on uranium proposed with PHELIX [7].

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Nuclear anapole moments from beams of multicharged ions

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Parity-nonconservation effects in neutral atoms are under intense experimental and theoretical investigations. The most accurate analysis has been performed for Cs atoms [1, 2]. The theoretical interpretation of this experiment requires highly accurate calculations of the atomic structure including relativistic effects, electron-electron correlations, the Breit interaction, and radiative corrections. It would be highly desirable to have a different source of information on weak interactions at low energies available, which does not suffer from rather involved theoretical interpretations as in the case of many-electron atoms. Such a scenario could be provided by studying P-odd effects in multicharged ions. P-odd effects, which depend explicitly on the nuclear spin, can be dominated by the contact electromagnetic interaction of electrons with the nuclear anapole moment [3].

In heliumlike ions, there is a unique opportunity to observe a net nuclear spin-dependent P-odd effect due to the near-degeneracy of the 2^1S_0 and 2^3P_1 levels for nuclear charge numbers close to $Z \simeq 32$. In work [4], we have proposed to measure the angular asymmetry of the radiation of a polarized ion beam due to the contribution of the nuclear anapole moment to the hyperfine-quenched decay of the 2^1S_0 level. A method for measuring hyperfine-quenched decays in heliumlike ions using the beam-foil time-of-flight technique has been elaborated in works [5, 6]. Its application to the problem under consideration seems to be quite effective.

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Part VIII

Quantum Electrodynamics

Resent results and current status of the muon (g-2) experiment at BNL

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The muon (g-2) experiment E821 is currently in progress at Brookhaven National Laboratory. Four data taking runs for positive muons and one run for negative muons were successfully accomplished in 1997-2000 and 2001, respectively. Results of the 1997, 1998 and 1999 runs have been published while data analysis for the 2000 and 2001 runs is currently in progress. Our 1997 and 1998 results are comparable in precision with last CERN measurement, within experimental errors they are all consistent with each other and with current theoretical value $a_\mu(th)$. However our 1999 result, with a precision comparable with that of $a_\mu(th)$, was 2.6 standard deviations higher than $a_\mu(th)$, though consistent with previous measurements within their errors. This deviation, which might indicate a sign of new physics beyond the Standard Model, caused great activity among people working for (g-2) theory and for new physics. In few months, however, some mistake in calculations of hadronic light-by-light scattering to muon (g-2) value was found and as a result difference between $a_\mu(exp)$ and $a_\mu(th)$ was reduced to 1.5 standard deviations. That makes upcoming results from 2000 and 2001 runs even more intriguing.

Theory of Muon $g - 2$: Current Status

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The latest measurement [1] of muon $g - 2$ at the Brookhaven National Laboratory disagreed with the theory by 2.6 s.d., suggesting possible existence of new physics beyond the Standard Model. The discrepancy has since been reduced to 1.6 s.d. by a discovery of sign error in the π^0 -pole contribution to the muon $g - 2$ [2, 3]. Nevertheless there is a strong interest in enhancing the credibility of theory of muon $g - 2$ in view of the imminent improvement of the BNL measurement.

This paper is a progress report of the current work on the QED part of theoretical prediction. Our effort is focused on enhancing the reliability of evaluation of the α^4 QED term, by providing alternate and independent evaluation as much as possible, and by improving numerical precision of all terms by an extensive computer work.

The situation on reliability may be summarized as follows: The 469 Feynman diagrams of order α^4 contributing to the difference $a_\mu - a_e$ can be classified into four categories:

- (1) Those evaluated by two or more independent methods. 139 diagrams belong to this category.
- (2) Those evaluated by one method, but structure of integrand was verified by extensive cross-check and by comparison with analytically known α^3 diagrams. 204 diagrams.
- (3) Those evaluated by one method only. Limited cross-checking. 96 diagrams.
- (4) Those evaluated by one method only. No cross-checking thus far. 30 diagrams.

At present an effort is under way to reduce the size of category (4).

Meanwhile, numerical precision of all categories are being upgraded by an extensive numerical work using the Monte-Carlo integration routine VEGAS. Already a substantial improvement has been achieved for all diagrams. Earlier evaluation of some integrals has been found to suffer from poor sampling statistics, resulting in overly optimistic error-bars. Fortunately, the dominant contribution comes from diagrams of category (2), which had been evaluated with reasonable statistics.

