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QED effects in heavy few-electron ions

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Abstract

Accurate calculations of the binding energies, the hyperfine splitting, the bound-electron g-factor, and the parity nonconservation effects in heavy few-electron ions are considered. The calculations include the relativistic, quantum electrodynamic (QED), electron-correlation, and nuclear effects. The theoretical results are compared with available experimental data. A special attention is focused on tests of QED in a strong Coulomb field.

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1. Introduction

Accurate calculations of heavy few-electron ions must be performed in the framework of the rigorous quantum electrodynamic (QED) formalism. The basic methods of quantum electrodynamics were formulated to the beginning of 1930s, almost immediately after creation of quantum mechanics. This theory provided description of such low-order processes as emission and absorption of photons and creation and annihilation of electron-positron pairs. However, application of this theory to some higher-order effects gave infinite results. This problem remained unsolved until the late 1940's when Lamb and Retherford discovered the $2s - 2p_{1/2}$ splitting (Lamb shift) in hydrogen. This discovery stimulated theorists to complete the creation of QED since it was believed that this splitting is of quantum electrodynamic origin. First evaluation of the Lamb shift was performed by Bethe who used Kramer's idea of the mass renormalization. A consequent QED formalism was developed by Dyson, Feynman, Schwinger, and Tomonaga. They showed that all infinities can be removed from the theory by so-called renormalization procedure. The basic idea of this procedure is the following. The electron mass and the electron charge, which originally occur in the theory, are not directly measurable quantities. All physical quantities calculated within QED become finite if they are expressed in terms of the physical electron mass and charge, parameters which can directly be measured in experiment. All calculations in QED are based on the perturbation theory in the fine structure constant $\alpha \approx 1/137.036$. The individual terms of the perturbation series are conveniently represented by so-called Feynman diagrams.

Before the beginning of 1970s investigations of QED effects in atomic systems were mainly restricted to low-Z atoms such as hydrogen or helium (here and below, Z is the nuclear charge number). In these systems, in addition to the small parameter α, there is another small parameter, which is αZ. For this reason, all calculations of low-Z atoms were based on the expansion in α and αZ.

A great progress in experimental investigations of heavy few-electron ions, which was made for the last decades (see [1,2] and references therein), has required accurate QED calculations for these systems. Investigations of heavy few-electron ions play a special role in tests of quantum electrodynamics. This is due to two reasons. First, in contrast to low-Z atoms, the parameter αZ is not small and, therefore, the calculations must be performed without any expansion in αZ [3]. Second, in contrast to heavy neutral atoms, the electron-correlation effects can be calculated to high accuracy using pertubation theory in the parameter $1/Z$. For this reason, the QED effects are not masked by large electron-correlation effects, as is the case in neutral atoms. This provides an excellent opportunity to test QED at strong electric fields.

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The calculations of high-Z few-electron ions are generally based on perturbation theory. To zeroth order, one can consider that electrons interact only with the Coulomb field of the nucleus. The interelectronic-interaction and QED effects are accounted for by perturbation theory in the parameters $1/Z$ and α, respectively. This leads to quantum electrodynamics in the Furry picture. To formulate the perturbation theory for calculations of the energy levels, transition and scattering amplitudes, it is convenient to use the two-time Green function method [4]. For very heavy ions the parameter $1/Z$ becomes comparable with α and, therefore, all the corrections may be classified by the parameter α only. In the present paper, we consider the current status of these calculations.

Relativistic units ($\hbar = c = 1$) are used in the paper.

2. Binding energies in heavy few-electron ions

2.1. H-like ions

To calculate the binding energy in a hydrogenlike ion, we may start with the Dirac equation,

$$(\alpha \cdot \mathbf{p} + \beta m + V_{\rm C}(r))\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{1}$$

where $V_{\rm C}(r)$ is the Coulomb potential induced by the nucleus. For the point-nucleus case, this equation leads to the binding energy

$$E_{nj} - mc^2 = -\frac{(\alpha Z)^2}{2\nu^2}\frac{2}{1+(\alpha Z/\nu)^2+\sqrt{1+(\alpha Z/\nu)^2}}mc^2, \tag{2}$$

where $\nu = n + \sqrt{(j+1/2)^2-(\alpha Z)^2} - (j+1/2)$, n is the principal quantum number, and j is the total angular momentum. To get the binding energy to a higher accuracy, we have to evaluate the quantum electrodynamic and nuclear corrections.

The finite-nuclear-size correction can be obtained by solving the Dirac equation with the potential induced by an extended-charge nucleus and taking the difference between the energies for the extended and the point-nucleus model. This can be done either numerically (see, e.g., Ref. [5]) or analytically [6]. To a relative accuracy of $\sim 0.2\%$, in the range $Z = 1$–100 the finite-nuclear-size correction is given by the following approximate formulas [6]:

$$\Delta E_{ns} = \frac{(\alpha Z)^2}{10n}[1+(\alpha Z)^2 f_{ns}(\alpha Z)]\left(2\frac{\alpha Z}{n}\frac{R}{(\hbar/mc)}\right)^{2\gamma} mc^2, \tag{3}$$

