Evidence for the absence of regularization corrections to the partial-wave renormalization procedure in one-loop self-energy calculations in external fields

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The equivalence of the covariant renormalization and the partial-wave renormalization (PWR) approaches is proven explicitly for the one-loop self-energy (SE) correction of a bound electron state in the presence of external perturbation potentials. No ''spurious'' correction terms to the noncovariant 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 method for performing PWR utilizing the relativistic *B*-spline approach for 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 a level of accuracy of about 0.1% no spurious terms are generated in numerical calculations of the SE in magnetic fields.

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I. INTRODUCTION

The partial-wave renormalization (PWR) approach was proposed a few years ago [1,2] as a convenient but noncovariant method to perform renormalization numerically in bound-state QED calculations. It was successfully applied first in exact numerical calculations of the self-energy and vacuum-polarization correction of order α [1,3,4] and further applied in exact calculations of QED corrections of order α^2 [5,6] (α is the fine-structure constant). A fair agreement between the results obtained within different numerical approaches can be stated (see, e.g., the results for the effective self-energy correction in Refs. [6,7]). Nevertheless, questions about the equivalence between the covariant renormalization and the numerical PWR scheme and conjectures about the possible occurrence of *spurious terms* in numerical calculations of higher-order QED effects have been raised in the past [8,9]. In Ref. [9] this issue was anticipated qualitatively in connection with problems encountered in the numerical evaluation of the screened Lamb shift when noncovariant, numerical renormalization schemes are employed. Persson *et al.* [8] made an attempt to derive such spurious correction terms to the PWR analytically. To our knowledge this is the first and only reference in which corresponding terms have been presented explicitly. They considered the exact self-energy correction of a bound electron state in the presence of an additional Coulomb-type screening potential V_c which is treated perturbatively. Formulating the PWR by employing the Pauli-Villars regularization, a generic, regulator-independent correction term that could contribute to the level shift of a bound state $|a\rangle$ is derived from corresponding counterterms [see Eq. (44) of Ref. [8]]:

$$\mathcal{E}^a(\Lambda\to\infty) = -\frac{\alpha}{2\pi}\langle a|[V_c(r)-\overline{V}_c]\ln(r)|a\rangle,$$

$$\overline{V}_c = \langle a|V_c(r)|a\rangle. \qquad (1)$$

Although for the particular situation under consideration the correction term cancels because it occurs with opposite sign in different subgroups of diagrams, the authors conjectured that this may not always be the case in calculations of higher-order QED effects and that the PWR and covariant renormalization could lead to results that differ generically by terms of the form of Eq. (1). The conclusions drawn in [8] received further support from numerical results for the self-energy (SE) including a perturbing $1/r$ potential [10].

In this paper we wish to address first the question about the occurrence of spurious terms of the generic type (1). Therefore, we reinvestigate the problem considered in Ref. [8]. In conclusion we find no indication for spurious terms generated by the numerical PWR method in the case of one-loop SE calculations in external fields. The correction (1) is shown to be due to an improper treatment of the unphysical high-energy contribution to the SE.

Recalculating the examples given in Ref. [10], we find that the spurious terms originate again from a similar unphysical high-energy contribution.

Finally, we investigate the problem of the spurious terms in an external magnetic field. In Ref. [8] it was conjectured that in the case of external magnetic perturbation the spurious contribution to SE should remain. Employing an approach developed here for the PWR in a magnetic field that is based on the basis set expansion for the Dirac equation due to Chen and Goldman [11] we prove the absence of the spurious terms for the QED corrections to the bound-electron g factor numerically on a level of accuracy of about 0.1%.

II. EQUIVALENCE BETWEEN THE COVARIANT AND PARTIAL-WAVE RENORMALIZATIONS

In Ref. [8] a generic correction term between the PWR and covariant renormalization contributing to the energy shift of a bound-electron state $|a\rangle$ interacting with a spherically symmetric perturbation potential V_c was derived within the Pauli-Villars regularization scheme. The authors obtain a spurious correction term to the PWR from both the

Λ-dependent wave-function correction and the vertex correction [see Eqs. (36) and (39) of Ref. [8]]:

$$\mathcal{E}^a(\Lambda)=\frac{2\alpha}{\pi}\sum_{l=0}^{\infty}\int_0^{\infty}dk\frac{k^2(2l+1)}{k'(k+k')^2}\langle a|j_l^2(kr)[V_c(r)-\overline{V}_c]|a\rangle$$

$$=\frac{2\alpha}{\pi}\sum_{l=0}^{\infty}\int_0^{\infty}dk f_l^a(k,\Lambda), \tag{2}$$

where Λ denotes the Pauli-Villars regulator and $k'=\sqrt{k^2+\Lambda^2}$. Without going through the details of the derivations given in Ref. [8] we take Eq. (2) as the starting point of the following considerations. Note that the integral over the momentum k will be finite for each partial wave l. The k and r dependence of the integrand ensures a sufficient convergence of both integrals, which allows one to interchange the order of integrations. For any finite value $r>0$ the integral over k is sufficiently convergent, i.e., the integrand falls off as $\sim 1/k^3$ for asymptotic values of k. On the other hand the contribution to the matrix element arising from the integration over r from $r=0$ to some arbitrarily small value $r=r_0$ will be negligible. In the following considerations (Sec. II A) we keep the usual order of integrations as dictated by the PWR approach (see, e.g., [1]), i.e., the matrix element is evaluated before the integration over k is performed.