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G factors of bound particles in quantum electrodynamics

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The g factors of bound particles can be presented in the form [1, 2]:

$$g(\text{H} - \text{atom}) = 2 + \Delta g_{\text{rel}} + \Delta g_{\text{rad}} + \Delta g_{\text{rec}} + \dots \quad (17)$$

In this study the quasipotential method for calculating relativistic Δg_{rel} , radiative Δg_{rad} and recoil Δg_{rec} corrections to the g factors of bound particles with arbitrary spin was used. It was found that the expression for the electron g factor contains nuclear spin-dependent contributions in the following form [3]:

$$g_{\text{e bound}} = g_{\text{e}} \left\{ 1 - \frac{m_2^2 (Z\alpha)^2}{3(m_1 + m_2)^2} \left[1 - \frac{3\kappa_1}{2(1 + \kappa_1)} - \frac{3}{2}(1 - K_{s_1}) - \right. \right. \quad (18)$$

$$\left. \left. - \frac{3}{2} \frac{m_1^2}{m_2^2} \left(1 - K_{s_2} - \frac{2}{3} ZK_{s_2} \right) + \frac{m_1}{2(m_1 + m_2)(1 + \kappa_1)} \left(1 + Z \frac{m_1}{m_2} \right) \right] \right\},$$

where $K_{S_i} = \langle \Sigma_i^2 / 3 \rangle$, $g_{\text{e}}/2 = 1 + \kappa$, $m_{1,2}$ are the masses of bound particles. These contributions appear upon taking into account, in the particle interaction operator, terms that are nonlinear in the spin operator Σ . Effects quadratic in the operator Σ appear

- in the matrix element of electromagnetic current for the particle with arbitrary spin;
- in the expressions for the Lorentz transformation of corresponding spin tensors;
- in the transformation law of the bound state wave function in the case of the particles with arbitrary spin.

The quantity $(\Sigma \cdot \mathbf{q})^2$ can be presented as the sum of the contact and quadrupole terms:

$$\Sigma_i \Sigma_j q_i q_j = \frac{1}{3} \mathbf{q}^2 \Sigma_i \Sigma_i + \left(q_i q_j - \frac{1}{3} \mathbf{q}^2 \delta_{ij} \right) \Sigma_i \Sigma_j. \quad (19)$$

The contact term contributes to the energy spectrum of the system, while the quadrupole term determines the correction to the quadrupole moment of the nucleus. The results that we obtained for the contributions to the g factors of particles are determined by the contact terms in eq. (3). The numerical value of the correction to the electron g factor in deuterium is equal to 0.001×10^{-9} .

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Regularization Corrections to the Partial-Wave Renormalization Procedure

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The equivalence of the covariant renormalization and the partial-wave renormalization (PWR) approach is proven explicitly for the one-loop self-energy correction (SE) of a bound electron state in the presence of external perturbation potentials. No "spurious" correction terms to the non-covariant PWR scheme are generated for Coulomb-type screening potentials and for external magnetic fields. It is shown that in numerical calculations of the SE with Coulombic perturbation potential "spurious" terms result from an improper treatment of the unphysical high-energy contribution. A new method for performing the PWR utilizing the relativistic B-spline approach for the construction of the Dirac spectrum in external magnetic fields is proposed. This method is applied for calculating QED corrections to the bound-electron g -factor in H-like ions. Within the level of accuracy of about 0.1% no "spurious" terms are generated in numerical calculations of the SE in magnetic fields.

Magnetic moment of the bound electron

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Precise measurements of the magnetic moment in low- Z hydrogen-like ions with spinless nuclei [1] are an important source of information about the electron mass. To extract a value of the electron mass from the experimental data, theory has to provide the highly accurate account of bound-state effects. At present, the theoretical uncertainty is mainly due to the lack of precision in the numerical result [2] for the first radiative correction to the bound electron magnetic moment.

I describe the analytic calculation of the order $\alpha(Z\alpha)^4$ correction and the reason of its enhancement. Calculation of the next order, $\alpha^2(Z\alpha)^4$ correction in the spirit of the NRQED approach [3] is also discussed.

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Part IX

Advanced Quantum Mechanics

Collisional excitation transfer in helium

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Collisional excitation transfer processes in $He^* - He$ binary encounters have been widely studied in electron beam interaction experiments and by means of time-resolved spectroscopy technique with pulse electron or laser excitation. The breaking of Wigner spin conservation rules for the levels with orbital moment $l > 2$ has been established certainly. The strong singlet-triplet mixing of the wave functions allows one to consider 1L and 3L sublevels as a whole.

As a result of time resolved kinetic studies of $He^* - He$ collisions in due time one of us (VBS) took into account a conception of the block of the collisional mixed excited states with $l > 2$ [1]. This model allows the analysis of kinetics for the excitation transfer to be simplified. Here we demonstrate the efficiency of this approach for the treatment of the collisional and radiative relaxation of He^* ($n = 5 - 10$) levels population after the pulse excitation.