$$\Delta E_{np_{1/2}} = \frac{(\alpha Z)^4}{40}\frac{n^2-1}{n^3}[1+(\alpha Z)^2 f_{np_{1/2}}(\alpha Z)] \times \left(2\frac{\alpha Z}{n}\frac{R}{(\hbar/mc)}\right)^{2\gamma} mc^2, \tag{4}$$

where $\gamma = \sqrt{1-(\alpha Z)^2}$,

$f_{1s}(\alpha Z) = 1.380 - 0.162\alpha Z + 1.612(\alpha Z)^2$,

$f_{2s}(\alpha Z) = 1.508 + 0.215\alpha Z + 1.332(\alpha Z)^2$,

$f_{2p_{1/2}}(\alpha Z) = 1.615 + 4.319\alpha Z - 9.152(\alpha Z)^2 + 11.87(\alpha Z)^3$,

and R is an effective radius of the nuclear charge distribution defined by

$$R = \left\{\frac{5}{3}\langle r^2\rangle\left[1-\frac{3}{4}(\alpha Z)^2\left(\frac{3}{25}\frac{\langle r^4\rangle}{\langle r^2\rangle^2}-\frac{1}{7}\right)\right]\right\}^{1/2}. \tag{5}$$

The corresponding formulas for other states can be found in Ref. [6]. We note that, in contrast to the nonrelativistic case where the corresponding correction is completely defined by the root-mean-square radius, in heavy ions the higher order moments of the nuclear charge distribution are required to determine the nuclear-size correction on a 1% accuracy level. For instance, in case of $Z = 92$ to gain the precision $\sim 0.2\%$, it is necessary to know the moment $\langle r^4\rangle$.

The next corrections one should take into account are the QED corrections of first order in α. They are determined by the self-energy (SE) and vacuum-polarization (VP) diagrams (Fig. 1a and b). The contribution of the self-energy diagram (Fig. 1a) combined with the corresponding mass counterterm is given by:

$$\Delta E = 2i\alpha\int_{-\infty}^{\infty}{\rm d}\omega\int{\rm d}\mathbf{x}_1\int{\rm d}\mathbf{x}_2\psi_a^\dagger(\mathbf{x}_1)\alpha^\mu G(E_a-\omega,\mathbf{x}_1,\mathbf{x}_2) \times D_{\mu\nu}(\omega,\mathbf{x}_1-\mathbf{x}_2)\alpha^\nu\psi_a(\mathbf{x}_2) - \delta m\int{\rm d}\mathbf{x}\overline{\psi}_a(\mathbf{x})\psi_a(\mathbf{x}) \tag{6}$$

Here $\psi_a(\mathbf{x})$ is the Dirac-Coulomb wave function of the state under consideration, $\overline{\psi} = \psi^\dagger\gamma_0$, $G(\omega,\mathbf{x}_1,\mathbf{x}_2)$ is the Coulomb Green function, $D_{\mu\nu}(\omega,\mathbf{x}_1-\mathbf{x}_2)$ is the photon propagator, $\alpha^\mu = (1,\alpha)$, and α is a vector incorporating the Dirac matrices. The first evaluation of the SE correction for heavy ions was performed by Desiderio and Johnson [7] who employed the method suggested by Brown, Langer, and Schaefer [8]. Later, Mohr [9] developed another method which allowed him to perform a high precision evaluation of this correction in the range $Z = 10$–110. An alternative approach to this problem was worked out in Refs. [10–12]. The most accurate calculations of the SE correction to all orders in αZ were performed by Mohr [13] and by Indelicato and Mohr [14] for the point-nucleus case and by Mohr and Soff [15] for the case of extended nuclei. The highest accuracy for low-Z ions was achieved by Jentschura et al. [16].

The formal expression for the vacuum-polarization correction (Fig. 1b) is given by

$$\Delta E = \frac{\alpha}{2\pi i}\int_{-\infty}^{\infty}{\rm d}\omega\int{\rm d}\mathbf{x}_1\int{\rm d}\mathbf{x}_2\psi_a^\dagger(\mathbf{x}_1)\frac{1}{|\mathbf{x}_1-\mathbf{x}_2|} \times [{\rm Tr}G(\omega,\mathbf{x}_2,\mathbf{x}_2)]\psi_a(\mathbf{x}_1). \tag{7}$$

This expression is ultraviolet divergent. It can be renormalized by dividing into two parts. The first part corresponds to the first

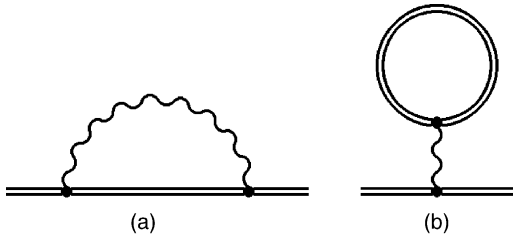

Fig. 1. First-order self-energy and vacuum-polarization diagrams.

nonzero term in the potential expansion of the Coulomb Green function in powers of αZ. This part, so-called Uehling part, becomes finite due to the charge renormalization and its evaluation causes no problem. The second part, so-called Wichmann–Kroll (WK) part, accounts for all higher order terms of the αZ-expansion. Despite this part being finite, the regularization is still needed due to a spurious gauge-dependent piece of the light-by-light scattering contribution. Calculations of the WK contribution in a wide range of Z were performed first by Soff and Mohr [17] for the extended nucleus case and by Manakov et al. [18] for the point-nucleus case. The most accurate results for some specific ions were obtained by Persson et al. [19].