Suppose we could interchange the summation over l with all the integrations involved, then the correction term Eq. (2) evidently vanishes in view of the identity

$$\sum_{l=0}^{\infty}(2l+1)j_l^2(kr)=1 \tag{3}$$

after the integration over r is performed. Accordingly, the PWR approach and the covariant renormalization would be equivalent, leading to identical results for the renormalized energy shift. Thus, one could try to prove explicitly whether or not Weierstrass' theorem for uniformly convergent functional series holds in the case of the generic correction term (2). In the following we shall demonstrate that the functional series (2) is uniformly convergent.

A. Proof of uniform convergence

The infinite summation over partial waves l may be decomposed into a finite sum $0\leqslant l\leqslant L-1$, with $L\gg 1$ and the remaining infinite sum over $l\geqslant L$. Accordingly, it is sufficient to focus on the remaining infinite sum. For this purpose we may substitute $k=t/(1-t)$, which transforms the indefinite integral over k involved in the generic expression (2) into a definite integral:

$$\mathcal{E}_L^a(\Lambda)=\frac{2\alpha}{\pi}\sum_{l=L}^{\infty}\int_0^1 dt f_l^a(t/(1-t),\Lambda). \tag{4}$$

As the next step we have to find an upper bound (majorante) u_l^a for each term f_l^a of the functional series for all $t\in[0,1]$ and for a fixed but large $\Lambda\gg 1$ such that $|f_l^a(t/(1-t),\Lambda)|<u_l^a(\Lambda)$ and $\Sigma_{l=L}^{\infty}u_l^a(\Lambda)=C^a(\Lambda)<\infty$ hold.

If Weierstrass' criterion of uniform convergence is valid, we can interchange the summation over l with the integration over t and thus over r as well. One key point for finding a convergent majorante series is to estimate appropriately the square of the spherical Bessel functions involved. We rewrite Eq. (4) in the following form:

$$\mathcal{E}_L^a(\Lambda)=\frac{2\alpha}{\pi}\sum_{l=L}^{\infty}\int_0^1 dt\frac{t^{2+\beta}}{(1-t)^{1+\beta}}\frac{(2l+1)\langle a|\{([(1-t)/rt])^{\beta}\,j_l^2(rt/(1-t))\}r^{\beta}[V_c(r)-\overline{V}_c]|a\rangle}{\sqrt{t^2+(1-t)^2\Lambda^2}\,[t+\sqrt{t^2+(1-t)^2\Lambda^2}]^2}, \tag{5}$$

where $\beta>0$. Note that the integrand of the integral (5) has a complicated analytical structure when extended into the complex t plane. Accordingly, the integral over t must be understood as being performed along a suitably chosen contour from the very beginning. The choice of the contour of integration will be done below. The integral (5) is difficult to handle analytically in closed form. Therefore, we may now employ the following estimates for the two factors involved in the integrand:

$$|\{\sqrt{t^2+(1-t)^2\Lambda^2}[t+\sqrt{t^2+(1-t)^2\Lambda^2}]^2\}^{-1}|\leqslant\tfrac{1}{4},\Lambda\gg 1, \tag{6}$$

and for all $l\geqslant L\gg 1$ and for all complex arguments z inside a bounded region of the complex t plane (see Appendix A)

$$|F_l(z,\beta)|=\left|\frac{j_l^2(z)}{z^{\beta}}\right|\leqslant(1+\beta)\frac{j_l^2(a'_{l,1})}{(a'_{l,1})^{\beta}}\leqslant c_{\beta}\left(l+\frac{1}{2}\right)^{-5/3-\beta}$$

$$\times[1-\mathcal{O}(l^{-\epsilon})],\quad \epsilon>0. \tag{7}$$

Here $a'_{l,1}$ denotes the position of the first maximum of the spherical Bessel function j_l and c_{β} denotes some finite constant. We should point out that the second inequality (7) strongly overestimates the function F_l by a constant value, which is even larger than the first (the largest) maximum of the function itself. Although the integral over t in Eq. (5) is convergent, one should be careful when treating the high-energy ($t\to 1$) region, which can actually now generate unphysical spurious terms as a consequence of the approximations performed above. We could restore or simulate the asymptotics by introducing some appropriately chosen convergence factor, e.g., $e^{-\mu t/(1-t)}$ with $\mu>0$, if needed.

Taking the absolute value of Eq. (5) together with the approximations (6) and (7) we can write

$$|\mathcal{E}_L^a(\Lambda)| \leqslant \frac{2\alpha}{\pi} \sum_{l=L}^{\infty} \left| \int_0^1 dt \frac{t^{2+\beta}}{(1-t)^{1+\beta}} \right| \frac{c_\beta}{2} \left(l+\frac{1}{2} \right)^{-2/3-\beta} \times |\langle a| r^\beta [V_c(r) - \overline{V}_c] |a\rangle|. \tag{8}$$

We observe the occurrence of Euler's Beta function in the expression above as a consequence of the estimates performed. The Beta function is defined via the integral [see formulas (6.2.1) and (6.2.2) in Ref. [12]]

$$B(z,w) := \int_0^1 dt t^{z-1}(1-t)^{w-1} = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)}. \tag{9}$$

Note that for certain values of the arguments z and w the integration over t has to be extended into the complex plane. Keeping in mind the analytical continuation, we can write

$$\left| \int_0^1 dt \frac{t^{2+\beta}}{(1-t)^{1+\beta}} \right| = \int_0^1 dt |B(3+\beta,-\beta)| = \int_0^1 dt \frac{\Gamma(3+\beta)\Gamma(1-\beta)}{\beta\Gamma(3)}. \tag{10}$$