The sensitivity analysis method was developed to estimate the parameters (collisional rate constants) of the dynamical system from the experimental relaxation signals [2]. The technique considered for estimating the parameters allows the statement of the problem of joint processing of the whole collection of experimental data relating to different excited levels, obtained at different concentrations of colliding particles, without resorting to decomposition into exponential components, but working with the parameters of the physical model described by a set of differential equations. The processing of the data obtained in the investigation of the collision processes in helium showed that the most complete information on the kinetics of excitation transfer can be obtained by simultaneous processing of the decay curves for as large a number of the levels related to each other as possible. The results obtained verify the working model proposed in [1] and imply the participation of mixed states with large orbital quantum numbers in the singlet-triplet transfer of excitation energy. It is shown that an unusual humpbacked form of the decay curves can be described by the collisional processes within alone principle quantum number n . More accurate estimations for the rate constants of the most significant collision processes was obtained. Its dependence of the n and orbital quantum number selection rules are discussed.

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Radiative kinetics of hydrogen atom: semiclassical approach

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Although hydrogen atom represents the simplest quantum system, the radiative constants for its excited levels do not have a convenient and accurate analytical representation. This fact causes certain difficulties in analyzing different phenomena evolving coherent laser beams interaction and light manipulation with Rydberg states. In this connection we would like to attract attention to the semiclassical treatment of radiative processes developed in [1, 2, 3] and report on formulas for some important rate constants.

Information on the dipole matrix elements $R_{qq'} = \langle q' | r | q \rangle$ involving two states (the index q incorporates quantum numbers $q = \{n, l\}$) is of much importance for many spectroscopy problem. In [2] it was shown that

$$R_{qq'} = \frac{L_c^2}{\pi\omega} \frac{1}{\sqrt{n^3 \cdot (n')^3}} \left[-\frac{\sqrt{\pi}}{x} \Phi'(x) + \Delta l_q \sqrt{\frac{\pi}{x}} \Phi(x) \right]; \quad (20)$$

$$x = \left(\frac{\omega L_c^3}{2} \right)^{2/3}; \quad \Delta l_q = \Delta l + \frac{\varepsilon + \varepsilon'}{5\omega L_c}; \quad \omega = \varepsilon' - \varepsilon > 0, \quad (21)$$

where $\Phi(x)$ is the Airy function, $L_c = (l+l'+1)/2$, $\Delta l = l' - l = \pm 1$, $c=137$ is the velocity of light (in atomic units), $\varepsilon = -1/(2n^2)$ gives the energies of levels, and ω corresponds to the frequency of the optical transition under consideration.

Another explicit formula describing radiative lifetimes $\tau_q = A_q^{-1}$ of the individual excited state q of the hydrogen atom reads [1]:

$$A_q = \frac{4}{\sqrt{3}\pi c^3 n^3} \frac{G(n, l)}{(l+0.5)^2}; \quad G_{l>0} = 1 + \frac{1}{5} \frac{p^2 \ln(p^2)}{1-p^2} + 0.110 \cdot p^2; \quad p = \frac{l+0.5}{n}; \quad (22)$$

$$G_{l=0} = \frac{1}{20} \left[1 + 16 \frac{p^2 \ln(p^2)}{1-p^2} \left(1 + \frac{39}{56} p^2 \right) + 33.4 \cdot p^2 \right]. \quad (23)$$

An analyze of effective radiative lifetimes occurring due to multiple light scattering in an optical dense atoms vapor is presented in [3].

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Universal Classical Approach for Rydberg Atomic Spectral Line Shapes

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Rydberg spectral line shapes are of great interest both in astrophysics and laboratory plasmas. Their calculations on the basis of the standard broadening theory face with the problem of taking into account radiative transitions between a large number of atomic states. With the help of the standard Gordon formulas [1].

It is natural to use in the case a classical approach which just the goal of present paper. We start from pure classical Born [2] results for Fourier components of atomic dipolar momenta expressed the intensities of Stark components in terms of double series in parabolic quantum numbers n_1, n_2, m , which take the following form for Z -components of dipole momentums:

$$Z_{\Delta n_1 \Delta n_2}^{\Delta m=0} \sim \frac{1}{\Delta n} \left\{ \sigma_2 J_{\Delta n_1}(\Delta n \sigma_1) J'_{\Delta n_2}(\Delta n \sigma_2) - \sigma_1 J'_{\Delta n_1}(\Delta n \sigma_1) J_{\Delta n_2}(\Delta n \sigma_2) \right\}, \quad (24)$$

Here $J(x)$ are Bessel functions, $\Delta n, \Delta n_1, \Delta n_2$ are changes in principle and parabolic quantum numbers,

$$\sigma_1 = \sqrt{(n+s-1)^2 - m^2}/2n, \quad \sigma_2 = \sqrt{(n-s-1)^2 - m^2}/2n, \quad s = n_1 - n_2. \quad (25)$$

When $n \gg 1$ and $\Delta n \ll n$ the variable K separates the spectral line intensity into large scale blocks of order of n whereas the variable s describes the variation of the intensities on small scale inside these large blocks. The only few of Bessel functions corresponding to a couple of K values ($K = 0, 1, 2$) are significant in es. (24). Thus for $\Delta n = 1$ the results coincide with Gulyaev data [3]. Analogues analytical result can be obtained for the case $\Delta n \sim n \gg 1$.