The QED corrections of second order in α are determined by diagrams presented in Fig. 2. Most of these diagrams can be calculated using the methods developed for the first-order SE and VP corrections [20–26]. The most demanding problem is to evaluate the SE–SE diagrams [27] and the V(SE)P diagram (the diagram with a photon line inside the VP loop) [28]. The loop-after-loop SE–SE diagram was first evaluated by Mitrushenkov et al. [29]. A partial evaluation of the other SE–SE diagrams was performed by Mallampalli and Sapirstein [30]. The residual SE–SE terms were first calculated by Yerokhin and Shabaev [31]. Finally, in Refs. [32] the whole gauge invariant set of the SE–SE diagrams was evaluated in the range $Z = 10$–100. As to the S(VP)E diagram, to date it was evaluated only in the Uehling approximation [20,21].

The calculations discussed above are based on the approximation in which the nucleus is considered as a source of the external Coulomb field. It defines quantum electrodynamics within the external field approximation. The first step beyond this approximation would consist in evaluation of the nuclear recoil correction. As is known, in the nonrelativisic theory of a hydrogenlike atom the recoil effect can easily be taken into account by using the electron reduced mass $\mu = mM/(m + M)$. A rigorous relativistic theory of the recoil effect can be formulated only in the framework of QED. In case of a hydrogenlike atom, a closed formula for the recoil effect to first order in m/M and to all orders in αZ was derived in Ref. [33] (see also [34] and references therein). According to this formula, the recoil correction is given by the sum of a low-order term $\Delta E_{\rm L}$ and a higher order term $\Delta E_{\rm H}$, where

$$\Delta E_{\rm L} = \frac{1}{2M}\langle a|[\mathbf{p}^2 - (\mathbf{D}(0)\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{D}(0))]|a\rangle, \tag{8}$$

$$\Delta E_{\rm H} = \frac{i}{2\pi M}\int_{-\infty}^{\infty} {\rm d}\omega\, \langle a|\left(\mathbf{D}(\omega) - \frac{[\mathbf{p}, V_{\rm C}]}{\omega + i0}\right) \times G(\omega + E_a)\left(\mathbf{D}(\omega) + \frac{[\mathbf{p}, V_{\rm C}]}{\omega + i0}\right)|a\rangle. \tag{9}$$

Here $\mathbf{p}$ is the momentum operator, $G(\omega)$ is the Coulomb Green function, $D_m(\omega) = -4\pi\alpha Z\alpha_l D_{lm}(\omega)$, and $D_{ik}(\omega, r)$ is the transverse part of the photon propagator in the Coulomb gauge. In Eq. (9), the scalar product is implicit. The term $\Delta E_{\rm L}$ contains all the recoil corrections within the $(\alpha Z)^4 m^2/M$ approximation. For the point-nucleus case, it can easily be calculated analytically [33]

$$\Delta E_{\rm L} = \frac{m^2 - E_a^2}{2M}. \tag{10}$$

The term $\Delta E_{\rm H}$ contains the contribution of order $(\alpha Z)^5 m^2/M$ and all contributions of higher order in αZ which are not accounted for by the $\Delta E_{\rm L}$ term. Numerical evaluations of the recoil correction to all orders in αZ were performed in Refs. [35,36] for point and extended nuclei, respectively.

Finally, one should take into account the nuclear polarization correction, which sets the ultimate limit of accuracy up to which QED can be tested in atomic systems. This correction is determined by the electron–nucleus interaction diagrams in which the

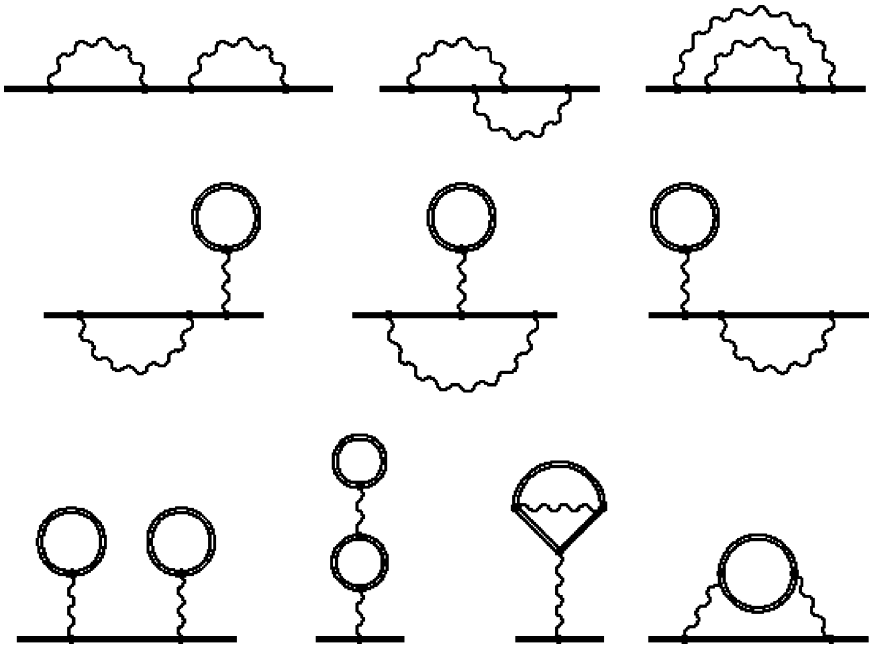

Fig. 2. Second-order one-electron Feynman diagrams.