The analytical continuation of the Beta function is provided by the reflection formula for the Gamma function [see (6.1.17) in Ref. [12]]: $\Gamma(1-w) = -w\Gamma(-w) = \pi/\sin(\pi w)$ for $0 < \mathrm{Re}\{w\} < 1$. The rigorous treatment of the integral (9), when evaluating it for the particular values $z = 3+\beta$ and $w = -\beta$, is provided by contour integration (see, e.g., Ref. [13]). It is performed along Pochhammer's closed contour $\mathcal{C}_P$ on the Riemann surface of the integrand $t^{z-1}(1-t)^{w-1}$ and relates the integral in Eq. (8) and the Beta function (9) for arbitrary arguments z and w to a product of Gamma functions according to

$$e^{-\pi i(z+w)} \oint_{\mathcal{C}_P} \frac{dt t^{z-1}}{(1-t)^{1-w}} = e^{-\pi i(z+w)} [1 - e^{2\pi i w} + e^{2\pi i(z+w)} - e^{2\pi i z}] \int_0^1 \frac{dt t^{z-1}}{(1-t)^{1-w}} = -4 \sin(\pi z) \sin(\pi w) B(z,w). \tag{11}$$

Thus, we are led to the final expression for the finite majorante series:

$$\sum_{l=L}^{\infty} \left| f_l^a \left(\frac{t}{1-t}, \Lambda \right) \right| \leqslant \frac{\Gamma(3+\beta)\Gamma(1-\beta)c_\beta}{4\beta} |\langle a| r^\beta [V_c(r) - \overline{V}_c] |a\rangle| \sum_{l=L}^{\infty} \left(l+\frac{1}{2} \right)^{-2/3-\beta}. \tag{12}$$

For $1/3 < \beta < 1$ the sum over l is convergent and can be expressed in terms of incomplete Zeta functions. Having derived a convergent majorante series the uniform convergence for the functional series (4) is proved. This indeed allows the interchange of the summation over l with all the integrations involved. As result the generic correction term (2) is equal to zero. Thus, the spurious logarithmic terms derived by Persson *et al.* [8] do not occur. This demonstrates the equivalence between the covariant renormalization and the noncovariant PWR approach when applied to the problem under consideration.

B. Comment on the missing term

We would like to point out that the evaluation of the correction term (2) as it has been performed in Ref. [8] is incomplete and that the logarithmic correction term Eq. (1) appears as an artifact of the way the expression has been evaluated. In Ref. [8], Eq. (2) was evaluated according to the limiting process

$$\mathcal{E}_1^a(\Lambda) + \mathcal{E}_2^a(\Lambda) = \frac{2\alpha}{\pi} \sum_{l=0}^{\infty} \lim_{K\to\infty} \left[\int_0^{K\tilde{r}/r} dk f_l^a(k,\Lambda) + \int_{K\tilde{r}/r}^{K} dk f_l^a(k,\Lambda) \right], \tag{13}$$

where $\tilde{r}$ is some average value of the coordinate r. Following the arguments in Ref. [8] the second term $\mathcal{E}_2^a$ vanishes in the limit $K\to\infty$, while the first part $\mathcal{E}_1^a$ generates the spurious term (1). In contrast to Ref. [8] let us now take into account the third term, which is supposed to be zero when K tends to infinity,

$$\mathcal{E}_3^a(\Lambda) = \frac{2\alpha}{\pi} \sum_{l=0}^{\infty} \lim_{K\to\infty} \int_K^{\infty} f_l^a(k,\Lambda). \tag{14}$$

Consider the sum of the second and third terms, i.e.,

$$\mathcal{E}_2^a(\Lambda) + \mathcal{E}_3^a(\Lambda) = \frac{2\alpha}{\pi} \sum_{l=0}^{\infty} \lim_{K\to\infty} \lim_{\mu\to 0} \int_{K\tilde{r}/r}^{\infty} dk e^{-\mu k} f_l^a(k,\Lambda). \tag{15}$$

The regulator $e^{-\mu k}$ is introduced for reasons of simplicity in order to guarantee a finite integral over k at the upper integration limit, if the factor j_l^2 is absent. For finite values of the parameter μ this regularization will generate some large but r-independent constant, which, however, cancels in the matrix element. Similarly, one may include the regulator $e^{-\mu/k}$ in $\mathcal{E}_1^a$ to derive the same result (1).

Now we can employ the same arguments that were used in Ref. [8] for calculating $\mathcal{E}_1^a$. The authors of [8] argue that the order between the integration over r and the summation over l can be interchanged for the following reasons: (a) the r-independent part of the k integrand does not contribute to the matrix element $\langle a| \cdots |a\rangle$, and (b) the convergence of the k integral thus does not depend on the Bessel function j_l^2.