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Radiative cascade following dielectronic recombination

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The DR electron capture results in a strongly nonequilibrium atomic level population with respect to values of orbital quantum numbers l which are much smaller as compared with principle quantum numbers n . Every population event is accompanied by radiative - collisional cascade resulting in a change of initial nl - distributions. The main mechanism responsible for nl -redistribution is radiative cascade when the plasma density is relatively low. Such situation are usual for atoms and multicharged ions under coronal equilibrium conditions in astrophysics as well as in rarefied laboratory plasmas (storage rings, tokamaks, stellarators, etc).

The process under consideration looks as follows: a free electron with the energy E less than the ion core excitation energy $\hbar\omega_c$ excites the core and is captured at a highly excited (Rydberg) energy state with large values of principle (n) and orbital (l) quantum numbers, then the core is stabilized by the radiative transition at the core frequency ω_c and we look for a radiative cascade of the captured electron over Rydberg atomic state n, l .

The general idea of a quasiclassical approach to the radiative cascade is to use classical kinetic equations for electron energy and angular momentum losses in the Coulomb field instead of quantum kinetic equations. As result one can obtain the limiting cases for the n, l distribution:

$$f(n, l) = N_e B(Z, T) Z^4 l^3 \{(\pi\sqrt{3}/2)n^3 + 2.42l^3 n^*\}, \quad n \ll n^*(l) \quad (26)$$

$$f(n, l) = N_e B(Z, T) Z^4 l^3 n^{*3} \{(\pi\sqrt{3}/2) + l^3/n^2\}, \quad n \gg n^*(l) \quad (27)$$

where

$$n^*(l, Z) = \left[\frac{3c^3(2l+1)}{4\pi\omega_c^2} G[\omega_c(l+1/2)^3/(3Z^2)] \right]^{1/3}, \quad (28)$$

$$G(u) = u[K_{1/3}^2(u) + K_{2/3}^2(u)] \quad (29)$$

(K are standard MacDonal functions),

$$B(T, Z) = (2/3)(2\pi/T)^{3/2} (g_j/g_i) \omega^2 f_{ij} \exp(-\omega/T). \quad (30)$$

The first terms of eqs. (26) and (27) are due to direct population whereas last terms are due to cascade ones.

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Perturbation theory for hydrogen Stark line intensities

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The Stark shift and splitting for arbitrary energy levels in hydrogen have been calculated up to very high orders in electric field F . However, the information in the line intensity dependence on field still remains very limited. The field dependence of the line intensity had been observed first in [1] for the E1 transitions between highly excited Rydberg states. Corresponding numerical calculations were confined to the particular case of experiment and could not be used for different atomic lines.

In this communication we report on the possibility to derive power series in F for intensities of hydrogen radiation lines [2] with the use of perturbation theory (PT) and the Sturm-series expansion for the Coulomb Green function in parabolic coordinates. The line intensity in field F is presented as the power series F as follows:

$$I_{nn'}(F) = I_{nn'}(0) \left(1 + \sum_{N=1}^{\infty} F^N \beta_{nn'}^{(N)} \right),$$

where $I_{nn'}(0)$ is intensity in the zero-field limit. The factors for the corrections to intensity in field come from corrections to the two factors of the radiation intensity $I_{n,n'} \sim \omega_{nn'}^4 |d_{nn'}|^2$, i.e. the line frequency $\omega_{nn'}$ and the dipole matrix element $d_{nn'}$, which involves perturbed wave functions of upper and lower states.

We develop the method for deriving the wave function in the form of power series with field-independent coefficients, which makes it possible to use in calculations computer algebra routines. This method takes naturally into account the field-induced mixing to the initial and final Stark levels of all atomic eigenstates with different principal quantum numbers n , including continuum.

We have derived the analytical results for the hydrogen Stark line intensity in dc electric field in the first, second, third, and fourth orders in the field strength. The numerical calculations have been carried out for the lines of Lyman and Balmer series and analytical properties of corresponding field-induced corrections have been analysed. The effect of the field dependence of intensity provides additional spectroscopic information about the atomic structure, which can be used for optical diagnostics of fields exerted on the atom and for control of the radiation and absorption of light by matter.

Our approach may be used also for the interaction of an atom with a charged particle or a system of particles in the case when the inverse of the distance from the atomic nucleus is used as the small parameter for perturbation theory.

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Atomic and collisional properties of highly-excited Hydrogen and Deuterium.

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The first goal of this research is to provide precise total energies and frequencies for transitions between metastable 2s and highly excited states of H and D. All known QED and relativistic corrections have been included in the calculation. Interest in these transitions has been sparked by the possibility of creating ultra-cold samples of 2s hydrogen. Starting from this metastable state Rydberg levels can be accessed more easily.

