One-loop self-energy correction in a strong binding field

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Abstract

A new scheme for the numerical evaluation of the one-loop self-energy correction to all orders in $Z\alpha$ is presented. The scheme proposed inherits the attractive features of the standard potential-expansion method but yields a partial-wave expansion that converges more rapidly than in all other methods reported in the literature.

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Introduction

Calculations of the one-loop self-energy correction to all orders in the parameter $Z\alpha$ (Z is the nuclear charge number and α is the fine structure constant) have a long history. The first correct evaluation of this correction was performed for several high-Z ions by Desiderio and Johnson [1] using the method proposed by Brown, Langer, and Schaefer [2]. Another, much more accurate and powerful method was developed by Mohr [3], who carried out high-precision calculations of this correction in a wide range of Z for the ground and the first excited states of H-like ions [4–6]. Various extensions of this method provided highly accurate evaluations of the self-energy correction for higher excited states [7, 8], for the extended-nucleus Coulomb potential [9], and for very small nuclear charge numbers [10–12]. Indelicato and Mohr [13, 14] presented an important modification of the method, in which renormalization is performed completely in coordinate space.

A different method for evaluation of the self-energy correction, which can be conventionally termed as the potential-expansion method, was introduced by Snyderman and Blundell [15–17]. Various numerical schemes based on this method were presented by other groups [18, 19].

There are also other methods developed for evaluation of the self-energy correction which have been less widely used so far. A noncovariant method of the so-called partial-wave renormalization was developed by Persson, Lindgren, and Salomonson [20] and by Quiney and Grant [21, 22]. Another method proposed by Labzowsky and Goidenko [23] is based on the multiple commutator expansion of the general expressions.

Closely related to the self-energy is the other dominant QED effect, the vacuum-polarization. The first evaluations of this correction to all orders in $Z\alpha$ were performed by Soff and Mohr [24] and by Manakov, Nekipelov, and Fainstein [25]. More accurate calculations of the vacuum-polarization correction were carried out later by other groups [26, 27].

Evaluation of the self-energy correction for a tightly bound electron is nontrivial, to a large extent, due to the fact that this correction involves the Dirac-Coulomb Green function that is not presently known in the closed analytical form (contrary to the nonrelativistic Coulomb Green function). Consequently, the self-energy correction is expressed as an infinite expansion over the angular momentum of the virtual photon (or, equivalently, the total angular momentum of the virtual electron states $j = |\kappa| - 1/2$, where κ is the relativistic angular-momentum parameter of the Dirac equation). This expansion (further referred to as the partial-wave expansion) greatly complicates calculations of the self-energy corrections.

In the method by Mohr [3], the summation of the partial-wave expansion was performed numerically before integrations over radial coordinates. A large number of terms included into the summation ($\sim 10^4$) and usage of the quadruple arithmetics ensured a high accuracy of the numerical results obtained but made the computation rather time consuming. In the extension of this method by Jentschura *et al.* [10–12], several millions of expansion terms included into computation were reported, which became possible due to an elaborate convergence-acceleration technique developed by the authors and an extensive usage of modern parallel computer systems.

On the contrary, calculations based on the potential-expansion method [16–19] are usually performed with much smaller numbers of partial-wave expansion terms actually included into the computation ($\sim 15-40$). This is achieved (*i*) by employing a more complete set of renormalization terms that are calculated separately in a closed form, (*ii*) by performing the radial integrations before the partial-wave summation (for the discussion of how this influences the convergence rate see Eqs. (1), (2) of Ref. [14] and the related text there), and (*iii*) by using extrapolation to estimate the contribution of the tail of the expansion. The price to pay is a more complex structure of the subtraction terms (especially, in coordinate space) and the necessity to keep the accuracy of numerical integrations well under control for each partial-wave term, in order to provide a reasonable extrapolation for the tail of the expansion. Still, the method is computationally very cheap and can be directly generalized for calculations of higher-order QED diagrams, where the self-energy loop enters as a subgraph. These advantages have determined the fact that most calculations of higher-order self-energy corrections have been performed up to now by extensions of the potential-expansion method.