The rigorous treatment of interchanging summations and integrations requires the validity of Weierstrass' criterion as we demonstrated in Sec. II A. Employing the arguments (a) and (b) above, we assume that in Eq. (15) the summation can

be interchanged with all integrations and limits involved. Using the identity Eq. (3) we arrive at

$$\begin{aligned}
&\mathcal{E}_2^a(\Lambda)+\mathcal{E}_3^a(\Lambda)\\
&\quad=\frac{2\alpha}{\pi}\lim_{K\to\infty}\lim_{\mu\to 0}\left\langle a\left|[V_c(r)-\overline{V}_c]\right.\right.\\
&\qquad\left.\left.\times\int_{K\tilde{r}\mu/r}^{\infty}\frac{d\xi e^{-\xi}}{\xi\sqrt{1+(\mu\Lambda/\xi)^2}[1+\sqrt{1+(\mu\Lambda/\xi)^2}]^2}\right|a\right\rangle\\
&\quad=\frac{\alpha}{2\pi}\lim_{K\to\infty}\lim_{\mu\to 0}\left\langle a\left|[V_c(r)-\overline{V}_c]\right.\right.\\
&\qquad\left.\left.\times\left[E_1\left(\frac{K\tilde{r}\mu}{r}\right)+O\left(\frac{\mu^4\Lambda K\tilde{r}}{r}\right)\right]\right|a\right\rangle. \qquad (16)
\end{aligned}$$

To obtain this result we performed the limit $\mu\to 0$ in the integrand first. Expanding the exponential integral for small arguments $E_1(K\tilde{r}\mu/r)=[-\gamma-\ln(K\tilde{r}\mu/r]+O(K\tilde{r}\mu/r)$ and taking the limit $\Lambda\to\infty$ of Eq. (16) one ends up with

$$\mathcal{E}_2^a+\mathcal{E}_3^a=\frac{\alpha}{2\pi}\langle a|[V_c(r)-\overline{V}_c]\ln(r)|a\rangle. \qquad (17)$$

Thus, we obtain the logarithmic potential term as the remaining cutoff-independent contribution. It carries an opposite overall sign and will cancel in the total sum. Moreover, we could introduce a unique regulator $e^{-\mu(1/k+k)}$ in expression (2) and thus avoid any (unnecessary) decomposition of the k integral and the introduction of $\tilde{r}$. Interchanging and performing the summation over l first one is left with

$$\begin{aligned}
\mathcal{E}^a(\Lambda)=\frac{\alpha}{2\pi}\lim_{\mu\to 0}\langle a|[V_c(r)-\overline{V}_c]2\{K_0(2\mu)-\Lambda^2K_2(2\mu)\\
+\tfrac{15}{16}\Lambda^4K_4(2\mu)+\cdots\}|a\rangle=0. \qquad (18)
\end{aligned}$$

All terms in the curly brackets vanish when the matrix element is evaluated. The calculation performed above indicates that the occurrence of the spurious logarithmic term (and maybe others as well) strongly depends on the analytical and numerical treatment of the high-energy contribution to the SE.

III. A NUMERICAL ANALYSIS OF SPURIOUS TERMS

In Ref. [10] the occurrence of spurious terms was reported in connection with numerical evaluations of the SE correction in one-electron ions with nuclear charge Z in the presence of additional Coulombic perturbation potentials. We will show, however, that this is due to an improper treatment of the high-energy contribution to the SE. The total expression for the SE correction of a bound-electron state $|a\rangle$ can always be represented in the form (see [14] for details)

$$\Delta E_a^{\mathrm{SE}}=\sum_n\ \langle an|\hat{\Sigma}|na\rangle, \qquad (19)$$

TABLE I. ΔE_a^{SE} and $\Delta E_a^{\mathrm{SE,WF}}$ for U^{91+} as a function of the energy cutoff k of the negative and the positive Dirac spectrum [see Eqs. (19) and (20)]. All energy values in a.u.

	Covariant	$k=5$	$k=10$	$k=\infty$	PWR
ΔE_a^{SE}	13.0714 [a]	12.9781	13.2190	13.2114	
$\Delta E_a^{\mathrm{SE,WF}}$	0.4626 [b]	0.4671	0.4914	0.5695	0.5598 [c]

[a]Reference [22].
[b]Reference [16].
[c]Reference [10].

where $\hat{\Sigma}$ denotes the nonlocal electron self-energy operator and the labels n run over the complete Dirac spectrum. The SE correction in the external field together with an additional perturbation potential can be divided into three parts: the wave-function correction, the vertex correction, and the derivative (or reference state) correction [8]. We will concentrate here on the wave-function correction due to the self-energy (SE,WF). This correction can be obtained from the lowest-order ΔE_a^{SE} correction by a replacement of the unperturbed wave function $|a\rangle$ by its first-order perturbation theory correction

$$|a\rangle\to\sum_n{}'\ \frac{|n\rangle\langle n|V|a\rangle}{E_a-E_n},$$

where V denotes the perturbation potential. The prime indicates that the term with $E_a=E_n$ is omitted from the sum. The energy correction $\Delta E_a^{\mathrm{SE,WF}}$ can be written as

$$\begin{aligned}
\Delta E_a^{\mathrm{SE,WF}}=\sum_{n,m}{}'\ \left\{\frac{\langle an|\hat{\Sigma}|nm\rangle\langle m|V|a\rangle}{E_a-E_m}\right.\\
\left.+\frac{\langle a|V|m\rangle\langle mn|\hat{\Sigma}|na\rangle}{E_m-E_a}\right\}. \qquad (20)
\end{aligned}$$

Within the B-spline approximation the complete Dirac spectrum is represented by a purely discrete one and terminates at some large number $N=4L(\nu+s-2)$, which is determined by the number of partial waves L, the order s of the B-spline functions, and the number of grid points ν. We may restrict the summation over the energy of the intermediate states in both Eqs. (19) and (20) by the condition $|E_n|\leqslant kmc^2$. The numerical results for the energy corrections as a function of the cutoff parameter k are shown in Table I. Where the lowest-order SE [Eq. (19)] is concerned its exact value in U^{91+} $(Z=92)$ is already obtained for $k=5$ within an accuracy of about 0.7%. Any further enlargement of the summation interval does not lead to any improvement of the accuracy. We should note that the accuracy also depends on the number of partial waves taken into account and on the number of grid points. In our case we typically used $L=6$, and $\nu\simeq 140$ together with spline functions of order $s=9$. The quoted accuracy is sufficient for our purposes since the contribution of the spurious term obtained in [10] is supposed to be much larger (about 20%).