A second reason for our research is fueled by interest in collisions between highly-excited hydrogen atoms. Long-range alkali-metal Rydberg molecules have been predicted [1, 2]. The corresponding potentials show oscillatory behavior that strongly depends on the quantum defect of the Rydberg level. We do a theoretical search for these states in hydrogen dimers where (nonrelativistic) atomic energies are independent of the electronic orbital angular momentum.

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Paschen-Back effect in Helium spectra revisited

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Development of new methods for magneto-optical trapping and cooling atoms stimulates high-precision considerations of spectral properties for simplest atomic systems in field. The dependence on a magnetic field B for intensity of Helium triplet radiation lines, corresponding to transitions $n^3P_J \rightarrow 2^3S_1$ ($J = 0, 1, 2$), is caused by mixing the fine-structure sublevels of the upper n^3P_J state ($J = 0, 1, 2$).

We have calculated variation of Helium line intensities induced by paramagnetic mixing of fine-structure sublevels in 2^3P_J -states. In a low-field limit (anomalous Zeeman effect) there are 18 lines (six π - and twelve σ -lines), corresponding to the radiation transitions $|2^3PJM\rangle \rightarrow |2^3S_1 M'\rangle$, with symmetric splitting relative the triplet lines with frequencies ω_2 , ω_1 and ω_0 of a free atom, with line intensities proportional to coefficients of angular momentum algebra in LS-coupling scheme (Fig.1a, the lines numbered from the lowest frequency, intensity proportional to the line height).

For $B \sim 0.1 \div 1$ T the Paschen-Back effect appears first in states $|2^3P_{1,2}\rangle$, together with an additional π -line 19, which corresponds to a strictly forbidden π -transition $|2^3P_1\rangle \rightarrow |2^3S_1\rangle$ with $M = 0$. The π -lines 4, 13 and σ -lines 1,2,14,15 disappear. The lines 16, 17, 18, originated from the state $J = 0$, also begin to change their intensities, due to mixing all states $J = 0, 1, 2$. This effect had not been accounted for in [1], therefore a picture of line intensities presented in [1] for $B = 0.85$ T differs essentially from the 3-level diagonalization result (Fig.1b). In a strong field, $B > 4$ T, only 9 lines remain visible. They form three groups by three σ^+ , σ^- and π lines, with equal intensities (the π -line 6 of Fig.1c joins 12).

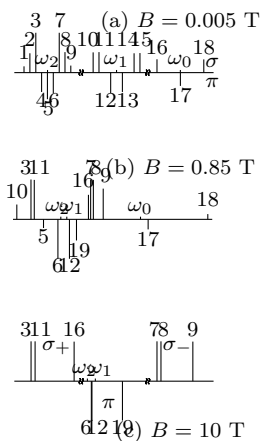


Figure 1: Splitting and intensities of the $|2^3P\rangle \rightarrow |2^3S\rangle$ lines for three field values.

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Diamagnetic Effect on the Intensity of Helium Radiation Lines

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The diamagnetic interaction determines the dependence on a magnetic field for the matrix elements of Helium radiation lines, which duly transforms into the line intensity dependence on field. The line intensity behaviour in a magnetic field for transitions between Hydrogen-like states with high orbital quantum numbers does not differ from that of the Hydrogen lines, considered in detail in [1]. In this communication we discuss only the lines involving the non-degenerate S, P and D Helium states.

The change in the matrix elements of a radiation transition is due to the magnetically induced corrections to the wave functions of the initial $|1\rangle$ and final $|0\rangle$ states. The diamagnetic corrections may be resolved in power series of the square field B , so that the dipole transition matrix element may be presented as

$$d_{if}(B) = d_{10} \left(1 + \sum_{s=1}^{\infty} q_{10}^{(s)} B^{2s} \right). \quad (31)$$

We confine ourselves to the first-order correction described by the coefficient q_{10} , which may be written in terms of the ratio between the second-order and first-order matrix elements, $\langle 1|\hat{d}_{\mu}G'_{E_0}\hat{V}_D + \hat{V}_DG'_{E_1}\hat{d}_{\mu}|0\rangle$ and $\langle 1|\hat{d}_{\mu}|0\rangle$, where G'_E is the reduced Green function, \hat{V}_D — the operator for diamagnetic interaction, \hat{d}_{μ} — the dipole moment operator with $\mu = 0$ for π -transition, $\mu = 1$ for σ -transition. In calculating matrix elements the model potential method has been used, similar to calculations for alkali atoms [2]. The radiation matrix element for the head lines both for singlet and triplet series of the $nP \rightarrow n_0S$ transitions ($n_0 = 1$ and 2) are reduced by the magnetic field ($q < 0$). The matrix elements for the other lines are enhanced ($q > 0$). A simple asymptotic relation (for large n) between q and the effective principal quantum number $\nu_{nP} = 1/\sqrt{-2E_{nP}}$ of the upper (initial) nP -level can be derived, $q^{\pi,\sigma} \approx a^{\pi,\sigma}\nu_{nP}^6$, where $a^{\sigma} \approx 2a^{\pi} \approx 0.4$.

