Radiative corrections to hydrogenlike ions and heavy alkali-metal atoms in a magnetic field

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A fully covariant scheme of renormalization is developed for the evaluation of radiative corrections to the energy levels of atoms and ions in an external magnetic field. Bound-state QED corrections to g factors are calculated for H-like ions in the ground state with nuclear charge numbers $1 \leqslant Z \leqslant 90$ and for the ns valence electrons in the atoms Cs, Ba^+, and Fr. It is shown that these corrections should be taken into account in the comparison with experimental data for neutral atoms.

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I. INTRODUCTION

The evaluation of quantum electrodynamical (QED) effects for highly charged ions (HCI) in an external magnetic field, i.e., the QED corrections to the g factors of bound electrons has been the topic of intensive experimental [1–4] and theoretical [5–8] investigations during the last years. In hydrogenlike HCI the QED corrections play a dominant role and their investigation is important for testing bound-state QED in strong fields. In Ref. [9] it has been pointed out that QED corrections could be also nonnegligible for ns valence electrons in heavy alkali atoms.

First calculations of the electron self-energy (SE) corrections to the bound-electron g factors in H-like ions have been performed within the framework of the partial-wave renormalization (PWR) method developed in Ref. [10,11]. However, later it has been observed that the PWR approach when being applied to the evaluation of the SE correction for a bound electron in an additional external field, considered as a perturbation, generates the so-called ''spurious'' terms, arising due to the ''noncovariant'' character of the PWR approach [12]. The PWR procedure consists of the partial-wave expansion of the SE contribution and of the corresponding counterterm. Then both expansions are subtracted term by term leading finally to a finite, renormalized expression for the energy shift. For the lowest-order electron SE (without additional external fields) this procedure has been shown to converge to the correct limit, but for the SE in the presence of an additional external field, according to Ref. [12], finite ''spurious'' terms arise. An explicit expression for such ''spurious'' terms has been provided in Ref. [12]. In the case of a Coulombic external perturbation these ''spurious'' terms cancel between the different contributions to the perturbation-theory (PT) corrections to SE matrix elements: the corrections to the wave functions, the vertex, and the reference-state correction. This conclusion has been confirmed later by numerical evaluations [13] for additional perturbations to the central Coulomb potential.

In Ref. [12] it has also been stated that in the case of an external magnetic field the ''spurious'' terms in perturbation theory do not cancel and that some ''spurious'' contribution remains after collecting all the contributions.

The situation with the ''spurious'' terms has been clarified in Ref. [14], where it has been proven that these terms result from an improper treatment of the unphysical high-energy contribution. Utilizing the nonperturbative method for performing the PWR with the B-spline approximation to the Dirac spectrum in an external magnetic field, it was shown that no ''spurious'' terms are generated in numerical calculations of the SE in the magnetic field within a level of accuracy of about 0.1%. Still one has to be careful with the high-energy region when performing PWR calculations.

The ''spurious'' terms problem does not occur within an another approach to the evaluation of the electron SE in an external field [6–8], which is called ''covariant'' contrary to the PWR procedure that is performed noncovariantly in coordinate space. Within the covariant approach all the Feynman graphs, corresponding to the SE in an external field are expanded in powers of the Coulomb potential of the nucleus. The terms of this expansion [zero-potential (ZP) and one-potential (OP) terms] containing ultraviolet divergences are explicitly isolated. These divergent terms are renormalized covariantly in momentum space by standard QED methods developed for free electrons. All higher-order terms of the potential expansion (the many-potential term) are convergent and can be evaluated directly in coordinate space. In Refs. [6–8], they were calculated as the difference between the unrenormalized initial expression for the SE and unrenormalized zero-potential and one-potential terms.

Contrary to this the many-potential term is evaluated directly in the present paper.

The corrections for ns valence electrons in alkali-metal atoms have been estimated earlier in Ref. [9] by defining an effective nuclear charge number Z_{eff} and comparing the QED corrections in the magnetic field with values in HCI. In the present paper these corrections are obtained by direct calculations.

The paper is organized as follows: In Sec. II we formulate the problem of the evaluation of radiative corrections to the bound-electron g factor and analyze different types of corrections. Section III is devoted to the covariant regularization of the nondiagonal matrix elements for the ZP and OP terms of the electron SE. In Sec. IV, the evaluation of the many-potential (MP) term for the nondiagonal electron SE is con-

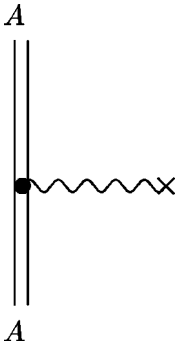

FIG. 1. The Feynman graph describing the interaction of the atomic electron in state A with the external field. The double solid line denotes the bound electron and wavy line with the cross at the end denotes the external field.

sidered. The results of Sec. III are employed in Sec. V for the evaluation of the SE correction to the wave function in the magnetic field and partly for the vertex correction in the magnetic field. The remainder of the vertex correction (which is ultraviolet and infrared finite) is calculated with the help of a nonperturbative approach in Sec. VI. In Sec. VII the numerical results for H-like ions are provided in comparison with results of different existing calculations. In Sec. VII the radiative corrections to the g factors for ns electrons in alkali-metal atoms are determined and the role of these corrections in modern bound-electron g-factor calculations for heavy atoms is analyzed.

II. RADIATIVE CORRECTIONS TO THE BOUND-ELECTRON g FACTOR

The magnetic dipole moment $\vec{\mu}$ of a bound electron is connected with its total angular momentum $\vec{j}$ by

$$\vec{\mu}=-g_j\frac{e}{2m}\vec{j}=-g_j\frac{\mu_B}{\hbar}\vec{j}, \tag{1}$$

where e is the electron charge $(e>0)$, m is the electron mass, μ_B is the Bohr magneton, and g_j is the gyromagnetic ratio. For an electron in an ns state, g_j coincides with the bound-electron g factor.