The one-loop self-energy correction is traditionally represented in terms of the dimensionless function $F(Z\alpha)$, which is connected to the energy shift (in units $\hbar = c = m = 1$) by

$$\Delta E = \frac{\alpha}{\pi}\,\frac{(Z\alpha)^4}{n^3}\,F(Z\alpha)\,, \tag{1}$$

where n is the principal quantum number. Practical calculations performed within the potential-expansion method in the Feynman gauge show that the general behavior of individual partial-wave expansion contributions to the function $F(Z\alpha)$ roughly follows the dependence

$$F_{|\kappa|} \approx \frac{n^3}{10\,(Z\alpha)^2\,|\kappa|^3}\,. \tag{2}$$

This makes clear that, while the nominal rate of convergence of the partial-wave expansion is always close to $|\kappa|^{-3}$ in this method, the actual convergence is governed by the parameter $n^3/(Z\alpha)^2$, whose numerical value can be rather large for excited states and small nuclear-charge numbers. Taking into account that the extension of the partial-wave summation beyond the typical limit of $|\kappa| = 30 - 40$ leads to serious technical problems within the numerical scheme employed, we conclude that the parameter $n^3/(Z\alpha)^2$ defines the region of the practical applicability of the potential-expansion method.

Similar situation persists in calculations of self-energy corrections to higher orders of perturbation theory. In such calculations, the convergence of the partial-wave expansion also worsens with decrease of Z and increase of n. In particular, a slow convergence of this expansion turned out to be the factor limiting the accuracy in evaluations of the self-energy correction to the $1s$ and $2s$ hyperfine splitting in low-Z ions [28–30]. This convergence also posed serious problems in calculations of the self-energy correction to the bound-electron g factor in light H-like ions [31–34].

The convergence rate of the partial-wave expansion becomes most crucial in the case of two-loop self-energy corrections, for which the summation should be performed over two independent expansion parameters, both of which are unbound [35, 36]. A calculation of the two-loop self-energy correction for very low nuclear charge numbers (and, specifically, for hydrogen) is a challenging problem, which apparently cannot be solved within a straightforward generalization of the potential-expansion method. (The present status of calculations of the two-loop self-energy correction can be found in Ref. [37]). One of the problems to be solved to this end is to find a way to improve the convergence properties of the partial-wave expansion.

The goal of the present investigation is to formulate a scheme for evaluation of the one-loop self-energy correction, which yield the fastest convergence of the partial-wave expansion among the methods reported so far in the literature.

I. FORMALISM

The energy shift of a bound electron due to the first-order self-energy correction is given by the real part of the expression

$$\begin{aligned}\Delta E \;=\; & 2i\alpha \int_{-\infty}^{\infty} d\omega \int d\boldsymbol{x}_1\, d\boldsymbol{x}_2\, \psi_a^{\dagger}(\boldsymbol{x}_1)\, \alpha_\mu\, G(\varepsilon_a - \omega, \boldsymbol{x}_1, \boldsymbol{x}_2)\, \alpha_\nu\, \psi_a(\boldsymbol{x}_2)\, D^{\mu\nu}(\omega, \boldsymbol{x}_{12}) \\ & - \delta m \int d\boldsymbol{x}\, \psi_a^{\dagger}(\boldsymbol{x})\, \beta\, \psi_a(\boldsymbol{x})\,, \end{aligned} \tag{3}$$

where $\alpha_\mu = (1, \boldsymbol{\alpha})$, $\boldsymbol{\alpha}$ and β are the Dirac matrices, $G(\omega, \boldsymbol{x}_1, \boldsymbol{x}_2) = [\omega - \mathcal{H}(1 - i0)]^{-1}$, $\mathcal{H} = \mathcal{H}_0 + V(x)$, $\mathcal{H}_0 = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta$ is the free Dirac Hamiltonian, $V(x)$ is a local potential (not necessarily the Coulomb one), and δm is the mass counterterm. $D^{\mu\nu}$ is the photon propagator defined in the Feynman gauge as

$$D^{\mu\nu}(\omega, \boldsymbol{x}_{12}) = g^{\mu\nu} \frac{\exp(i\sqrt{\omega^2 + i0}\, x_{12})}{4\pi\, x_{12}} \,, \tag{4}$$

where $x_{12} = |\boldsymbol{x}_{12}| = |\boldsymbol{x}_1 - \boldsymbol{x}_2|$, and the branch of the square root is fixed by the condition $\mathrm{Im}(\sqrt{\omega^2 + i0}) > 0$. In Eq. (3) it is assumed that the unrenormalized part of the expression and the mass counterterm are regularized in a certain covariant way and that the limit removing the regularization is taken after the cancellation of the divergent terms.