A magnetic field also induces dipole transitions with selection rules for the orbital angular momentum $|\Delta l| \geq 3$. The relation of intensity for these lines to the intensity of field-free dipole-allowed transitions may be written as $I_{n_3l+3 \rightarrow nl} = \eta I_{n_1l+1 \rightarrow nl} B^4$. This effect is caused mainly by the mixing of $|n_1l + 1\rangle$ -states and $|n_3l + 3\rangle$ -states. The asymptotic behaviour of the coefficient η may be described by equation $\eta = b\nu^{12}$, where ν is the principal quantum number of the upper $|n_3l + 3\rangle$ state. For singlet lines of $|n_3^1F\rangle \rightarrow |1^1S\rangle$ transitions $b \approx 6 \times 10^4$ is about 200 times larger than for $|n_3^1F\rangle \rightarrow |1^1S\rangle$ transitions and 500 times larger than for the triplet $|n_3^3F\rangle \rightarrow |2^3S\rangle$ transitions.

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Precise theory of the Stark effect on hydrogen- and helium-like atoms

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A general approach is presented for calculating the higher-order terms of series in powers of the electric field for the hydrogen- and helium-like atomic systems. In the present paper we modify and extend the degenerate theory in several ways. We consider the problem of the atomic structure in the presence of a uniform electric field using rather general angular momentum arguments to show how the different susceptibilities (independent non-zero irreducible parts) contribute.

The Z-dependent perturbation theory is applied to obtain higher-order perturbation terms. Calculations of polarizabilities and hyperpolarizabilities are carried out using sums of oscillator strengths and, alternatively, with the excited electron Green's function. In the case of helium-like atoms, an estimate is given based on the model potential method for the contribution of an infinite series over the bound states, including the integral over the continuum, for second- and higher-order matrix elements [1, 2].

In connection with precise laser spectroscopy measurements which have been carried out and planned, we have calculated the higher-order susceptibilities for the ground and excited states of hydrogen- and helium-like atoms ($1snp\ ^3P_0$ and $1snp\ ^3P_0$ terms with $n = 2 - 5$). In particular, the present study may be important for the further experimental investigations of the anticrossing measurements in helium by using microwave cavity spectroscopy [3]. On the other hand, the hyperpolarizabilities themselves are of current interest because of their relevance to optical harmonic generation through the interaction of intense beams of light with atoms.

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Long-Range Atom-Metal-Surface Interaction and Interference of Atomic States

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New results for the observation of the stationary interference pattern of hydrogen atomic states are presented.

In a paper the process of interaction of a hydrogen atom with a metal surface is used as a part of the scheme of an atomic interferometer [1]. The key point is a very high sensitivity of the interferometric pattern to small perturbations of its components. Therefore this scheme turns out to be a convenient tool for precision studies of long-range interaction of metastable hydrogen atoms with metal surfaces. In particular, recent experiments [2] showed that the scale of interaction strongly depends on the microcrystalline structure of the metal surface. In these experiments we used the slits formed by massive plates of gold-silver alloy and pure palladium. It was found that for both metals the mixing amplitude displayed a severalfold, by the factor of 5–7, increasing after annealing. These important results can serve in benefit of a significant role played by conductive electrons from the surface layer.

Discussions on our experiment and a possible theoretical explanation are presented. We consider here two quite different interpretations of the effect, which were proposed in [3, 4]. According to work [3] the $2S$ atom and individual electrons located in a thin surface layer of metal form a huge number of EPR-pairs given rise to a coherent admixture of the $2P$ -state. In contrast to this mechanism, the interpretation given in [4] is based on the "physical locality" and the hydrogen atom in a beam is treated as a wave packet. Small parts of the center-of-mass wave function, i.e. tails of halo, can penetrate the metal surface up to a high field area that results in a coherent mixing of the $2S$ and $2P$ states.

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Low energy electron collisions with atomic oxygen

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The wave functions of neutral oxygen exhibit large correlation corrections and strong term dependence of the one-electron orbitals. Accurate representation of wave functions has been obtained on the basis of non-orthogonal orbitals. The non-orthogonal orbitals provide much greater flexibility in the choice of target wave functions than the orthogonal orbitals and also allow to include correlation with a minimum number of configurations and correlated orbitals. Both the correlation and relaxation effects are found to be important.