Table 1
Individual contributions to the ground-state binding energy in $^{238}U^{91+}$, in eV

Point-nucleus binding energy	−132279.93(1)
Finite nuclear size	198.33(52)
First-order SE	355.05
First-order VP	−88.60
Second-order QED	−1.26(33)
Nuclear recoil	0.46
Nuclear polarization	−0.20(10)
Lamb shift theory	463.78(62)
Lamb shift experiment [41]	460.2(4.6)

The Lamb shift is defined as a part of the binding energy that is beyond its point-nucleus value given by Eq. (2).

intermediate states of the nucleus are excited. It was evaluated by Plunien and Soff [37] and by Nefiodov et al. [38].

The individual contributions to the ground-state binding energy in $^{238}U^{91+}$ are given in Table 1. The uncertainty of the Dirac binding energy comes from the uncertainty of the $R_\infty hc$ constant [39]. The finite-nuclear-size correction is evaluated for the Fermi model of the nuclear charge distribution with $\langle r^2\rangle^{1/2} = 5.8507(72)$ fm [40]. The uncertainty of this correction is estimated by adding quadratically two errors, one obtained by varying the root-mean-square radius and the other obtained by changing the model of the nuclear-charge distribution from the Fermi to the homogeneously-charged-sphere model. As one can see from the table, the present status of the theory and experiment on heavy H-like ions provides a test of QED on the level of about 2%.

2.2. Li-like ions

To date, the highest accuracy was achieved in experiments on the $2p_{1/2,3/2} - 2s$ transitions in heavy Li-like ions [42–45]. In these systems, in addition to the one-electron contributions discussed above, one has to evaluate two- and three-electron contributions. To first order in α, the two-electron contribution is determined by the one-photon exchange diagram (Fig. 3) whose calculation causes no problem. To second order in α, one should account for the two-photon exchange diagrams (Fig. 4) and the self-energy and vacuum-polarization screening diagrams (Fig. 5). The two-photon exchange diagrams were evaluated by different authors [46–50]. The results of these calculations are in a good agreement with each other. The complete calculation of

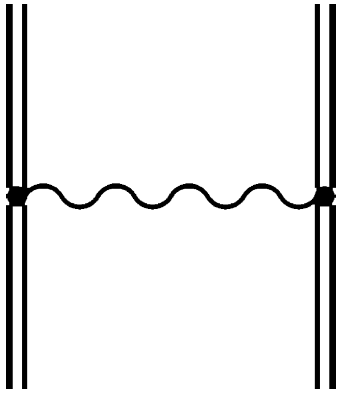

Fig. 3. One-photon exchange diagram.

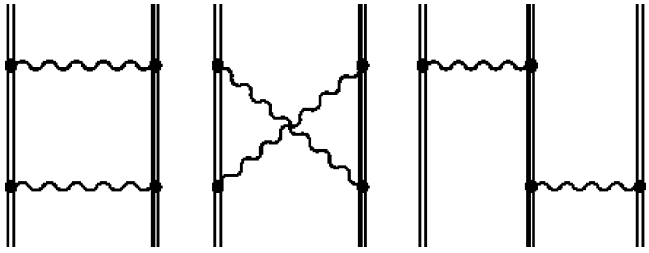

Fig. 4. Two-photon exchange diagrams.

the vacuum-polarization screening diagrams was performed in Ref. [51]. The self-energy screening diagrams were evaluated in Refs. [52,47]. To gain the accuracy required by the experiments, in addition to higher order one-electron QED corrections, one should evaluate the interelectronic-interaction corrections of third and higher orders in the parameter $1/Z$. Such evaluations within the framework of the Breit approximation were accomplished in Refs. [53,54,48].

The individual contributions to the $2p_{1/2} - 2s$ transition energy in Li-like uranium are presented in Table 2. The total theoretical value of the transition energy, 280.66(22) eV, agrees well with the related experimental values, 280.59(10) eV [42] and 280.52(10) eV [45]. Comparing the first- and second-order QED contributions, −42.93 eV and 1.45(18) eV, respectively, with the total theoretical and experimental uncertainties, we conclude that the present status of the theory for Li-like uranium provides

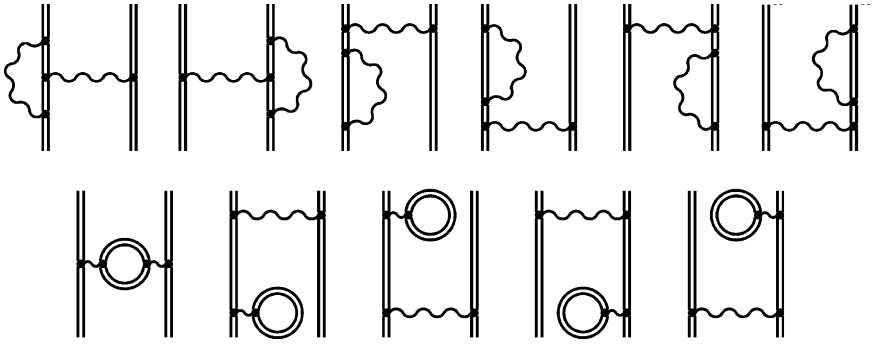

Fig. 5. Self-energy and vacuum-polarization screening diagrams.