Ultraviolet divergencies in Eq. (3) can be conveniently isolated by separating the first two terms in the expansion of the bound-electron propagator G in terms of the binding potential V,

$$G(E, \boldsymbol{x}_1, \boldsymbol{x}_2) = G^{(0)}(E, \boldsymbol{x}_1, \boldsymbol{x}_2) + G^{(1)}(E, \boldsymbol{x}_1, \boldsymbol{x}_2) + G^{(2+)}(E, \boldsymbol{x}_1, \boldsymbol{x}_2) \,, \tag{5}$$

where $G^{(0)} = [\omega - \mathcal{H}_0(1 - i0)]^{-1}$ is the free Dirac Green function, $G^{(1)}$ is the first-order expansion term

$$G^{(1)}(E, \boldsymbol{x}_1, \boldsymbol{x}_2) = \int d\boldsymbol{z}\, G^{(0)}(E, \boldsymbol{x}_1, \boldsymbol{z})\, V(z)\, G^{(0)}(E, \boldsymbol{z}, \boldsymbol{x}_2) \,, \tag{6}$$

and $G^{(2+)}$ is the remainder. The three terms in Eq. (5), after substitution into Eq. (3), lead to the separation of the self-energy correction into the zero-potential, one-potential, and many-potential parts [15]:

$$\Delta E = \Delta E_{\text{zero}} + \Delta E_{\text{one}} + \Delta E_{\text{many}} \,, \tag{7}$$

with the mass-counterterm part naturally ascribed to the zero-potential term. Converting the first two terms into momentum space and cancelling the ultraviolet divergences, one obtains:

$$\Delta E_{\text{zero}} = \int \frac{d\boldsymbol{p}}{(2\pi)^3}\, \overline{\psi}_a(\boldsymbol{p})\, \Sigma_R^{(0)}(\varepsilon_a, \boldsymbol{p})\, \psi_a(\boldsymbol{p}) \,, \tag{8}$$

$$\Delta E_{\text{one}} = \int \frac{d\boldsymbol{p}_1}{(2\pi)^3} \frac{d\boldsymbol{p}_2}{(2\pi)^3}\, \overline{\psi}_a(\boldsymbol{p}_1)\, \Gamma_R^0(\varepsilon_a, \boldsymbol{p}_1; \varepsilon_a, \boldsymbol{p}_2)\, V(\boldsymbol{q})\, \psi_a(\boldsymbol{p}_2) \,, \tag{9}$$

where $\boldsymbol{q} = \boldsymbol{p}_1 - \boldsymbol{p}_2$, $\overline{\psi}_a(\boldsymbol{p}) = \psi_a^\dagger(\boldsymbol{p})\, \gamma^0$, and $\Sigma_R^{(0)}(p)$ and $\Gamma_R^\mu(p_1, p_2)$ are the renormalized free self-energy and vertex functions (for their exact definition and calculational formulas see, *e.g.*, Ref. [19]).

The many-potential term is represented by the following expression

$$\Delta E_{\rm many} = 2i\alpha \int_C d\omega \int d\boldsymbol{x}_1\, d\boldsymbol{x}_2\, \psi_a^{\dagger}(\boldsymbol{x}_1)\, \alpha_\mu \\ \times G^{(2+)}(\varepsilon_a - \omega, \boldsymbol{x}_1, \boldsymbol{x}_2)\, \alpha_\nu\, \psi_a(\boldsymbol{x}_2)\, D^{\mu\nu}(\omega, \boldsymbol{x}_{12})\,, \tag{10}$$