The energy correction for a bound electron in the state A in an external magnetic field $\vec{B}$ reads

$$E_A(B)=-\langle A|\vec{\mu}\cdot\vec{B}|A\rangle. \tag{2}$$

The same quantity can be expressed also using the vector potential $\vec{A}$ for an external field:

$$E_A(B)=\langle A|\vec{\alpha}\cdot e\vec{A}|A\rangle, \tag{3}$$

where $\vec{\alpha}$ is the Dirac matrix. We use here relativistic units $m=c=\hbar=1$. Expression (3) corresponds to the Feynman graph is shown in Fig. 1.

In the case of a homogeneous magnetic field

$$\vec{A}=-\frac{1}{2}(\vec{r}\times\vec{B}), \tag{4}$$

where $\vec{r}$ is the radius vector for an electron in an atom. Considering a static field aligned in the z direction and using Eqs. (1)–(3), we obtain the expression for the g factor of a bound ns electron, first derived by Breit [15]:

$$g^{\rm bound}=\frac{2}{\mu_B B_z}\langle A|\vec{\alpha}\cdot e\vec{A}|A\rangle. \tag{5}$$

This value differs from the free-electron value $g^{\rm free}=2$, which follows from the Dirac equation. The radiative corrections change the value $g^{\rm free}_{\rm rad}$ [16] as

$$g^{\rm free}_{\rm rad}=2.002\,319\,304\,386(20), \tag{6}$$

where

$$\delta g^{\rm free}_{\rm QED}=2319.30\times10^{-6} \tag{7}$$

is the QED correction to the free-electron g factor. The major part of $\delta g^{\rm free}_{\rm QED}$ is incorporated in the Schwinger term:

$$\delta g^{\rm free}_{\rm Sch}=\frac{\alpha}{\pi}=2322.82\times10^{-6}. \tag{8}$$

The bound-electron corrections to the g factor are defined as $\delta g=g^{\rm bound}-g^{\rm free}$. In particular, the relativistic correction $\delta g_{\rm rel}$ is defined as the difference between the value of Eq. (5) and $g^{\rm free}=2$ [15]. The integration over the angles in Eq. (5) yields

$$\delta g_{\rm rel}=\frac{4}{3}\int_0^\infty dr\ \ g_{ns}(r)rf_{ns}(r)-2, \tag{9}$$

where $g_{ns}(r)$ and $f_ns(r)$ are the upper and the lower radial Dirac wave functions for the ns electron, normalized to

$$\int_0^\infty dr\ \ [g^2_{ns}(r)+f^2_{ns}(r)]=1. \tag{10}$$

The inclusion of bound-state QED corrections requires the evaluation of the contribution from the Feynman graphs given in Fig. 2. The Figs. 2(a) and 2(b) correspond to the electron self-energy corrections to the wave function (SE-WF), Fig. 2(c) represents the vertex correction (VER). Figures 2(d)–2(f) describe the vacuum polarization corrections (VP).

For Figs. 2(a) and 2(b), apart from the renormalization problem, there is a problem of treating the singularity connected to the presence of the reference state A in the summations over intermediate electron states. This reference-state problem is usually treated within the framework of the adiabatic S-matrix approach due to Gell-Mann and Low [17], as generalized by Sucher [18]. This approach has been applied first to the bound-state QED problems in Ref. [19]. A detailed description of this approach can be found in Ref.

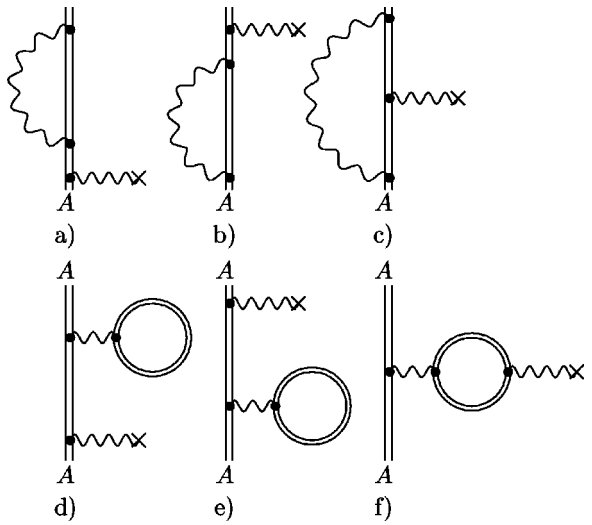

FIG. 2. The Feynman graphs corresponding to the lowest-order QED corrections to the interaction of the bound electron with the external field. The wavy line denotes the virtual photon. The other symbols are explained in Fig. 1.

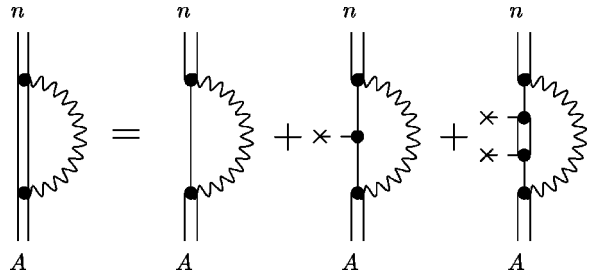

FIG. 3. Graphical representation of the electron self-energy regularization. The dashed line with the cross of the end denotes the nuclear Coulomb potential V. The other notations are the same as in Figs. 1 and 2. The indices A, n correspond to the two different atomic states.

[20]. An other QED methods for solving the same problem are the Green function method [21] and the line profile approach [22,23].

It is convenient to divide the contribution of Figs. 2(a) and 2(b) into two parts, namely irreducible and reducible ones. The irreducible part contains no reference state A in the sums over intermediate electron states. The calculation of the reducible part should be combined with the calculation of the vertex contribution.