Table 2
The $2p_{1/2} - 2s$ transition energy in $^{238}U^{89+}$, in eV

One-photon exchange	368.83
One-electron nuclear size	−33.27(8)
First-order QED	−42.93
Two-photon exchange within the Breit approximation	−13.54
Two-photon exchange beyond the Breit approximation	0.17
SE and VP screening	1.16
Three- and more photon exchange	0.16(7)
Nuclear recoil	−0.07
Nuclear polarization	0.03(1)
One-electron second-order QED	0.12(18)
Total theory	280.66(21)
Experiment [42]	280.59(10)
Experiment [45]	280.52(10)

a test of QED on a 0.5% level to first order in α and on a 15% level to second order in α.

2.3. He-like ions

In Refs. [55,56], the two-electron contribution to the ground-state energy of helium-like ions was measured. It was done by comparing the ionization energies of helium-like and hydrogen-like ions. This experiment is of special importance since to date the two-electron contribution is the only measured value which has been calculated to the second order in α. As in case of Li-like ions, the lowest order two-electron contribution is determined by the one-photon exchange diagram. The contributions of second order in α are given by the two-photon exchange diagrams and by the SE and VP screening diagrams. The two-photon exchange contribution was first evaluated by Blundell et al. [57] and by Lindgren et al. [58]. This contribution can be conventionally divided into two parts: one which corresponds to the Breit approximation and the other which is beyond the Breit approximation. The VP and SE screening diagrams for the ground-state were evaluated in Refs. [59–62]. The corresponding calculations for excited states of He-like ions were performed in Refs. [63–65,48,49,66,67].

In Table 3, we present the individual contributions to the two-electron binding energy of the ground-state in He-like uranium. The two-photon exchange contribution is divided into two parts as described above. The Breit contribution and the higher order QED corrections are evaluated as in Ref. [67]. As one can see from the table, to test the screened QED effects, the experimental precision should be improved by an order of magnitude.

Table 3
The two-electron binding energy of the ground state in $^{238}U^{90+}$, in eV

One-photon exchange	2265.90(1)
Two- and more photon exchange within the Breit approximation	−11.96
Two-photon exchange beyond the Breit approximation	−0.85
SE screening	−9.78
VP screening	2.63
Higher order QED	−0.05(18)
Total theory	2245.89(18)
Experiment [56]	2248(9)

3. Hyperfine splitting in heavy ions

High-precision measurements of the hyperfine splitting (HFS) in heavy hydrogen-like ions [68–72] have triggered a great interest to theoretical calculations of this effect. The ground-state hyperfine splitting of a hydrogen-like ion is conveniently written as [73]:

$$\Delta E_\mu = \frac{4}{3}\alpha(\alpha Z)^3 \frac{\mu}{\mu_N}\frac{m}{m_p}\frac{2I+1}{2I}mc^2 \times\{A(\alpha Z)(1-\delta)(1-\varepsilon)+x_{rad}\}. \quad (11)$$

Here m_p is the proton mass, μ is the nuclear magnetic moment, μ_N is the nuclear magneton, and I is the nuclear spin. $A(\alpha Z)$ denotes the relativistic factor

$$A(\alpha Z) = \frac{1}{\gamma(2\gamma-1)} = 1 + \frac{3}{2}(\alpha Z)^2 + \frac{17}{8}(\alpha Z)^4 + \cdots, \quad (12)$$

δ is the nuclear-charge distribution correction, ε is the nuclear magnetization distribution correction (so-called Bohr–Weisskopf correction), and x_{rad} is the QED correction. The most accurate calculations of the QED corrections were performed in Refs. [74–76]. The uncertainty of the theoretical predictions is mainly determined by the uncertainty of the Bohr–Weisskopf (BW) effect. In calculations, based on the single-particle nuclear model [73,77,74,78], which provide a reasonable agreement with the experiments (see, e.g., Ref. [4]), this uncertainty may amount up to about 100% of the BW effect and is generally larger than the total QED contribution. More elaborated calculations, based on many-particle nuclear models [79,80], do not provide a desirable agreement with the experiments.