The collision calculations are carried out by using the new R-matrix code in which non-orthogonal orbitals are used for describing both the target states and the R-matrix basis functions. A B-spline basis is used for the description of continuum functions in the internal region. The eigenproblem in the B-spline basis leads to a generalized eigenvalue problem. For an accurate determination of electron flux through the boundary, we do not impose any boundary conditions on the radial basis functions at the outer edge of the box. The amplitudes of the wave functions at the boundary which are needed for construction of the R-matrix are simply given by the coefficient of the last spline; the only spline which has non zero value at the boundary. The completeness of the B-spline basis ensures that no Buttle correction to the R-matrix elements is required. The use of non-orthogonal orbitals considerably simplifies the structure of the bound part of close-coupling expansion, that leads to substantial reduction in pseudo-resonances. The convergence of the close-coupling expansion has been tested in a systematic way by including 8, 16 and 26 target states of oxygen [1]. A significant part of the polarizability of low-lying states arises from transitions to the continuum. This implies that the close-coupling expansion should also take into account the possible loss of flux into the continuum. The effect of coupling to the continuum is simulated through the use of well-chosen pseudo-states and autoionizing states in the close-coupling expansion [2].

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Anomalous is not anomalous. Part II/V. A chiral symmetry breaking (CSB) theory for atom H.

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Part II of this series [1] deals with natural antihydrogen H-states, already detected in molecule H_2 [2, 3]. H-handedness results from a parity operator in a molecular Hamiltonian, acting on Coulomb interactions in a 4-unit charge system. This is insoluble and its stability is a problem [4] as solutions are constrained by models. In 4-unit charge systems in bonds the parity operator for atom handedness acts on a Coulomb term. There is a connection between states of different atomic handedness and those in Coulomb quadruplet $\pm(1 \pm 1/n)$ [2, 3]. Within atom H, this inter-atomic parity operator (the atom-antiatom switch) makes sense only if, in the H Hamiltonian, it acts on the Coulomb electron-proton attraction. If so, it must leave a fingerprint of antihydrogen states in the spectrum of natural H. To explain this, we review chiral and achiral behavior in connection with an attractive Coulomb field. As in [2, 3], we start from scratch. We reconsider symmetry, a set of simple rules for positions of vertices of a structure or for numbers on a reference frame. Chirality is the absence, achirality the presence of (a) symmetry. We define a continuous chirality measure (CCM) [6] for atom H by offering a theoretical basis for Avnir's folding/unfolding technique [6] and use a 19th century Walden inversion as model. With these tools, a chiral symmetry breaking (CSB) theory for atom H is derived, which produces a small correction to Bohr theory. This matches observed data with errors of 10^{-11} . The predicted CSB fine structure reduces errors to 10^{-13} . With CSB, H ns singlet states can be hydrogenic H or antihydrogenic \bar{H} . CSB theory provides an alternative explanation for Lamb-shifts, for non-annihilating antihydrogen-states in bond H_2 [2, 3] and for the anomaly of the free electron magnetic moment. Term 1s2s for artificial antihydrogen, available with the ongoing CERN-AD experiment, is discussed. Simple CSB theory and complex bound state QED are different. The validation of the complicated framework of modern bound state QED may be problematic.

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Relativistic dipole dynamical polarizability of the $ns_{1/2}$ -states in hydrogenic atoms. New analytic results

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A novel closed-form analytic representation for the linear response wave function,

$$\delta\Psi_i(\mathbf{r}, E) \equiv \left(c\boldsymbol{\alpha}\hat{\mathbf{p}} + mc^2\beta - Ze^2/r - E \right)^{-1} \boldsymbol{\alpha}|i\rangle,$$

of the arbitrary relativistic hydrogenic $|i\rangle = ns_{1/2}$ -level exposed to a uniform dipole radiation of frequency ω is reported (see [1, 2] and references therein). This result has been derived using relativistic generalization of the Podolsky–Sternheimer–Dalgarno–Lewis method, that is, by means of direct analytically solving appropriate inhomogeneous E -dependent Dirac equation, thus requiring no prior knowledge of the relativistic Coulomb Green’s function. The utility of the formulas obtained for numerous potential applications is illustrated by analytical and numerical calculations of the two-photon relativistic dipole transition amplitudes between $1s_{1/2}$ - and $2s_{1/2}$ hydrogenic levels, together with relativistic dipole dynamic and static polarizabilities (RDP) of these states at $\hbar\omega = |E - \varepsilon_{ns_{1/2}}|$ lying both below and above respective ionization thresholds $|\varepsilon_{ns_{1/2}}|$. Our analytic technology enables, in particular, these two last cases to be considered on the same footing, which favors the current approach against those formerly reported in literature. As an interesting by-product application of the above general result, we have succeeded first in casting, for several lowest n , the *static* DPs $\alpha_{ns_{1/2}}(0)$ into explicit analytic form. At $n = 1, 2$ and $1 \leq Z \leq 137$, however, the exact results appear to be virtually indistinguishable numerically from appropriate expansions up to order $(\alpha Z)^6$, $\alpha \approx 1/137$:

$$\begin{aligned} \alpha_{1s_{1/2}}(0) &= \frac{9a_0^3}{2Z^4} \left(1 - \frac{28}{27}(\alpha Z)^2 + \frac{31 + 2\pi^2}{432}(\alpha Z)^4 + \frac{150\pi^2 + 216\eta_1 - 1273}{31104}(\alpha Z)^6 \right), \\ \alpha_{2s_{1/2}}(0) &= \frac{120a_0^3}{Z^4} \left(1 - \frac{367}{240}(\alpha Z)^2 + \frac{9535 + 840\pi^2 + 1728\zeta(3)}{34560}(\alpha Z)^4 \right. \\ &\quad \left. + \frac{3270\pi^2 + 5184\eta_2 + 167292\zeta(3) - 235397}{518400}(\alpha Z)^6 \right). \end{aligned}$$

Here, $\zeta(3) = 1.202\dots$ is the value of the Riemann zeta function, $\eta_1 = 0.11698\dots$ and $\eta_2 = 0.037487\dots$ are the sums of two certain series, a_0 is the Bohr’s radius. Although interesting in its own right, the study presented is strongly motivated due to its utility for highly accurate numerical simulations of ionization probabilities and line profiles in resonant multi-photon processes with simplest atoms [2]. We demonstrate this by carrying out such calculation for the ground state 2+1-photon resonant ionization of positronium.

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Two-photon transitions in the H_2 molecule and its μ -isotopes

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We present new results of *ab initio* calculations of the two-photon transitions probabilities between the ground and electronically/muonically excited discrete levels in the H_2 molecule and its neutral μ -isotope, $ppe^- \mu^-$, at internuclear separations $R \geq 0.5 a.u.$ Apart from its conspicuous academic interest, this study is currently of major practical importance due to dramatic technical advances enabling a wide range of energy levels of the H_2 molecule to be measured to better than 0.03 cm^{-1} accuracy [1, 2]. Despite much lower experimental resolution attainable nowadays with $(pp\mu^-)^+$ and $ppe^- \mu^-$ molecules, detailed theoretical data on the two-photon (de)excitation rates in these fundamental systems are of relevance for an adequate interpretation of the $2s_{1/2} - 2p_{3/2}$ energy separation measurements in isotopes of the muonic hydrogen atom, which are presently underway at PSI [3]. For both the H_2 molecule and its μ^- -isotopes, currently available theoretical information on the two-photon transition amplitudes is either lacking or incomplete, which urges further *ab initio* investigation intended to fill this gap.

It is demonstrated that the two-photon amplitudes of interest can be described, at each fixed internuclear separation R , using the following variational ansatz to determine auxiliary N -particle wave function $\Psi^{(1)}$ of the system:

$$\mathcal{I} = \langle \Psi^{(1)} | \widehat{H}_0 - E_0 | \Psi^{(1)} \rangle + 2 \langle \Psi^{(1)} | \sum_{q=1}^N \hat{\mathbf{n}} \cdot \mathbf{r}_q | \Psi^{(0)} \rangle, \quad \delta \mathcal{I} = 0.$$

Here, $\Psi^{(0)}(\mathbf{r}_i, \mathbf{R})$ and E_0 denote the unperturbed wave function and the corresponding energy of the system; these are the eigenfunction and eigenenergy of the unperturbed Hamiltonian: $\widehat{H}_0 \Psi^{(0)} = E_0 \Psi^{(0)}$. Hence, the function $\Psi^{(1)}$ incorporates an admixture to $\Psi^{(0)}$ of all unperturbed states due to the external dipole perturbation $\widehat{V} = \sum_{q=1}^N \hat{\mathbf{n}} \cdot \mathbf{r}_q$. The quality of $\Psi^{(1)}$ computed thereby was controlled by calculating it also directly, using conventional perturbative “sum-over-states” technique, as well as by comparing results of independent calculations based on $\Psi^{(1)}$ of the ground state static dipole polarizabilities at equilibrium ($\alpha^{(H_2)} = 0.82 a.u.$, $R = 0.7 a.u.$) with available data ($\alpha^{(H_2)} = 0.802 a.u.$ [4]). The overall accuracy of the transition probabilities values computed so far is limited by unaccounted portion of interparticle correlations and inaccuracy in values of the Franck-Condon factors, thus leaving room for certain improvements of the scheme developed.

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Postdeadline contributions

Weak Charge of ^{133}Cs

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Measurements of parity nonconservation (PNC) in atoms provide sensitive tests of extensions to the Standard Model of electroweak interactions. Measurements of atomic PNC have been made at the 1% level of accuracy in several heavy atoms and to 0.3% in cesium. Combining the precisely measured PNC amplitude in cesium with the most accurate available atomic structure calculations, including corrections from the Breit interaction, vacuum polarization, the nuclear skin effect, gives a value of the weak charge of cesium that differs from that predicted by the Standard Model by about 2 standard deviations.