where $G^{(2+)} = G - G^{(0)} - G^{(1)}$ and the contour C of the ω integration does not necessarily go along the real axis but can be chosen differently in order to simplify the numerical evaluation of this expression. In our approach, we employ the contour C_{LH} that consists of the low-energy part (C_L) and the high-energy part (C_H) and is similar to the one introduced in our previous work [19]. The low-energy part of the contour C_L extends from $-\varepsilon_0 - i0$ to $-i0$ on the lower bank of the branch cut of the photon propagator and from $+i0$ to $\varepsilon_0 + i0$ on the upper bank of the cut. In order to avoid appearance of poles of the electron propagator near the integration contour, each part of C_L is bent into the complex plane if the calculation is performed for excited states. (The analytical structure of the integrand and a possible choice of the contour are discussed in detail in Ref. [19].) The high-energy part of the contour is $C_H = [\varepsilon_0 + i0, \varepsilon_0 + i\infty) + (\varepsilon_0 - i\infty, \varepsilon_0 - i0]$. The parameter ε_0 separating the low- and the high-energy part of the contour is chosen to be $\varepsilon_0 = Z\alpha\, \varepsilon_a$ in this work. (It is assumed that the condition $\varepsilon_a - \varepsilon_{1s} < \varepsilon_0$ is fulfilled for the states under consideration, where ε_{1s} is the ground-state energy.)

Due to a lack of a closed-form representation for the Dirac Coulomb Green function, the evaluation of the many-potential term has to be performed by expanding G (and, therefore, $G^{(2+)}$) into eigenfunctions of the Dirac angular momentum with the eigenvalue κ. As discussed in Introduction, the convergence rate of the resulting partial-wave expansion is of crucial importance for the numerical evaluation of the self-energy correction.

Until this moment, our description closely followed the standard potential-expansion method [15]. We would like now to modify this method in order to achieve a better convergence of the partial-wave expansion in the many-potential term $\Delta E_{\rm many}$. To this end, we look for an approximation $G_a^{(2+)}$ to the function $G^{(2+)}$ that fulfills the following requirements: (*i*) it can be evaluated in a closed form (*i.e.*, without the partial-wave expansion) and (*ii*) the difference $G^{(2+)} - G_a^{(2+)}$ inserted into Eq. (10) yields a rapidly converging partial-wave series.

We start with the expansion of the bound-electron Green function in terms of the binding potential,

$$
\begin{aligned}
G(E,\boldsymbol{x}_1,\boldsymbol{x}_2) \;=\; & G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2) + \int d\boldsymbol{z}\, G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{z})\, V(z)\, G^{(0)}(E,\boldsymbol{z},\boldsymbol{x}_2) \\
& + \int d\boldsymbol{z}_1\, d\boldsymbol{z}_2\, G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{z}_1)\, V(z_1)\, G^{(0)}(E,\boldsymbol{z}_1,\boldsymbol{z}_2)\, V(z_2)\, G^{(0)}(E,\boldsymbol{z}_2,\boldsymbol{x}_2) + \ldots\,.
\end{aligned}
\tag{11}
$$

It is well known that the dominant contribution to radial integrals like those that appear in Eq. (10) originates from the region where the radial arguments are close to each other, $\boldsymbol{x}_1 \approx \boldsymbol{x}_2$. This region is also responsible for the part of the partial-wave expansion of the Green function that has the slowest asymptotic convergence in $1/|\kappa|$ [3]. We now assume that in this region one can neglect the commutators of the potential V with the free Green function $G^{(0)}$. Commuting V out to the left in Eq. (11) and repeatedly employing the identity

$$
\int d\boldsymbol{z}\, G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{z})\, G^{(0)}(E,\boldsymbol{z},\boldsymbol{x}_2) = -\frac{\partial}{\partial E}\, G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2)\,, \tag{12}
$$

we obtain the approximation G_a to the bound-electron Green function G,

$$
\begin{aligned}
G_a(E,\boldsymbol{x}_1,\boldsymbol{x}_2) \;=\; & G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2) + [-V(x_1)]\, \frac{\partial}{\partial E}\, G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2) \\
& + [-V(x_1)]^2\, \frac{\partial^2}{\partial^2 E}\, G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2) + \ldots\,.
\end{aligned}
\tag{13}
$$

This expansion has a form of the Taylor series and can be formally summed up, yielding

$$
G_a(E,\boldsymbol{x}_1,\boldsymbol{x}_2) = G^{(0)}(E+\Omega,\boldsymbol{x}_1,\boldsymbol{x}_2)\,, \tag{14}
$$

where $\Omega = -V(x_1) = Z\alpha/x_1$. It should be noted that the idea of commuting the potential V outside in the one-potential term was first proposed by Mohr [3], who proved that this procedure does not influence the asymptotic ultraviolet behavior of this term (we recall that ultraviolet divergences originate from the region $\boldsymbol{x}_1 \approx \boldsymbol{x}_2$ in configuration space). Later, it was also demonstrated [13, 14] that all ultraviolet divergences in the one-loop self-energy correction could be identified by isolating several first terms of the expansion of the potential V and the reference-state wave functions ψ_a around the point $\boldsymbol{x}_1 = \boldsymbol{x}_2$.