A new method to determine the BW effect was recently developed in Ref. [81]. With this method, the BW correction to the hyperfine splitting in hydrogen-like ^{209}Bi, ^{203}Tl, and ^{205}Tl was determined using experimental data on the hyperfine splitting in the corresponding muonic atoms [82,83]. The parameters of the nuclear magnetization distribution were chosen to reproduce the experimental values of the nuclear magnetic moment as well as the BW effect in muonic atoms extracted from the corresponding experiments. The single-particle and configuration-mixing nuclear models were considered. To increase the precision of determining the BW contribution, the QED corrections for muonic atoms have been evaluated. In Table 4, the BW correction to the HFS in electronic H-like ions, derived from the experiments on muonic atoms, is compared with the BW correction obtained by direct calculations within the single- and many-particle nuclear models. Taking into account that the uncertainty of the

Table 4
The Bohr–Weisskopf correction ε, derived from experiments on muonic atoms [81], is compared with previous direct evaluations of this effect within the single-particle [77,78] and the many-particle [79,80] nuclear model

	$^{209}Bi^{82+}$	$^{205}Tl^{80+}$	$^{203}Tl^{80+}$
Elizarov et al. [81]	0.0123(15)	0.0193(27)	0.0155(40)
Shabaev [78]	0.0118	0.0179	0.0179
Labzowsky et al. [77]	0.0131		
Tomaselli et al. [79]	0.0210		
Sen'kov and Dmitriev [80]	0.0095(+7, −38)		

Table 5
Hyperfine splitting in H-like ions, in eV

	Theory [81]	Theory [78]	Experiment
$^{203}Tl^{80+}$	3.220(20)	3.229(17)	3.21351(25) [72]
$^{205}Tl^{80+}$	3.238(9)	3.261(18)	3.24410(29) [72]
$^{209}Bi^{82+}$	5.098(7)	5.101(27)	5.0840(8) [68]

single-particle results may amount up to 30–100%, we conclude that the ε values, based on experiments with muonic atoms, have a better accuracy.

In Table 5, we compare the total theoretical results for the HFS in H-like ions with experiment. As one can see from the table, the results based on experiments with muonic atoms are closer to the experimental ones, compared to the results based on the direct calculations within the single-particle nuclear model. However, due to a higher accuracy of the former results, a small discrepancy between the theory and experiment occurs for $^{209}Bi^{82+}$. It can also be seen that in case of two isotopes of Tl, the results of Ref. [81] are much closer to the related experimental values than in case of Bi. Since, in contrast to the Tl isotopes, the bismuth nucleus has a nonzero electric-quadrupole moment, one may expect that the discrepancy between the theory and experiment is caused by a large contribution of the electric-quadrupole splitting in muonic bismuth. It is known that the first-order electric-quadrupole splitting vanishes for s states. However, the second-order effect is nonzero and, in principle, it may be significant for muonic atoms. This is due to a relatively large role of the electric-quadrupole HFS interaction in muonic atoms compared to electronic ones. Our numerical evaluation of this effect showed that, whereas it changes the HFS in muonic bismuth by about −3.4 eV, it almost does not affect the BW value presented in Table 4.

One of the main goals of the HFS experiments with heavy H-like ions was to probe the magnetic sector of QED in the presence of a strong Coulomb field. The analysis of the theoretical results showed, however, that the QED corrections to the HFS in heavy H-like ions are strongly masked by the uncertainty of the BW effect. This makes unfeasible tests of QED by a direct comparison of theory and experiment on the HFS in heavy H-like ions. An opportunity for QED tests has been found by considering a specific difference of the ground-state HFS values in H- and Li-like ions [84]. Namely, it was shown that the difference

$$\Delta' E = \Delta E^{(2s)} - \xi \Delta E^{(1s)}, \tag{13}$$

where $\Delta E^{(1s)}$ and $\Delta E^{(2s)}$ are the HFS in H- and Li-like ions of the same isotope, is very stable with respect to variations of the nuclear model, if the parameter ξ is chosen to cancel the BW corrections in the right-hand side of Eq. (13). The parameter ξ is almost independent of the nuclear structure and, therefore, can be calculated to a high accuracy. In case of Bi, the calculations yield $\xi = 0.16885$ and $\Delta' E = -61.27(4)$. The non-QED and QED contributions amount to −61.52(4) and 0.24(1), respectively. It means that the QED contribution is six times larger than the current total theoretical uncertainty. This provides good perspectives for tests of QED in the HFS experiments. In particular, it can be shown that this method allows one to test QED on level of a few percent, provided the HFS is measured to accuracy $\sim 10^{-6}$.

4. Bound-electron g-factor

The g-factor of a hydrogenlike ion with a spinless nucleus can be defined as

$$g^{(e)} = -\frac{\langle JM_J|\mu_z^{(e)}|JM_J\rangle}{\mu_B M_J}, \tag{14}$$

where $\mu^{(e)}$ is the operator of the magnetic moment of electron and μ_B is the Bohr magneton. For the $1s$ state, a simple relativistic calculation based on the Dirac equation yields

$$g_D = 2 - \tfrac{4}{3}(1 - \sqrt{1-(\alpha Z)^2}). \tag{15}$$

The total g-factor value can be written as

$$g^{(e)} = g_D + \Delta g_{QED} + \Delta g_{rec} + \Delta g_{NS}, \tag{16}$$

where Δg_{QED} is the QED correction, Δg_{rec} is the nuclear recoil correction, and Δg_{NS} is the finite-nuclear-size correction. High-precision measurements of the bound-electron g-factor in H-like carbon [85,86] and oxygen [87] have stimulated successful theoretical calculations of this effect (see Refs. [88–94] and references therein). In particular, these studies provided a new determination of the electron mass to an accuracy which is four times better than that of the 1998 CODATA value. As a result, the 2002 CODATA value for the electron mass [39] is derived from the g-factor measurements. An extension of these experiments to higher-Z systems, which is anticipated in the near future, could lead also to an independent determination of the fine structure constant.