The total bound-state QED correction consists of the following contributions:

$$\delta g^{\rm bound}_{\rm QED} = \delta g^{\rm bound}_{\rm SE\text{-}WF,irr} + \delta g^{\rm bound}_{\rm SE\text{-}WF,red} + \delta g^{\rm bound}_{\rm VER} + \delta g^{\rm bound}_{\rm VP}. \tag{11}$$

The irreducible SE-WF contribution to the g factor of the bound electron reads

$$\delta g^{\rm bound}_{\rm SE\text{-}WF,\,irr} = \frac{2}{\mu_B B_z} \sum_{n\neq A} \frac{(\hat{\Sigma}^{\rm ren}(E_A))_{An}(\vec{\alpha}\cdot e\vec{A})_{nA} + (\vec{\alpha}\cdot e\vec{A})_{An}(\hat{\Sigma}^{\rm ren}(E_A))_{nA}}{E_A - E_n}, \tag{12}$$

where $\hat{\Sigma}^{\rm ren}(E_A)$ is the renormalized expression for the lowest-order electron self-energy operator and $\hat{F}_{An}$ denotes a matrix element $A|\hat{F}|n$. The evaluation of the matrix element of $\hat{\Sigma}^{\rm ren}(E_A)$ will be considered in Secs. III–V. The evaluation of $\delta g^{\rm bound}_{\rm SE\text{-}WF,red}$ and $\delta g^{\rm bound}_{\rm VER}$ will be discussed in Secs. IV–VI.

Let us now turn to $\delta g^{\rm bound}_{\rm VP}$. The contribution of the Figs. 2(d) and 2(e) resembles Eq. (12), but the matrix elements of the electron self-energy operator $\hat{\Sigma}^{\rm ren}$ are replaced by the matrix elements of the vacuum polarization operator $\hat{\Pi}^{\rm ren}$:

$$\delta g^{\rm bound}_{\rm VP} = \frac{2}{\mu_B B_z} \times \sum_{n\neq A} \frac{(\hat{\Pi}^{\rm ren})_{An}(\vec{\alpha}\cdot e\vec{A})_{nA} + (\vec{\alpha}\cdot e\vec{A})_{An}(\hat{\Pi}^{\rm ren})_{nA}}{E_A - E_n}. \tag{13}$$

Since the operator $\hat{\Pi}^{\rm ren}$ does not depend on energy, there is no reducible VP contribution.

For the evaluation of the correction (13), we employ the commonly used Uehling approximation in which the polarization operator is replaced by the Uehling potential:

$$\hat{\Pi}^{\rm ren} \approx V_{\rm Uehl} = -\frac{2\alpha Z}{3\pi r}\int_0^\infty e^{-2r\chi}\left(1+\frac{1}{\chi}\right)\frac{\sqrt{\chi^2+1}}{\chi^2}\,d\chi. \tag{14}$$

Expression (14) is written in atomic units. The Uehling approximation is valid with an inaccuracy of about 10% when calculating energy levels of H-like ions for all Z values up to $Z=92$. The same holds true for the VP corrections to the bound-electron g factor [8].

The Uehling contributions to Fig. 2(f) is exactly zero [5]. Neglecting again the high-order terms, we omit thus fully the contribution of Fig. 2(f).

The purpose of this paper is twofold. First, we check the MP contribution to $\delta g^{\rm bound}_{\rm SE\text{-}WF,red}$ and $\delta g^{\rm bound}_{\rm VER}$ that has not yet been calculated fully covariantly. Second, we check the estimates for $\delta g^{\rm bound}_{\rm QED}$ given earlier in Ref. [9] for ns valence electrons in alkali-metal atoms. For both these purposes an accuracy of 10% would be rather sufficient: (1) the noncovariantly calculated part of the MP contribution to $\delta g^{\rm bound}_{\rm QED}$ is

relatively small and (2) other than $\delta g^{\rm bound}_{\rm QED}$, corrections to the bound-electron g factors in alkali-metal atoms are not known with accuracy higher than 0.1 $\delta g^{\rm bound}_{\rm QED}$.

Therefore, we accept the Uehling approximation for $\delta g^{\rm bound}_{\rm VP}$ and do not repeat the known results for H-like ions in this approximation. For alkali-metal atoms the numerical results for $\delta g^{\rm bound}_{\rm VP}$ have been elaborated in Refs. [9,14].

III. REGULARIZATION OF THE NONDIAGONAL SE MATRIX ELEMENT

The divergences in the SE operator can be isolated by expanding the electron propagator in powers of the nuclear Coulomb potential V. The structure of this expansion can be presented in the form

$$\frac{1}{z-\hat{h}_{\rm bou}(1-i0)}=\frac{1}{z-\hat{h}_{\rm free}(1-i0)}+\left(\frac{1}{z-\hat{h}_{\rm free}(1-i0)}\right)V\left(\frac{1}{z-\hat{h}_{\rm free}(1-i0)}\right)+\left(\frac{1}{z-\hat{h}_{\rm free}(1-i0)}\right)V\left(\frac{1}{z-\hat{h}_{\rm bou}(1-i0)}\right)V\left(\frac{1}{z-\hat{h}_{\rm free}(1-i0)}\right), \tag{15}$$

where $\hat{h}_{\rm bou}$ and $\hat{h}_{\rm free}$ denote the Dirac operators for the bound and the free electron, respectively.

This expansion in the Feynman graph representation is depicted in Fig. 3 for the nondiagonal matrix element of the electron self-energy operator $\hat{\Sigma}$. The first term of the expression (15) is called usually the ZP term, the second term is the OP term, and the third term is the MP term. All divergences are contained in the ZP and the OP terms, the MP term is finite.