Expression (14) yields an approximation for the bound-electron Green function that has a form of the free Green function with a shifted energy argument. Taking into account that the free Green function is known in a closed form [3]

$$
G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2) = -\left[\left(\frac{c}{x_{12}} + \frac{1}{x_{12}^2}\right) i\boldsymbol{\alpha}\cdot\boldsymbol{x}_{12} + \beta + E\right] \frac{\exp[-c\,x_{12}]}{4\pi x_{12}}\,, \tag{15}
$$

($c = \sqrt{1-E^2}$), we can employ this expression for the evaluation of G_a. The corresponding approximation for the function $G^{(2+)}$ is obtained by subtracting the first two terms of the Taylor expansion from G_a,

$$G_a^{(2+)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2) = G^{(0)}(E+\Omega,\boldsymbol{x}_1,\boldsymbol{x}_2) - G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2) - \Omega\,\frac{\partial}{\partial E}\,G^{(0)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2)\,. \tag{16}$$

According to the derivation, the functions $G_a(E,\boldsymbol{x}_1,\boldsymbol{x}_2)$ and $G_a^{(2+)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2)$ approximate, correspondingly, $G(E,\boldsymbol{x}_1,\boldsymbol{x}_2)$ and $G^{(2+)}(E,\boldsymbol{x}_1,\boldsymbol{x}_2)$ in the region where $\boldsymbol{x}_1 \approx \boldsymbol{x}_2$. This means, in particular, that instead of the original expression for Ω in Eq. (14), $\Omega = Z\alpha/x_1$, one can use its arbitrary symmetrization with respect to x_1 and x_2. In our actual calculations, the following choice of Ω was employed

$$\Omega = \frac{2Z\alpha}{x_1+x_2}\,, \tag{17}$$

which turned out to be more convenient from the numerical point of view.

We now use the approximate expression for the Green function obtained above in order to separate the many-potential term (10) into two parts, one of which contains $G_a^{(2+)}$ instead of $G^{(2+)}$ and is evaluated in a closed form in configuration space, whereas the remainder is calculated by summing a rapidly-converging partial-wave series. Bearing in mind that the partial-wave expansion for the low-energy part of Eq. (10) is already converging very fast (if the parameter ε_0 of the integration contour C_{LH} is chosen as described above), we apply this separation to the high-energy part only. The many-potential term, therefore, is written as the sum of the subtraction and remainder terms,

$$\Delta E_{\rm many} = \Delta E_{\rm many}^{\rm sub} + \Delta E_{\rm many}^{\rm remd}\,. \tag{18}$$

The subtraction term is obtained from the high-energy part of Eq. (10) by the substitution $G^{(2+)} \to G_a^{(2+)}$. Its explicit expression in the Feynman gauge reads

$$\begin{aligned}\Delta E_{\rm many}^{\rm sub} &= \frac{i\alpha}{2\pi}\int_{C_H} d\omega \int d\boldsymbol{x}_1\, d\boldsymbol{x}_2\, \psi_a^{\dagger}(\boldsymbol{x}_1)\,\alpha_\mu \\ &\quad\times G_a^{(2+)}(\varepsilon_a-\omega,\boldsymbol{x}_1,\boldsymbol{x}_2)\,\alpha^\mu\,\psi_a(\boldsymbol{x}_2)\,\frac{\exp(i\sqrt{\omega^2+i0}\,x_{12})}{x_{12}}\,.\end{aligned} \tag{19}$$

The remainder term is obtained from Eq. (10) by applying the substitution $G^{(2+)} \to G^{(2+)} - G_a^{(2+)}$ in the high-energy part.