For heavy H-like ions the theoretical uncertainty of the bound-electron g-factor is mainly determined by the nuclear effects [91,93]. This uncertainty becomes comparable with the binding QED corrections of second order in α and, therefore, strongly restricts probing QED in these investigations. However, in Ref. [95], it was shown that the uncertainty caused by the nuclear effects can be significantly reduced in a specific difference of the g-factors of H- and Li-like ions of the same isotope. This gives a good opportunity for tests of the magnetic sector of QED in the presence of a strong Coulomb field. The most accurate calculations of the g-factor of Li-like ions in the range $Z = 6$–92 were performed in Ref. [96].

The g-factor of a H-like ion with nonzero nuclear spin can be approximated as

$$g = g^{(e)} \frac{F(F+1) + j(j+1) - I(I+1)}{2F(F+1)} - \frac{m}{m_p} g_I \frac{F(F+1) + I(I+1) - j(j+1)}{2F(F+1)}. \tag{17}$$

Here m and m_p are the electron and the proton mass, respectively, $g^{(e)}$ is the bound-electron g-factor defined above, $g_I = \mu/\mu_n I$ is the nuclear g-factor, $\mu_n = |e|/2m_{pc}$ is the nuclear magneton, j and I are the electron and the nucleus angular momentum, respectively, and F is the total angular momentum of the ion. According to formula (17), the contribution of the nuclear

Table 6
The bound-electron g-factor in $^{209}Bi^{82+}$

Point-nucleus Dirac value	1.7276
QED	0.0029
Nuclear size correction	0.0005
Total theory	1.7310
Experiment [99]	1.7343(33)

g-factor is suppressed by factor m/m_p compared to the electronic g-factor. It follows that measurements of the g-factor of ions with nonzero nuclear spin with a 10^{-9} accuracy would provide determinations of the nuclear magnetic moments on the 10^{-6} accuracy level. Calculations of various corrections to formula (17) were presented in Ref. [97].

Another possibility for investigations of the g-factor of ions with nonzero nuclear spin was discussed in Ref. [98]. In that work, it was shown that the transition probability between the ground-state hyperfine splitting components of a hydrogenlike ion, including the QED and nuclear corrections, is given by

$$w = \frac{\alpha}{3}\frac{\omega^3}{m^2}\frac{I}{2I+1}\left[g^{(e)} - g_I\frac{m}{m_p}\right]^2, \tag{18}$$

where ω is the transition frequency. Formula (18) allows one to calculate the QED and nuclear corrections to the transition probability using the corresponding corrections to the bound-electron g-factor. In particular, it was found [98] that in cases of Pb and Bi, the QED and nuclear corrections increase the transition probability by about 0.3%. In Ref. [99], the life time of the upper hyperfine splitting component in $^{209}Bi^{82+}$ was measured to be $\tau_{exp} = 397.5(1.5)$ μs. This result is in a good agreement with the theoretical prediction [98] $\tau_{theo} = 399.01(19)$ μs. Using formula (18) and the experimental values of the hyperfine splitting and the transition probability in $^{209}Bi^{82+}$ [68,99], one finds the experimental value of the bound-electron g-factor in Bi to be 1.7343(33). The corresponding theoretical value is 1.7310. The values of the individual contributions to the bound-electron g-factor in Bi are given in Table 6. From this table, it can be seen that the QED correction is needed to obtain agreement between the theory and experiment.

5. Parity nonconservation effects with heavy ions

Investigations of parity nonconservation (PNC) effects in atomic systems play a prominent role in tests of the Standard Model (SM) [100]. The well-known cesium experiment by Wieman's group [101], compared to the most elaborated theoretical result (see Ref. [102] and references therein), provided the most accurate test of electroweak theory at the low-energy regime. Further improvement of tests of the Standard Model with neutral atoms, from theoretical side, is mainly limited by difficulties with accurate calculations of the electron-correlation effects. For this reason, the PNC experiments with heavy few-electron ions, where the electron-correlation effects can be evaluated to a high accuracy, seem highly desirable. The PNC effects in these systems were first discussed in Refs. [103–105]. For tests of the spin-independent part of the week interaction, a promising situation occurs in heavy He-like ions with the nuclear-charge number near $Z = 64$ and $Z = 92$, where two levels of the opposite parity, 2^1S_0 and 2^3P_0, are very close to each other. The study of PNC effects with these ions requires precise knowledge of the $2^1S_0 - 2^3P_0$ energy difference. The most accurate calculations of this difference, which include a complete set of two-electron QED corrections, were performed in Ref. [67]. In Table 7, the results of Ref. [67] are compared with the related data by other authors.