From Table I we conclude that the summation interval with $k=5$ for H-like U^{91+} provides a sufficient approximation (about 2% deviation) for $\Delta E_a^{\mathrm{SE,WF}}$. However, we have found that any further enlargement of this interval generates the spurious contribution as obtained in [10]. From the physical point of view a 20% contribution that originates from high energies larger than $5mc^2$ (compared to the binding energy $0.3mc^2$) is hardly understandable. Therefore, we conclude that the occurrence of the spurious contribution in the numerical calculations reported in Ref. [10] has a similar origin as the spurious term (1) derived analytically in Ref. [8], i.e., an improper treatment of the high-energy contribution to the SE within the PWR approach.

IV. CALCULATION OF QED CORRECTIONS TO THE g FACTOR

Now we show that the conclusion drawn in Ref. [8] concerning the inapplicability of the PWR approach to SE calculations in external magnetic fields also does not strictly hold. For this purpose we employ an approach to the evaluation of the SE that includes an external magnetic field in the Dirac equation from the beginning.

Accordingly, the problem reduces again to the evaluation of the lowest-order SE [Eq. (19)]. The Dirac equation with an external magnetic field is solved by means of an approach due to Chen and Goldman which we describe briefly in Appendix B.

Within this approach the vacuum-polarization and self-energy corrections to the electron g factor in hydrogenlike heavy ions will be calculated. First we calculate the vacuum-polarization effect in order to determine the values of the magnetic field strength where this method remains stable. After this we turn to the calculation of the self-energy correction in an external magnetic field within the PWR method.

A. Vacuum-polarization corrections to the electron g factor of hydrogenlike heavy ions

Vacuum-polarization (VP) corrections to the electron g factor for H-like highly charged ions (HCIs) have been calculated within the the Uehling approximation [15]. For calculations of the energy level of HCIs this approximation is valid with an accuracy of about 10% for all Z values. Within the Uehling approximation the VP correction of a bound-electron state $|a(B)\rangle$ including the external magnetic field is determined by the matrix element

$$\Delta E_a^{\mathrm{VP}}(B)=\left\langle a(B)\left|-\frac{Z}{r}S(r)\right|a(B)\right\rangle \equiv\left(-\frac{Z}{r}S(r)\right)_{a(B)a(B)}, \tag{21}$$

where

$$S(r)=\frac{2\alpha}{3\pi}\int_1^\infty e^{-2rx/\alpha}\left(1+\frac{1}{x^2}\right)\frac{\sqrt{x^2+1}}{x^2}dx \tag{22}$$

TABLE II. VP corrections to the electron g factor for the ground state of hydrogenlike ions.

Z	$\delta g_{1s}^{\mathrm{VP}}$, this work	$\delta g_{1s}^{\mathrm{VP}}$, Ref. [16]
1	-3.0×10^{-11}	
5	-4.0×10^{-9}	-4.2×10^{-9}
10	-6.4×10^{-8}	-6.37×10^{-8}
20	-9.37×10^{-7}	-9.41×10^{-7}
50	-3.32×10^{-5}	-3.32×10^{-5}
90	-4.3991×10^{-4}	-4.3995×10^{-4}

and α denotes the fine-structure constant (in atomic units $\alpha=1/c$). Then the correction to the g factor results as

$$\delta g_a^{\mathrm{VP}}=\frac{2[\Delta E_a^{\mathrm{VP}}(B)-\Delta E_a^{\mathrm{VP}}(0)]}{\mu_B B}, \tag{23}$$

where μ_B is Bohr's magneton (in atomic units $\mu_B=\frac{1}{2}$).

The results of the calculations for the $1s$ ground state of H-like ions in comparison with perturbation-theory results obtained within the Uehling approximation [16] are given in Table II. An agreement better than 0.01% was found for all Z values from 5 to 90. In these calculations values for the magnetic field strength $B=|\vec{B}|$ within the range of 1.0 a.u. $\leqslant B\leqslant 100.0$ a.u. have been used. The numerical results are stable within this range of B values.

B. Self-energy correction to the electron g factor in hydrogenlike heavy ions

For the evaluation of the self-energy correction in the external magnetic field we employ the original PWR scheme developed in [1,2] in combination with the approach due to Chen and Goldman [11] for solving the Dirac equation in cylindrically symmetric external magnetic fields.