Let us write down explicitly the renormalized expressions for the matrix elements $(\hat{\Sigma}^{\rm ren}_{\rm ZP}(E_A))_{An}$ and $(\hat{\Sigma}^{\rm ren}_{\rm OP}(E_A))_{An}$, following Refs. [24–26]. Then in the Feynman gauge

$$(\hat{\Sigma}^{\rm ren}_{\rm ZP}(E_A))_{An}=-\frac{\alpha}{(4\pi)^2}\int d^3p\,\Psi^+_A(\vec{p})\,\gamma_0\hat{\Sigma}_R(\vec{p},E_A)\Psi_n(\vec{p}), \tag{16}$$

where $\hat{\Sigma}_R$ is the free-electron self-energy operator off the mass shell:

$$\hat{\Sigma}_R(\vec{p},E_A)=(\not{p}-m)\left[2+\frac{\rho}{1-\rho}\left(1+\frac{2-\rho}{1-\rho}\ln\rho\right)\right]+\frac{\rho m}{1-\rho}\times\left(1-\frac{2-\rho}{1-\rho}\ln\rho\right)+(\not{p}-m)\ln\frac{\lambda^2}{m^2}. \tag{17}$$

Here $\not{p}=p_\mu\gamma^\mu$, $\rho=\rho(\vec{p},E_A)=(m^2-E_A^2+p^2)/m^2$, and λ is the fictitious photon mass that indicates the infrared divergence. This divergence arises in the expression for $\hat{\Sigma}_R(\vec{p},E_A)$ after renormalization.

The OP contribution can be expressed as

$$(\hat{\Sigma}^{\rm ren}_{\rm OP}(E_A))_{An}=-\frac{\alpha^2 Z}{(4\pi)^2}\int d^3p\,d^3q\,\Psi^+_A(\vec{p})\,\gamma_0\times\Lambda^0_R(\vec{p}E_A,\vec{q}E_A)\frac{1}{(\vec{p}-\vec{q})^2}\Psi_n(\vec{q}), \tag{18}$$

where Λ^0_R is the free-electron vertex part off the mass shell:

$$\Lambda^0_R(\vec{p}E_A,\vec{q}E_A)=\tilde{\Lambda}^0_R(\vec{p}E_A,\vec{q}E_A)+\ln\frac{\lambda^2}{m^2}. \tag{19}$$

The infrared divergences in $(\hat{\Sigma}^{\rm ren}_{\rm ZP}(E_A))_{An}$ and $(\hat{\Sigma}^{\rm ren}_{\rm OP}(E_A))_{An}$ contributions cancel due to the Ward identity and the Dirac equation [25,26].

The expression for $\tilde{\Lambda}^0_R(\vec{p}E_a,\vec{q}E_a)$, which is most convenient for numerical evaluations has been taken from [8,26]:

$$\begin{aligned}\Lambda^0_R(\vec{p}E,\vec{q}E)=\gamma_0[4\tilde{C}_{24}-2+2m_e^2C_0-4pp'(C_0+C_{11}+C_{12}+C_{23})-2p^2(C_{11}+C_{21})-2p'^2(C_{12}+C_{22})]+\not{p}p_0[4(C_{11}\\+C_{21})]+\not{p}p'_0[4(C_0+C_{11}+C_{12}+C_{23})]+\not{p}'p_0[4(C_0+C_{11}+C_{21}+C_{23})]+\not{p}'p'_0[4(C_{12}+C_{22})]\\-\not{p}\gamma_0\not{p}'[2(C_0+C_{11}+C_{12})]-p_0[4m_e(C_0+2C_{11})]-p'_0[4m_e(C_0+C_{12})].\end{aligned} \tag{20}$$

Here C_0, C_{ij} denote the Feynman parameter integrals:

$$m^2 C_0 = \int_0^1 dy \frac{1}{a} \ln\left(\frac{a+b}{b}\right), \tag{21}$$

$$m^2 C_{11} = -\int_0^1 dy \frac{y}{a}\left[1 - \frac{b}{a}\ln\left(\frac{a+b}{b}\right)\right], \tag{22}$$

$$m^2 C_{12} = -\int_0^1 dy \frac{1-y}{a}\left[1 - \frac{b}{a}\ln\left(\frac{a+b}{b}\right)\right], \tag{23}$$

$$m^2 C_{21} = \int_0^1 dy \frac{y^2}{a}\left[\frac{1}{2} - \frac{b}{a} + \left(\frac{b}{a}\right)^2 \ln\left(\frac{a+b}{b}\right)\right], \tag{24}$$

$$m^2 C_{22} = \int_0^1 dy \frac{(1-y)^2}{a}\left[\frac{1}{2} - \frac{b}{a} + \left(\frac{b}{a}\right)^2 \ln\left(\frac{a+b}{b}\right)\right], \tag{25}$$

$$m^2 C_{23} = \int_0^1 dy \frac{y(1-y)}{a}\left[\frac{1}{2} - \frac{b}{a} + \left(\frac{b}{a}\right)^2 \ln\left(\frac{a+b}{b}\right)\right], \tag{26}$$

$$m^2 C_{24} = \frac{1}{4}\left\{1 - \int_0^1 dy \frac{b}{a}\left[1 - \frac{b}{a}\ln\left(\frac{a+b}{b}\right)\right] - \int_0^1 dy \ln(a+b)\right\}, \tag{27}$$

in relativistic units $p_0 = q_0 = E_A$. Here $b = y\rho - (1-y)\rho'$ and $a + b = 1 - y(1-y)k^2/m^2$, where $k^2 = (\vec{p} - \vec{q})^2$ and ρ was defined in Eq. (17) [$\rho' = (m^2 - E_A^2 + q^2)/m^2$]. A different (equivalent) expression for Λ_R^0 was employed in Ref. [27].

While the numerical calculation of the integrals in Eqs. (16) and (18) was performed by means of standard integration methods, the wave functions in momentum space have to be generated at first via Fourier transformation of the *B*-spline representation of the coordinate-space wave function. The integrals in Eqs. (21)–(27) were evaluated by means of the Gaussian method with 32 integration points.