Table 7
The $2^3P_0 - 2^1S_0$ transition energy, in eV

Z	Artemyev et al. [67]	Andreev et al. [49]	Plante et al. [106]	Drake [107]
63	−0.224(69)	−0.591		−0.168
64	0.004(74)	−0.389	−0.170	0.067
65	0.32(12)	−0.153		0.328
66	0.495(84)	0.016	0.341	0.614
89	1.61(46)			1.731
90	0.61(46)		−0.095	0.718
91	−0.31(55)	−1.971		−0.209
92	−2.64(28)	−4.511	−2.639	−1.816

A feasible PNC experiment with heavy ions was suggested by Labzowsky et al. [108]. Instead of the standard measurement of the circular dichroism which is rather difficult to perform with X-ray radiation, it was proposed to study a one-photon $2^1S_0 - 1^1S_0$ transition in polarized He-like ions near $Z = 64$, where the 2^1S_0 and 2^3P_0 levels are almost degenerate. A one-photon M1 transition from 2^1S_0 to 1^1S_0 is possible through hyperfine induced mixing between the 2^1S_0 and 2^3S_1 levels. An additional possibility is admixture of the 2^3P_1 level due to the combined effects of weak interaction (mixing 2^1S_0 and 2^3P_0) and hyperfine interaction (mixing 2^3P_0 and 2^3P_1). As a result, the total amplitude of the one-photon $2^1S_0 - 1^1S_0$ transition is a mixture of the basic M1 and the additional E1 amplitude. However, if the lifetime of the 2^1S_0 state, which is mainly defined by the 2E1 two-photon transition to the ground-state, is comparable or smaller than the 2^3P_0 lifetime, a strong background may occur in the experiment. This is the case for gadolinium ($Z = 64$) but not for europium ($Z = 63$), where the 2^1S_0 level lives significantly longer than the 2^3P_0 level. For this reason, experiments with Eu^{61+} ions seem more promising [108].

The polarization of the ion in the 2^1S_0 state can be described by the density matrix [108]

$$\rho = \frac{1}{2I+1}\left[1 + \frac{3\lambda_0}{I+1}(\boldsymbol{\nu}\cdot\mathbf{I})\right], \tag{19}$$

where $\mathbf{I}$ is the operator of the total angular momentum, ν is the unit vector directed along the ion polarization, and λ_0 is the degree of polarization ($\lambda_0 \le 1$). The probability for the emission of a photon in direction $\mathbf{n}$ is given by [108]

$$dW(\mathbf{n}) = \frac{W_{M1}}{4\pi}[1 + \varepsilon(\boldsymbol{\nu}\cdot\mathbf{n})]d\Omega, \tag{20}$$

where W_{M1} is the total probability of the hfq M1 $2^1S_0 - 1^1S_0$ transition and ε is the asymmetry coefficient caused by the PNC effects. Our evaluation of this coefficient yields

$$\varepsilon = 6\lambda_0\frac{\sqrt{W_{E1}/W_{M1}}}{I+1}, \tag{21}$$

where W_{E1} is the total probability of the weak-hyperfine quenching E1 $2^1S_0 - 1^1S_0$ transition. We note that expression (21) differs by about a factor of 2 from the related expression derived in Ref. [108].

The experiment should consist in observing the difference of the transition probability (20) due to a change of the ion polarization direction or, equivalently, due to rotating the detector around the beam direction by an angle π. The value of this difference is proportional to the asymmetry parameter ε. Our calculation of this parameter for europium employing the transition energies from Ref. [67] (see Table 7) yields $\varepsilon \approx 0.0004\lambda_0$. This value is almost four times larger compared to that obtained in Ref. [108]. This is due to a change of the $2^1S_0 - 2^3P_0$ energy difference, compared to that used in Ref. [108], and due to the change of the expression for ε discussed above.

The experiment under consideration requires preparing and storing a polarized ion beam. A promising idea for preparation of polarized ion beams was suggested in Ref. [109].

6. Conclusion

In this paper we have considered the present status of calculations of the QED effects in heavy few-electron ions. Calculations of the PNC effects for heavy ions have also been discussed.

To date, the most accurate tests of QED effects on binding energies in a strong Coulomb field have been accomplished in heavy Li-like ions: on a 0.5% accuracy level to first order in α and on a 15% accuracy level to second order in α. An improvement of the experimental accuracy by an order of magnitude accompanied by more accurate determinations of higher order QED and nuclear-size effects would provide tests of QED beyond the external field approximation.

The theoretical value of the ground-state hyperfine splitting in H-like Bi, with the Bohr–Weisskopf correction determined using experimental data on the HFS in muonic Bi, deviates by 2σ from the corresponding experimental value. Taking into account the second-order electric-quadrupole HFS in muonic Bi, that was accomplished in the present paper, has not reduced this discrepancy.

High-precision measurements of the hyperfine splitting in heavy H- and Li-like ions of the same isotope are highly desirable. They would give a unique opportunity for tests of the magnetic sector of QED in the strongest electric field currently available for experimental study.

The QED theory of the bound-electron g-factor has been probed by direct measurements on hydrogen-like carbon and oxygen. These measurements have also provided a new determination of the electron mass with an accuracy which is four times better than that of the previously accepted value. Extentions of these measurements to higher-Z systems and to ions with nonzero nuclear spin would provide independent determinations of the fine structure constant and the nuclear magnetic moments.

Investigations of the PNC effects with heavy ions seem very promising for tests of the Standard Model. A new evaluation of the hyperfine- and weak-quenched one-photon transitions in He-like europium, performed in this paper, has lead to a four times increase of the PNC effect, compared to previous calculations.

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