The formula for the SE correction in an external magnetic field for the state $a(B)$ reads

$$\Delta E_a^{\mathrm{SE}}(B)$$

$$=\frac{\alpha}{\pi}\sum_{n(B)}\left(\frac{1-\vec{\alpha}_1\vec{\alpha}_2}{r_{12}}\int_0^\infty\frac{\sin(\kappa r_{12})\,d\kappa}{\kappa-E_n(1-i0)+E_a}\right)_{a(B)n(B)n(B)a(B)}-\delta m_a(B), \tag{24}$$

where the sum runs over the total Dirac spectrum, $\vec{\alpha}$ denote the Dirac matrices, $r_{12}=|\vec{r}_1-\vec{r}_2|$, and δm_a abbreviates the counterterm. According to [1,2] this counterterm follows from Eq. (24) by replacing the summation over bound states $n(B)$ by a corresponding integration over free-electron Dirac states and by replacing the bound-state energy $E_n(B)$ in the denominator by the free-electron energy ϵ. The bound states $a(B)$ are expanded in free-electron Dirac states $|\vec{p},\epsilon\rangle$ (where $\vec{p}$ is the electron momentum). The correction to the g factor that arises from the SE contribution reads

TABLE III. Self-energy corrections to the electron g factor for the ground state of H-like ions.

Z	$\delta g_{1s}^{\mathrm{SE}}$, this work	$\delta g_{1s}^{\mathrm{SE}}$, Ref. [16]	$\delta g_{1s}^{\mathrm{SE}}(\alpha Z$ expansion), Ref. [16]
1	$(2.31\pm0.01)\times10^{-3}$	2.322840×10^{-3}	2.32284×10^{-3}
5	$(2.32\pm0.01)\times10^{-3}$	2.323389×10^{-3}	2.323388×10^{-3}
10	$(2.321\pm0.009)\times10^{-3}$	2.325472×10^{-3}	2.3249028×10^{-3}
20	$(2.332\pm0.007)\times10^{-3}$	2.33692×10^{-3}	
50	$(2.469\pm0.012)\times10^{-3}$	2.47162×10^{-3}	
90	$(2.997\pm0.011)\times10^{-3}$	$3.04\,516\times10^{-3}$	

$$\delta g_a^{\mathrm{SE}}=\frac{2[\Delta E_a^{\mathrm{SE}}(B)-\Delta E_a^{\mathrm{SE}}(0)]}{\mu_B B}. \tag{25}$$

Numerical results for the ground states of H-like ions with different Z values are given in Table III in comparison with data obtained via perturbation theory [16] and from the αZ expansion (for low Z). As for the VP corrections, numerically stable results are provided for values of magnetic field strengths within the same range 1.0 a.u. $\leqslant B \leqslant 100.0$ a.u. For all Z values the deviations from the perturbation-theory results turn out to be smaller than 0.1%.

Thus, contrary to the statement made in [8], this provides numerical evidence for the absence of the spurious terms in calculations of the SE correction in external magnetic fields performed within the PWR approach at a level of accuracy better than 0.1%.

We should note that the accuracy achieved in our approach will not be sufficient for obtaining accurate values for bound-state QED corrections to electron g factors. The reason traces back to the fact that bound-state QED corrections are obtained via subtraction of the free-electron QED corrections from the values given in Tables II and III. This leads to severe numerical cancellations that diminish the accuracy of the net result significantly. However, it does not effect our conclusions concerning the spurious terms.

V. CONCLUSIONS

Summarizing, we have provided evidence for the absence of the ''renormalization corrections'' for the particular case of the SE in external fields. Contrary to the statements made in [8,10] we have found that via a proper treatment of the high-energy contribution to the SE such corrections can be avoided numerically and analytically. However, the proof presented here cannot exclude the possible existence of spurious corrections in more complicated situations, e.g., in connection with high-order QED corrections. In the particular case of the ''loop after loop'' second-order electron self-energy correction a discrepancy between results obtained within the PWR [17] approach and from the covariant renormalization scheme [18] and [19] has been reported. This may indicate that this problem requires further investigation.

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APPENDIX A: THE UPPER LIMIT FOR BESSEL FUNCTIONS

Let us consider first the real functions $F_l(x,\beta)=j_l^2(x)/x^\beta$ for values $\beta>0$ and $l\geqslant L\gg1$ over the interval $x\in[0,a_{l,1}]$. We adopt the notation of Ref. [12]. Let $a_{l,1}$ and $a'_{l,1}$ denote the location of the first zero and the first maximum of the spherical Bessel function $j_l(x)$, respectively. We employ the formulas (10.1.59) and (10.1.61) of Ref. [12]:

$$a'_{l,1}\approx\left(l+\frac{1}{2}\right)\left[1+0.8086\left(l+\frac{1}{2}\right)^{-2/3}\right][1-O(l^{-\epsilon})], \tag{A1}$$

$$j_l(a'_{l,1})\approx0.8458\left(l+\frac{1}{2}\right)^{-5/6}[1-O(l^{-\epsilon})] \tag{A2}$$

with $\epsilon>0$. Obviously, the zeros of the functions F_l and j_l coincide. For any $l>0$ and $\beta>0$ the function F_l has exactly one maximum within the interval $x\in[0,a_{l,1}]$ located at $x=b'_{l,1}$, i.e., $F'_l(b'_{l,1},\beta)=0$ and $F''_l(b'_{l,1},\beta)<0$. Derivatives with respect to x are indicated by primes. For the first derivative F'_l evaluated at $a'_{l,1}$, we find

$$F'_l(a'_{l,1},\beta)=\left.\left(\frac{2xj_l(x)j'_l(x)-\beta j_l^2(x)}{x^{\beta+1}}\right)\right|_{x=a'_{l,1}}$$

$$=-\beta\frac{j_l^2(a'_{l,1})}{(a'_{l,1})^{\beta+1}}=-\beta\frac{F_l(a'_{l,1},\beta)}{a'_{l,1}}<0. \tag{A3}$$