Calculational formulas for the remainder term $\Delta E_{\rm many}^{\rm remd}$ are obtained by obvious modifications of the corresponding expressions for the many-potential term that can be found, *e.g.*, in Ref. [19]. In order to bring the subtraction term into a form suitable for the numerical evaluation, one has first to perform the angular part of integrations over $\boldsymbol{x}_1$, $\boldsymbol{x}_2$ analytically. To do so, we utilize the fact that both $G_a^{(2+)}$ and the scalar part of the photon propagator depend on angular variables through $\boldsymbol{x}_{12}$ only. Their product can be written as

$$G_a^{(2+)}(\varepsilon_a-\omega,\boldsymbol{x}_1,\boldsymbol{x}_2)\,\frac{\exp(i\sqrt{\omega^2+i0}\,x_{12})}{x_{12}}=\mathcal{F}_1\,i\boldsymbol{\alpha}\cdot\boldsymbol{x}_{12}+\mathcal{F}_2\,\beta+\mathcal{F}_3\,. \tag{20}$$

Here, $\mathcal{F}_i\equiv\mathcal{F}_i(x_1,x_2,\xi)$ are scalar functions depending only on x_1, x_2, and $\xi=\hat{\boldsymbol{x}}_1\cdot\hat{\boldsymbol{x}}_2$, where $\hat{\boldsymbol{x}}=\boldsymbol{x}/x$. Explicit expressions for $\mathcal{F}_i$ are immediately obtained from the definition of the $G_a^{(2+)}$ (16) and the expression for the free Green function $G^{(0)}$ (15). The functions $\mathcal{F}_i$ can be expanded over the set of spherical harmonics by

$$\mathcal{F}_i(x_1,x_2,\xi)=4\pi\sum_{l,m}V_l^{(i)}(x_1,x_2)\,Y_{lm}(\hat{\boldsymbol{x}}_1)\,Y^*_{lm}(\hat{\boldsymbol{x}}_2)\,, \tag{21}$$

where

$$V_l^{(i)}(x_1,x_2)=\frac{1}{2}\int_{-1}^{1}d\xi\,\mathcal{F}_i(x_1,x_2,\xi)\,P_l(\xi) \tag{22}$$

and $P_l(\xi)$ is a Legendre polynomial. Substituting Eq. (21) into Eq. (19) and performing simple angular-momentum algebraic manipulations, we obtain the final result for the many-potential subtraction term that is suitable for the numerical evaluation,

$$\begin{aligned}\Delta E^{\rm sub}_{\rm many} &= 2i\alpha\int_{C_H}d\omega\int_0^{\infty}dx_1\,dx_2\int_{-1}^{1}d\xi\,(x_1x_2)^2\\ &\times\Big\{\mathcal{F}_1\,g_a(x_1)\,f_a(x_2)\,\big[x_1P_{\overline{l}_a}(\xi)-x_2P_{l_a}(\xi)\big]\\ &+\mathcal{F}_1\,f_a(x_1)\,g_a(x_2)\,\big[x_2P_{\overline{l}_a}(\xi)-x_1P_{l_a}(\xi)\big]\\ &+2\mathcal{F}_2\,\big[g_a(x_1)\,g_a(x_2)\,P_{l_a}(\xi)-f_a(x_1)\,f_a(x_2)\,P_{\overline{l}_a}(\xi)\big]\\ &-\mathcal{F}_3\,\big[g_a(x_1)\,g_a(x_2)\,P_{l_a}(\xi)+f_a(x_1)\,f_a(x_2)\,P_{\overline{l}_a}(\xi)\big]\Big\}\,,\end{aligned} \tag{23}$$

where $l_a=|\kappa_a+1/2|-1/2$, $\overline{l}_a=2j_a-l_a$, and $g_a(x)$ and $f_a(x)$ are the upper and the lower radial components of the reference-state wave function $\psi_a(\boldsymbol{x})$.

II. NUMERICAL EVALUATION

The numerical evaluation of the self-energy correction within the present scheme is in many respects similar to that in the standard potential-expansion method. Since the potential-expansion method is well documented (see, *e.g.*, a detailed description in Ref. [19]), here we concentrate on novel features of our evaluation as compared to the standard approach. They appear in the calculations of (*i*) the high-energy part of the many-potential remainder term $\Delta E^{\rm remd}_{\rm many}$ and (*ii*) the many-potential subtraction term $\Delta E^{\rm sub}_{\rm many}$.