IV. THE MP CONTRIBUTION TO THE NONDIAGONAL SE MATRIX ELEMENT

The expression for the MP contribution to the nondiagonal SE matrix element is

$$(\hat{\Sigma}^{\rm ren}_{\rm OP}(E_A))_{An} = -\frac{\alpha}{\pi}\sum_m \int_0^\infty dw\, {\rm Re}\left\{\sum_n \frac{1}{E_a - E_m - iw} \times \int d^3r_1 d^3r_2\, \phi_m^+(-w,\vec{r}_1)\Psi_A(\vec{r}_2)\frac{1 - \vec{\alpha}_1\vec{\alpha}_2}{r_{12}} \times \exp(-wr_{12})\Psi_n(\vec{r}_1)\phi_m(w,\vec{r}_2)\right\}. \tag{28}$$

Here the sum over m is extended over the total Dirac spectrum for the bound electron, $r_{12} = |\vec{r}_1 - \vec{r}_2|$ and $\vec{\alpha}_i$ are the Dirac matrices acting on the different wave functions. The function $\phi_m(w,\vec{r})$ is defined as

$$\phi_m(w,\vec{r}) = \sum_\nu \frac{(V(\vec{r}))_{\nu m}}{E_a - E_\nu - iw}\Psi_\nu(\vec{r}), \tag{29}$$

where the sum over ν is the extended over the total Dirac spectrum for the free electron, $\Psi_\nu(\vec{r})$ and E_ν denote the eigenfunctions and the eigenvalues for the free-electron Dirac equation.

The triple summation over the total Dirac spectrum in Eq. (28) (two summations over the free-electron spectrum and one summation over the bound-electron spectrum) were performed with the use of the *B*-spline approach [28]. The free-electron spectrum was obtained from the bound-electron spectrum with $Z = 0$. The number of grid points was 150 and the order of splines was equal to 8.

V. EVALUATION OF $\delta g^{\rm bound}_{\rm SE\text{-}WF}$ AND $\delta g^{\rm bound}_{\rm VER}$

We begin with the evaluation of $\delta g^{\rm bound}_{\rm SE\text{-}WF,irr}$ by the insertion of the expressions $(\hat{\Sigma}^{\rm ren}_{\rm ZP}(E_A))_{An}$, $(\hat{\Sigma}^{\rm ren}_{\rm OP}(E_A))_{An}$ and $(\hat{\Sigma}^{ren}_{\rm MP}(E_A))_{An}$, obtained in Secs. III and IV, in Eq. (12). Most easily this calculation is performed by introducing the wave function

$$\tilde{\Psi}_A(\vec{r}) = \sum_{n(E_a \neq E_n)} \frac{(e\vec{\alpha}\vec{A}(\vec{r}))_{An}}{E_A - E_n}\Psi_n(\vec{r}). \tag{30}$$

Then Eq. (12) reduces to

$$\delta g^{\rm bound}_{\rm SE\text{-}WF} = \frac{2}{\mu_B B_z}\{(\hat{\Sigma}^{\rm ren}(E_A))_{\tilde{A}A} + (\hat{\Sigma}^{\rm ren}(E_A))_{A\tilde{A}}\}. \tag{31}$$

The evaluation of the matrix elements $(\hat{\Sigma}^{\rm ren}_{\rm ZP}(E_A))_{\tilde{A}A}$ and $(\hat{\Sigma}^{\rm ren}_{\rm OP}(E_A))_{\tilde{A}A}$ is performed in the momentum space. The direct Fourier transformation of the potential (4) is not suitable for the numerical calculations. Therefore, we followed the procedure employed in Ref. [7]:

$$\vec{A}(\vec{r}) = \lim_{\zeta\to 0}\frac{1}{2}(\vec{r}\times\vec{B})\exp\{-(\zeta r/2)^2\}. \tag{32}$$

Then in momentum space we have

$$\vec{A}(\vec{p}) = \lim_{\zeta\to 0}\frac{i}{\pi^{3/2}\zeta^5}\exp\{-(p/\zeta)^2\}(\vec{p}\times\vec{B}). \tag{33}$$

For the practical calculation we used the value for ζ from 10^{-4} to 10^{-6} since the average value for p in the ion with the nuclear charge Z is $\overline{p} \sim Z$. Practically this means that the order of the magnitude of $\exp\{-(p/\zeta)^2\}$ is comparable with $(\pi^{3/2}\zeta^5)^{-1}$.

The reducible correction $\delta g^{\rm bound}_{\rm SE\text{-}WF,red}$ that corresponds to the irreducible correction (12) is given by

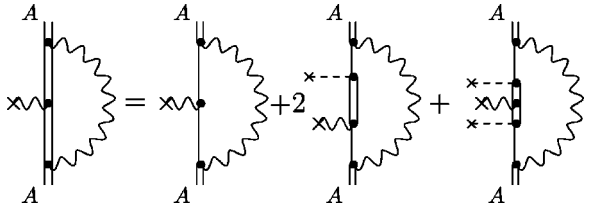

FIG. 4. The potential expansion of the vertex graph. The notations are the same as in Figs. 1–3.

$$\delta g^{\rm bound}_{\rm SE\text{-}WF,red}=\left\{\left[\frac{\partial}{\partial E}\hat{\Sigma}^{\rm ren}(E)\right]_{E=E_A}\right\}_{AA}(e\vec{\alpha}\vec{A}(\vec{r}))_{AA}. \tag{34}$$

The evaluation of the matrix element of $[(\partial/\partial E)\hat{\Sigma}^{\rm ren}(E)]_{E=E_A}$ in Eq. (34) is again performed with the use of the potential expansion (15) and the renormalized expressions for $\hat{\Sigma}^{\rm ren}_{\rm ZP}(E)$, and $\hat{\Sigma}^{\rm ren}_{\rm OP}(E)$, and $\hat{\Sigma}^{\rm ren}_{\rm MP}(E)$ [see Eqs. (16), (18), and (28)]. Unlike the case of $(\hat{\Sigma}^{\rm ren}(E_A))$, the in frared divergences do not cancel in $[(\partial/\partial E)\hat{\Sigma}^{\rm ren}(E)]_{E=E_A}$; the remaining infrared term reads

$$\frac{\alpha}{(4\pi)^2}\ln\frac{\lambda^2}{m_e^2}(e\vec{\alpha}\vec{A}(\vec{r}))_{AA}. \tag{35}$$

It will be canceled with the similar term in the vertex correction.