This implies that (1) $b'_{l,1}<a'_{l,1}$ and (2) F_l decreases monotonically over the interval $b'_{l,1}<x\leqslant a'_{l,1}$. Using the differential equation for j_l we derive for the second derivative

$$F''_l(a'_{l,1},\beta)=\left.\left(\beta(\beta+1)\frac{j_l^2(x)}{x^{\beta+2}}+2\frac{j_l(x)j''_l(x)}{x^\beta}\right)\right|_{x=a'_{l,1}}$$

$$=\{\beta(\beta+1)-2[(a'_{l,1})^2-l(l+1)]\}$$

$$\times\frac{j_l^2(a'_{l,1})}{(a'_{l,1})^{\beta+2}}<0, \tag{A4}$$

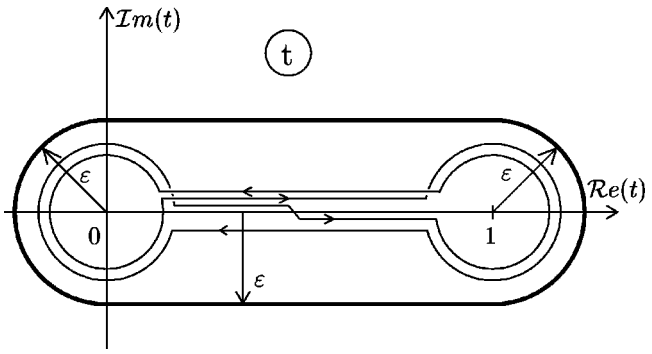

FIG. 1. The region of the complex t plane for which the approximation Eq. (A6) is valid. It includes Pochhammer's contour as depicted.

which holds for all values $0<\beta<L$, since $l\gg 1$. The fact that $F_l''(a'_{l,1},\beta)<0$ reveals that F_l has its point of inflection somewhere between $a'_{l,1}$ and $a_{l,1}$, i.e., F_l is a convex function over the interval $[b'_{l,1},a'_{l,1}]$. Accordingly, we can estimate the value of F_l at the position $b'_{l,1}$ of its first maximum, which finally provides an upper bound for the function F_l throughout the whole range $x\in[0,\infty)$:

$$F_l(b'_{l,1},\beta)\leqslant F_l(a'_{l,1},\beta)+|F_l'(a'_{l,1},\beta)||b'_{l,1}-a'_{l,1}| \leqslant(1+\beta)\,F_l(a'_{l,1},\beta). \tag{A5}$$

Here we used Eq. (A3) and the fact that $|b'_{l,1}-a'_{l,1}|\leqslant a'_{l,1}$. Finally, we arrive at

$$F_l(x,\beta)\leqslant(1+\beta)\frac{j_l^2(a'_{l,1})}{(a'_{l,1})^\beta}\leqslant c_\beta\left(l+\frac{1}{2}\right)^{-5/3-\beta}[1-\mathcal{O}(l^{-\epsilon})]. \tag{A6}$$

Where the proof is concerned we shall restrict consideration to values $0<\beta<1$ only.

To provide the function F as required along Pochhammer's contour we need to extend the considerations above into the complex plane. The function F is analytic in the complex plane $z=x+i\zeta$. A suitable region of the complex t plane [see Eq. (4)] that includes Pochhammer's contour is depicted in Fig. 1.

For small imaginary parts $0<\varepsilon\ll 1$ all steps of the derivation go through for complex arguments $z=x+i\zeta$ with $|\zeta|\leqslant\varepsilon$. The Taylor expansion yields

$$|F(z,\beta)|=\left|F(x,\beta)+i\zeta\left(\frac{\partial}{\partial\zeta}F(z,\beta)\right)\right|_{\zeta=0}|+\mathcal{O}(\zeta^2)| \leqslant|F(x,\beta)|+\varepsilon|F'(x,\beta)|+\mathcal{O}(\varepsilon^2), \tag{A7}$$

where $0<x<1$. Now we might define $\sup_{(0<x<\infty)}|F'(x,\beta)|\equiv M<\infty$ together with $\varepsilon=(l+1/2)^{-5/3-\beta}$. In view of Eq. (A6) we can write

$$|F(z,\beta)|\leqslant(c_\beta+M)\left(l+\frac{1}{2}\right)^{-5/3-\beta}[1-\mathcal{O}(l^{-\epsilon})]. \tag{A8}$$

APPENDIX B: FINITE BASIS SET SOLUTION OF THE DIRAC EQUATION FOR ATOMIC ELECTRONS IN EXTERNAL MAGNETIC FIELDS

The Dirac equation for a bound electron in an additional external magnetic field reads

$$\hat{H}\Psi=E\Psi, \tag{B1}$$

with

$$\hat{H}=\hat{H}_0+\hat{H}_m \tag{B2}$$

and

$$\hat{H}_0=\vec{\alpha}\cdot\vec{p}+\beta m+V_{\mathrm{C}}(\vec{r}), \tag{B3}$$

$$\hat{H}_m=\frac{1}{2}\vec{\alpha}\cdot[\vec{B}\times\vec{r}], \tag{B4}$$

where $\vec{\alpha},\beta$ denote the Dirac matrices, m is the electron mass, and $\vec{B}$ is the magnetic field strength. The magnetic field is supposed to be directed along the z axis: $\vec{B}=B\vec{e}_z$. $V_{\mathrm{C}}(\vec{r})$ is the Coulomb potential of a (pointlike or extended) nucleus. In Eqs. (B1)–(B4) atomic units are used.