The radial integrations over x_1 and x_2 in $\Delta E^{\rm sub}_{\rm many}$ and $\Delta E^{\rm remd}_{\rm many}$ are performed after the change of variables $(x_1, x_2) \to (r, y)$ [4]:

$$r = \min(x_1, x_2)/\max(x_1, x_2)\,, \quad y = 2\sqrt{1-\varepsilon_a^2}\, x_2\,. \tag{24}$$

Numerical evaluation of the radial integrals is complicated [specifically, for small values of the $\mathrm{Re}(\omega)$] by the presence of the function $G^{(0)}(E+\Omega)$ in the integrand. To understand this, one should recall that the analytical behavior of $G^{(0)}(E+\Omega)$ is governed by the parameter $c' = \sqrt{1-(E+\Omega)^2}$. Since in the high-energy part $E \equiv \varepsilon_a - \omega = \varepsilon_a - \varepsilon_0 - iw$ ($w \in \mathbb{R}$), the energy argument is

$$E + \Omega = \varepsilon_a - \varepsilon_0 - iw + \frac{2Z\alpha}{x_1 + x_2}\,. \tag{25}$$

For certain values of x_1 and x_2, $\mathrm{Re}(E+\Omega) = 1$. When w is small, a fast change of the phase of the square root $\sqrt{1-(E+\Omega)^2}$ occurs in the vicinity of this point, which can lead to a numerical instability of the radial integrations. This problem was handled by breaking the integration interval at the point where $\mathrm{Re}(E+\Omega) = 1$ and employing a larger number of integration points in this region.

The numerical evaluation of the subtraction term $\Delta E^{\rm sub}_{\rm many}$ involves an additional numerical integration (over ξ) as compared to that of $\Delta E^{\rm remd}_{\rm many}$. However, since the subtraction term is represented in a closed form (without a partial-wave expansion), its numerical evaluation can still be performed rather efficiently. The integration over ξ contains an integrable singularity at the point $x_{12} = 0$, which was handled by dividing the interval $\xi \in [-1, 1]$ into several parts and employing a sufficiently dense grid near the point $\xi = 1$.

III. RESULTS AND DISCUSSION

In Tables I, II, and III we present a comparison of two different schemes for the evaluation of the self-energy correction for the $1s$, $2s$, and $2p_{1/2}$ states. The labels "A" and "B" stand for the subtraction scheme introduced in this work and for the standard potential-expansion approach, respectively. The entry "Free" denotes the sum of the zero- and one-potential terms (this part is the same in both methods), "Subtraction" stands for the many-potential subtraction term $\Delta E^{\rm sub}_{\rm many}$ (absent in the standard approach), whereas the individual partial-wave expansion contributions correspond to the many-potential remainder term $\Delta E_{\rm many}^{\rm remd}$ and to the many-potential term $\Delta E_{\rm many}$ in the "A" and "B" schemes, respectively. The entry "Behavior" indicates the approximate dependence of the terms of the partial-wave expansion on $|\kappa|$ in the region of interest, *i.e.*, for $|\kappa| = 10 - 30$. The numbers in parentheses represent the uncertainties in the last digit. If no uncertainties are indicated, numerical values are believed to be accurate to all digits specified. Our results obtained within the two approaches are compared with the numerical values by Mohr [6].

The comparison of the data listed in the tables demonstrates that the additional subtraction introduced in this work leads to a significant improvement of the convergence of the partial-wave expansion in all the cases studied. This shows that the new approach is applicable for the evaluation of the self-energy correction in the low-Z region, where the standard potential-expansion approach fails to yield accurate results.

In the low-Z region, one has to deal with numerical cancellations between individual contributions to the self-energy correction. The origin of these cancellations are spurious terms of order $\alpha(Z\alpha)^2 \ln Z\alpha$ that appear in the Feynman gauge when the self-energy correction is separated into the zero, one, and many-potential terms [15] and that have to be cancelled numerically in order to obtain the physical contribution to order $\alpha(Z\alpha)^4$. In our approach, the numerical integrations can be relatively easily performed with sufficient accuracy, so that the numerical cancellations do not pose any serious problems. Even in the most difficult case, $Z = 1$, the numerical scheme proposed yields a result with a reasonable accuracy, $F_{1s}(1\alpha) = 10.316\,85(10)$, which is in a good agreement with the most precise value by Jentschura *et al.* [11], $F_{1s}(1\alpha) = 10.316\,793\,650(1)$.