The potential expansion for the vertex correction is depicted in Fig. 4. The three terms of this expansion are denoted as VER1, VER2, and VER3. Only the VER1 part is divergent. It can be treated exactly in the same manner as $(\hat{\Sigma}^{\rm ren}_{\rm OP}(E_A))_{AA}$ where the Coulomb potential $V(\vec{p}-\vec{q})=\alpha Z/(\vec{p}-\vec{q})^2$ is replaced by $e\vec{\alpha}\vec{A}(\vec{p})$, and $\vec{A}(\vec{p})$ is the vector potential of the external magnetic field Eq. (33). The infrared divergence that is present in Eq. (19) will be canceled by the infrared divergent term Eq. (35) in the SE-WF, red contribution [7,8].

The term VER2 is analogous to $(\hat{\Sigma}^{\rm ren}_{\rm MP}(E_A))_{AA}$. The only difference is that one of the functions $\phi_m(w,\vec{r})$ in the expression (28) should be replaced by the function, depending on $(e\vec{\alpha}\vec{A}(\vec{p}))$ instead of the Coulomb potential V. The term VER2 is finite. Now it remains to consider the finite contribution VER3 that will be described separately in the following section.

VI. EVALUATION OF $\delta g^{\rm bound}_{\rm VER3}$

The correction $\delta g^{\rm bound}_{\rm VER3}$, although finite, is the most difficult one to calculate numerically. It contains two bound-electron propagators and two free-electron propagators. To avoid computational difficulties, we shall apply the nonperturbative finite basis set method based on the exact solution of the Dirac equation for the atomic electron in the external magnetic field [29]. Accordingly, the correction $\delta g^{\rm bound}_{\rm VER3}$ results as

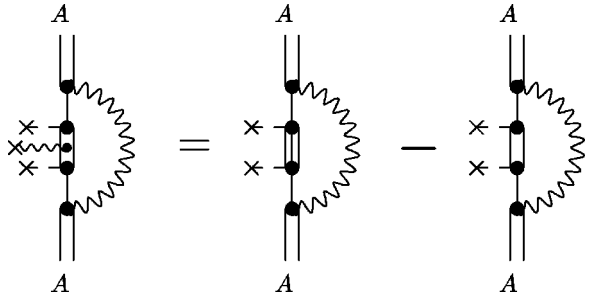

FIG. 5. Graphical representation of the evaluation of $\delta g^{\rm bound}_{\rm VER3}$. The triple solid line denotes the atomic electron in an external magnetic field. The other notations are the same as in Figs. 1–3.

$$\delta g^{\rm bound}_{\rm VER3}=\frac{(\hat{\Sigma}^{\rm ren}_{\rm MP}(E_A,B_z))_{AA}-(\hat{\Sigma}^{\rm ren}_{\rm MP}(E_A,0))_{AA}}{\mu_B B_z}. \tag{36}$$

It is understood that the magnetic field is included nonperturbatively only in the bound-electron propagator in Eq. (28) but not in the wave functions $\Psi_A(\vec{r})$. This situation is depicted in Fig. 5.

The Dirac equation for the atomic electron in an external magnetic field reads

$$\hat{H}\Psi=E\Psi, \tag{37}$$

with

$$\hat{H}=\hat{H}_0+\hat{H}_m \tag{38}$$

and

$$\hat{H}_0=\vec{\alpha}\cdot\vec{p}+\beta m+V(\vec{r}), \tag{39}$$

$$\hat{H}_{\rm m}=\frac{1}{2}\vec{\alpha}\cdot(\vec{B}\times\vec{r}), \tag{40}$$

where $\vec{\alpha}$ and β denote the Dirac matrices, c is the speed of light, and $\vec{B}$ is the magnetic-field strength. The magnetic field is supposed to be directed along the z axis, i.e., $\vec{B}=B\vec{e}_z$. For highly charged ions the potential $V(\vec{r})$ is the Coulomb potential of the nucleus (pointlike or extended). For the valence electrons in heavy alkali-metal atoms, $V(\vec{r})$ also includes the electron core potential. In Eqs. (37)–(40) atomic units are used.

The variational solution of the Dirac equation (37) is obtained according to [29] with the trial functions

$$\Psi^{\mu}(\vec{r})=\sum_{s=1}^{2\tilde{N}}\sum_{\kappa}^{\kappa_{\rm max}}a_s^{\kappa}\Psi_s^{\kappa\mu}(\vec{r}). \tag{41}$$

The electron wave functions $\Psi^{\mu}(\vec{r})$ in the magnetic field possess cylindrical symmetry and can be expanded with respect to a finite basis set of the functions $\Psi_s^{\kappa\mu}(\vec{r})$ of spherical symmetry. The index κ denotes the Dirac angular quantum number, μ corresponds to the total electron angular momen-

TABLE I. Self-energy corrections to the electron g factor for the ground state of H-like ions. In the brackets we represent the numerical results from Ref. [8]. All numbers have to be multiplied by 1×10^{-6}.