According to Ref. [11] the variational solution of the Dirac equation (B1) is obtained by means of trial functions

$$\Psi^\mu(\vec{r})=\sum_{I=1}^{I_{\max}}\sum_{\kappa}^{\kappa_{\max}}a^\kappa\Psi_I^{\kappa\mu}(\vec{r}). \tag{B5}$$

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 $\Psi_I^{\kappa\mu}(\vec{r})$ of spherical symmetry. The index κ denotes the Dirac angular quantum number, μ corresponds to the total electron angular momentum projection, a^κ are the variational coefficients, and $2\tilde{N}$ defines the number of basis set functions.

The next step employs the B-spline representation of the functions $\Psi_I^{\kappa\mu}(\vec{r})$:

$$\Psi_I^{\kappa\mu}(\vec{r})=\sum_{J=1}^{2N}b_{IJ}^\kappa\Phi_J^{\kappa\mu}(\vec{r}), \tag{B6}$$

with

$$\Phi_n^{\kappa\mu}(\vec{r})=\psi_n^\kappa\begin{pmatrix} i\dfrac{1}{r}\chi_{\kappa\mu}(\vec{r}/r)\\ 0\end{pmatrix}, \tag{B7}$$

$$\Phi_{N+n}^{\kappa\mu}(\vec{r})=\psi_n^\kappa\begin{pmatrix} 0\\ -i\dfrac{1}{r}\chi_{-\kappa\mu}(\vec{r}/r)\end{pmatrix}, \tag{B8}$$

where $n=1,\ldots,N$, ψ_n^κ denote the B-spline representations of the finite basis set of radial functions [20], and $\chi_{\kappa\mu}(\vec{r}/r)$ are the usual spherical spinors.

The variational solution of the Dirac equation (B1) with the trial functions (B5) reduces to the diagonalization of the Hamiltonian (B4) within the finite basis set defined by Eqs. (B5)–(B8). As a result one obtains the full set of solutions of the Dirac equation for the atomic electron in an external magnetic field.

In particular, the matrix elements of the operator $\hat{H}_m$ with the wave functions (B6)–(B8) are given by

$$\langle \Psi_n^{\kappa\mu} | \hat{H}_m | \Psi_{N+n'}^{\kappa'\mu'} \rangle = \frac{B}{2} r_{nn'}^{\kappa\kappa'} A_{\kappa\kappa'}, \tag{B9}$$

where

$$r_{nn'}^{\kappa\kappa'} = \int_0^\infty r \psi_n^\kappa(r) \psi_{n'}^{\kappa'}(r) dr, \tag{B10}$$

$$A_{\kappa\kappa'} = -i \int d\Omega \langle \chi_{\kappa\mu} | [\vec{\sigma} \times \vec{r}]_z | \chi_{-\kappa'\mu'} \rangle = \begin{cases} \dfrac{4\kappa\mu}{4\kappa^2 - 1}, & \text{for} \quad \kappa' = \kappa \\ \mathrm{sgn}(\kappa) \dfrac{[(|\kappa| + 1/2)^2 - \mu^2]^{1/2}}{2|\kappa| + 1}, & \text{for} \quad \kappa' = -\kappa \end{cases}. \tag{B11}$$

It is convenient to rearrange the summations in Eqs. (B5)–(B6) in such a way that the summation over partial waves L will be performed as the last one. In the B-spline approach one starts to count the states from the lowest negative energy state ($J=1$). Then the state with $J=N+1$ corresponds to the positive energy ground state $1s_{1/2}$.

Within the B-spline approach the H-like ion is included inside a spherical box of radius $R_{\mathrm{box}} \sim 50/Z$ a.u. The number of grid points was $N_g = 150$ and the order of splines $k=8$. This corresponds to $2N = 2(N_g + k - 2) = 314$ energy levels that approximately represent the Dirac spectrum. With this choice the inaccuracy of the spline approximation for the $1s_{1/2}$ state compared to the Chen and Goldman variational solution [11] becomes less than 10^{-8}. To test the accuracy of our approach we have calculated the Zeeman splitting of the $1s_{1/2}$ state in the hydrogen atom for different field strengths B.

TABLE IV. Results for the Zeeman splitting ΔE_Z for the ground state in neutral hydrogen obtained in the Chen and Goldman approach (CGA) [11] and in perturbation theory (PT). All values are given in atomic units (a.u). For the magnetic field strength 1 a.u. $= 2.35 \times 10^5$ T.

B	ΔE_Z (CGA)	ΔE_Z (PT)
0	0.500 006 656 6	0.500 006 656 6
10^{-5}	0.500 011 656 5	0.500 011 656 5
10^{-3}	0.500 506 398	0.500 506 647 7
10^{-1}	0.549 743 3	0.550 005 769 1
1	0.872 133	0.999 997 781 3

In Table IV the results for the corresponding Zeeman splittings are compared as evaluated within the approach Chen and Goldman and by means of perturbation theory. The latter have been obtained employing the standard formula [21]. The comparison reveals that for field strengths B up to 2×10^2 T the deviation from the perturbation-theory results is about 10^{-8} while for a field strength of about 2×10^4 T the deviation increase up to 10^{-3}. The latter is due to the strong distortion of the atomic structure by the magnetic field.

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