Z	$\delta g^{\rm bound}_{\rm SE\text{-}WF,irr(ZP+OP)}$	$\delta g^{\rm bound}_{\rm SE\text{-}WF,irr(MP)}$	$\delta g^{\rm bound}_{\rm SE\text{-}WF,(red+VER1)}$	$\delta g^{\rm bound}_{\rm VER2+VER3}$	$\delta g^{\rm bound}_{\rm VER3}$	$\delta g^{\rm bound}_{\rm SE}$
1	1.39	0.4012	2320.62	0.43	0.04	2322.84
	(1.39)	(0.1386)	(2320.78)	(0.53)		(2322.84)
10	66.46	12.51	2229.98	17.01	0.06	2325.96
	(66.46)	(12.28)	(2229.83)	(16.97)		(2325.54)
20	193.56	42.40	2076.05	29.14	0.07	2341.15
	(193.56)	(41.61)	(2073.50)	(29.20)		(2337.87)
30	356.80	81.90	1900.17	30.23	0.08	2369.10
	(356.81)	(80.37)	(1899.43)	(29.98)		(2366.59)
40	550.69	128.23	1730.55	13.73	0.08	2423.20
	(550.70)	(125.84)	(1729.58)	(13.27)		(2419.39)
50	774.06	181.98	1570.18	-19.39	0.09	2506.83
	(774.06)	(178.60)	(1569.42)	(-17.25)		(2504.83)
60	1027.85	246.31	1423.05	-62.20	0.10	2635.01
	(1027.87)	(241.80)	(1422.44)	(-58.20)		(2633.91)
70	1315.04	326.47	1289.79	-108.51	0.11	2822.79
	(1315.07)	(320.83)	(1290.52)	(-105.03)		(2821.39)
80	1641.51	430.04	1175.17	-157.67	0.13	3089.05
	(1641.52)	(423.97)	(1174.84)	(-151.87)		(3088.46)

tum projection, a_s^κ are the variational coefficients, and $2\tilde{N}$ defines the number of the basis-set functions.

The next step is the use of the B-spline approximation of the functions $\Psi_s^{\kappa\mu}(\vec{r})$ [29].

The variational solution of the Dirac equation (37) with the trial functions (41) reduces to the diagonalization of the Hamiltonian (38) within the finite basis set defined by Eq. (41). As a result one obtains the full set of solutions of the Dirac equation for the atomic electron in an external magnetic field.

Within the B-spline approach the H-like ion is enclosed inside of a spherical box of radius $R_{\rm box}\sim 50/Z$ a.u. The number of grid points was $N_g=150$ and the order of splines was $k=8$. This corresponds to $2N=2(N_g+k-2)=312$ energy levels that represent approximately the Dirac spectrum. With this choice the inaccuracy of the spline approximation for the $1s_{1/2}$ state compared to the variational solution [29] became less than 10^{-8} [14]. The comparison between the results of the evaluation of Zeeman splitting by the perturbation theory (PT) and by the nonperturbative approach [29] reveals that for field strengths B up to 2×10^2 T the deviation from the PT is about 10^{-8} while for a field strength of about 2×10^4 T the deviation increases up to 10^{-3}. The latter is due to the distortion of the atomic structure by the magnetic field.

In Ref. [14] the nonperturbative approach [29] has been used for the evaluation of the total correction $\delta g^{\rm bound}_{\rm QED}$. For H-like ions with $1\leqslant Z\leqslant 90$ the deviation from the accurate PT results [8] turned out to be less than 0.1%. This calculation accomplished to prove the absence of the spurious terms in the PWR approach (see the Introduction). However, this accuracy was not sufficient for obtaining accurate values for $\delta g^{\rm bound}_{\rm QED}$. The reason can be traced back to the fact that the $\delta g_{\rm QED}$ corrections are obtained via subtracting the free-electron QED corrections from the bound-electron QED corrections: $\delta g_{\rm QED}=\delta g^{\rm bound}_{\rm QED}-\delta g^{\rm free}_{\rm QED}$. Taking into account only the lowest-order QED corrections in $\delta g^{\rm bound}_{\rm QED}$, the Schwinger value for $\delta g^{\rm free}_{\rm QED}$ has to be used. This subtraction leads to severe numerical cancellations that diminish the accuracy of the net result. However, this is not the case when the nonperturbative approach is employed only for that part of $\delta g^{\rm bound}_{\rm QED}$, namely, for the $\delta g^{\rm bound}_{\rm VER3}$ contribution, which is far from dominating in the total result (see the sixth column of Table I). Thus we can expect that a level of accuracy of about 10% is still achieved in the present evaluation of $\delta g_{\rm QED}$.

VII. NUMERICAL RESULTS FOR H-LIKE IONS

The results of our calculation for the various contributions to $\delta g^{\rm bound}_{\rm SE}$ in comparison with the corresponding results obtained in Refs. [7,8] for H-like ions in the ground state are presented in Table I for different Z values. We should also note that the number presented in Ref. [6] are in close agreement with those given in Refs. [7,8]. The mean deviation of our results from Refs. [7,8] in the total $\delta g^{\rm bound}_{\rm SE}$ value amounts to 0.1%. This deviation originates from the use of the pointlike nucleus, while in Refs. [7,8] an extended nuclear model was employed. Moreover, in Refs. [7,8] a larger number of the partial-waves in the evaluation of $\delta g^{\rm bound}_{\rm SE\text{-}WF,irr\,(MP)}$ has been employed. However, these deviations are well within the limit of about 10% inaccuracy, which we have set.

VIII. RADIATIVE CORRECTIONS TO THE BOUND-ELECTRON g FACTORS FOR ns ELECTRONS IN ALKALI-METAL ATOMS

The electron g factor for the number of ns heavy atomic systems and in particular for alkali-metal atoms have been

TABLE II. QED corrections to the electron g factor for the ns valence electron in alkali metal atoms.

Z	Atom	State	$\delta g_{ns}^{\mathrm{VP}}$	$\delta g_{ns}^{\mathrm{SE,ver[1]+WF,red}}$	$\delta g_{ns}^{\mathrm{SE}}$	δg_{QED}
55	Cs	$6s$	-3.0×10^{-7}	2.29214×10^{-3}	2.32333×10^{-3}	2.9×10^{-7}
56	Ba^{+}	$6s$	-5.55×10^{-7}	2.29174×10^{-3}	2.32397×10^{-3}	5.9×10^{-7}
87	Fr	$7s$	-5.70×10^{-7}	2.291591×10^{-3}	2.32411×10^{-3}	7.2×10^{-7}

accurately measured, showing a clear deviation from the free-electron value g^{free} given by Eq. (6). Note that $\delta g_{\mathrm{QED}}^{\mathrm{free}} = g^{\mathrm{free}} - 2$ differs from the Schwinger value Eq. (8) since it includes higher-order QED terms. A large number of theoretical calculations of $\delta g = g^{\mathrm{bound}} - g^{\mathrm{free}}$ also exists for alkali-metal atoms [see Ref. [9]]. However, the deviation δg in light and in heavy atoms has a different origin. In light atoms the main contribution is due to the relativistic correction δg_{rel} [see Eq. (9)]. For a recent status of this correction, see [30]. In heavy atoms the core-valence correlation correction δg_{corr} dominates [31–35]. The Breit interaction between the valence and core electrons also leads to an observable contribution $\delta g_{\mathrm{Breit}}$ [31–35].

In most of the theoretical studies for the alkali-metal atoms it has been assumed that the correction δg_{QED} is negligible, i.e., the QED correction to the g factor is the same as for the free electron. However, recent calculations for hydrogenlike ions [7], which are also confirmed in the present paper, show that the deviation of the bound-state QED correction $\delta g_{\mathrm{QED}}^{\mathrm{bound}}$ from the free-electron value $\delta g_{\mathrm{QED}}^{\mathrm{free}}$ can be as large as 50% for high-Z values.

In Ref. [9] it was supposed that the correction δg_{QED} can be observable for heavy alkali-metal atoms. In this paper we confirm this conclusion, although the accurate value for δg_{QED} has decreased substantially compared to the estimates provided in Ref. [9].

The main problem with the estimates in Ref. [9] has been the comparison of the calculations of QED corrections for the ns electron in the alkali-metal atoms with the same corrections for the $1s$ electron in HCI. In this way, part of the QED corrections ($\delta g_{\mathrm{SE\text{-}WF,red}}^{\mathrm{bound}} + \delta g_{\mathrm{VER}}^{\mathrm{bound}}$) has been estimated. In this paper all calculations are performed directly following the lines described in Secs. III–VII. The evaluation of all the contributions is performed in the one-particle approximation. Approximate Dirac-Hartree-Fock (DHF) wave functions are employed. These wave functions are obtained in a local potential field that is fitted to the DHF potential as it has been described in Ref. [9].

For the summation over the Dirac spectrum we again used the B-spline approach with 150 grid points and the order of spline being equal to 8. The number of the partial-waves in the MP term varied around 10. Note that the size of the alkali metal atoms is much larger than the size of HCI. Therefore, we could use a radial box of the size $R_{\mathrm{box}} \sim 100$ a.u. Since the magnetic field grows rapidly with the size of the box we had to assume relatively small values for the magnetic field ($10\ \mathrm{T} \leqslant B_z \leqslant 100\ \mathrm{T}$) for the evaluation of $\delta g_{\mathrm{VER3}}^{\mathrm{bound}}$. This leads to the strong cancellations in Eq. (36) but does not affect seriously the accuracy of the total result due to the smallness of $\delta g_{\mathrm{VER3}}^{\mathrm{bound}}$ contribution.

The results of the calculations are given in Table II. In the fourth column the values of $\delta g_{\mathrm{VP}}^{\mathrm{bound}}$ are shown. In the fifth column we present the sum of the dominant contributions $\delta g_{\mathrm{SE\text{-}WF,red}}^{\mathrm{bound}} + \delta g_{\mathrm{VER1}}^{\mathrm{bound}}$. The total value of $\delta g_{\mathrm{SE}}^{\mathrm{bound}}$ is given in the sixth column and the value for $\delta g_{\mathrm{QED}} = \delta g_{\mathrm{QED}}^{\mathrm{bound}} - \delta g_{\mathrm{Sch}}^{\mathrm{free}}$ is given in the seventh column of Table II. The last value should be compared with the experimental data.

In Table III we collect the different contributions to $\delta g^{\mathrm{bound}}$ and compared them with experimental data for alkali-metal atoms. Here δg_{tot} denotes the sum of the δg_{rel}, δg_{corr}, and $\delta g_{\mathrm{Breit}}$. The correction δg_{QED} calculated in this work appears to be an order of magnitude smaller than the estimates given for Cs, Ba^{+}, and Fr in Ref. [9]. Still δg_{QED} is not negligible in case of Ba^{+}, where the most accurate experimental and theoretical data are known. Note that the theoretical error bars in Ref. [35] were introduced mainly to incorporate the possible QED corrections. Then the inclusion of δg_{QED} leads to a better agreement with the experimental value.

TABLE III. Different contributions for alkali-metal atoms. All numbers have to be multiplied by 1×10^{-6}.

Z	Atom	δg_{rel}	δg_{corr}	$\delta g_{\mathrm{Breit}}$	δg_{tot}	δg_{exp}	δg_{QED}
55	Cs	-50.00 [33]	366.00 [33]	1.00 [33]	317.00 [33]		
		-23.00 [32]	284.00 [32]	-7.00 [32]	254.00 [32]		
		-28.10 [9]				223.00 [36]	0.29
56	Ba^{+}	-55.39 [35]		-7.08 [35]	171.8 ± 3.0 [35]		
		-59.71 [9]				172.62 ± 0.03 [4]	0.59
87	Fr	-33.00 [32]	3370.00 [32]	-10.00 [32]	3327.00 [32]		
		-40.01 [9]				$2650. \pm 80.00$ [37]	0.72

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