In Table IV we present the numerical results for the self-energy correction in the region that was not previously tabulated in the literature, $5 < Z < 10$, and compare our numerical values for $Z = 5$ and 10 with evaluations by other authors. It is noteworthy that unlike the previous calculations summarized in Table IV, our evaluation is computationally very cheap. The time of the calculation for one value of Z is less than 1h on a modern personal computer. This feature makes the above approach very promising for extensions to the higher-order self-energy corrections.

To sum up, we have developed a highly efficient scheme for the evaluation of the one-loop self-energy correction for an electron bound in a symmetric local potential (not necessarily the Coulomb one). The approach presented inherits the attractive features of the standard potential-expansion method but yields a much better convergence rate for the resulting partial-wave expansion. As a result, the applicability of the potential-expansion method is extended into the region of large values of the parameter $n^3/(Z\alpha)^2$. We expect that the approach developed will allow one to

TABLE I: Individual contributions to the one-loop self-energy correction for the $1s$ state, in units of $F(Z\alpha)$. "A" denotes the new subtraction scheme, whereas "B" indicates the standard potential-expansion approach.

	$Z=5$		$Z=10$		$Z=92$	
	A	B	A	B	A	B
Free	$-767.728\,001$	$-767.728\,0$	$-184.021\,481$	$-184.021\,48$	$-0.171\,545$	$-0.171\,545$
Subtraction	$30.582\,424$		$11.527\,613$		$0.290\,350$	
$\lvert\kappa\rvert=1$	739.691 981	759.830 8	175.775 040	183.505 51	1.371 144	1.632 207
2	3.435 185	8.855 9	1.260 600	3.339 31	$-0.001\,514$	0.012 042
3	0.227 353	2.299 5	0.094 384	0.863 90	0.001 728	0.008 313
4	0.029 960	1.028 4	0.012 972	0.367 77	0.000 469	0.003 806
5	0.007 001	0.568 2	0.002 982	0.193 45	0.000 155	0.001 988
6	0.002 592	0.352 0	0.001 033	0.114 57	0.000 062	0.001 158
7	0.001 246	0.234 7	0.000 457	0.073 33	0.000 029	0.000 731
8	0.000 682	0.164 8	0.000 231	0.049 60	0.000 015	0.000 490
9	0.000 403	0.120 2	0.000 127	0.034 99	0.000 008	0.000 344
10	0.000 250	0.090 4	0.000 073	0.025 52	0.000 005	0.000 251
11	0.000 162	0.069 7	0.000 044	0.019 12	0.000 003	0.000 188
12	0.000 108	0.054 8	0.000 028	0.014 65	0.000 002	0.000 145
13	0.000 074	0.043 8	0.000 018	0.011 44	0.000 001	0.000 114
14	0.000 052	0.035 5	0.000 012	0.009 08	0.000 001	0.000 091
15	0.000 037	0.029 2	0.000 008	0.007 32	0.000 001	0.000 074
$\sum_{\lvert\kappa\rvert=16}^{35}$	0.000 115	0.167 8	0.000 020	0.038 82	0.000 002	0.000 420
$\sum_{\lvert\kappa\rvert=36}^{\infty}$ (extr.)	0.000 003(2)	0.034(3)	0.000 001(1)	0.007 2(4)	0.000 000	0.000 099(3)
Total	6.251 627(2)	6.252(3)	4.654 162(1)	4.654 1(4)	1.490 916	1.490 916(3)
Ref. [6]	6.251 627(8)		4.654 162 2(2)		1.490 916 0(3)	
Behavior	$30/\lvert\kappa\rvert^5$	$100/\lvert\kappa\rvert^3$	$100/\lvert\kappa\rvert^6$	$25/\lvert\kappa\rvert^3$	$0.5/\lvert\kappa\rvert^5$	$0.25/\lvert\kappa\rvert^3$

significantly improve accuracy of evaluations of the self-energy correction to the hyperfine splitting and of the screened self-energy correction in the low-Z region. In perspective, this approach can also serve as a basis for an evaluation of the two-loop self-energy correction for hydrogen.

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TABLE II: The same as Table I, but for the $2s$ state.

	$Z=5$		$Z=10$		$Z=92$	
	A	B	A	B	A	B
Free	$-1457.418\,809$	$-1457.418\,8$	$-356.528\,846$	$-356.528\,8$	$-1.962\,337$	$-1.962\,337$
Subtraction	$31.058\,101$		$11.890\,558$		$0.275\,605$	
$\lvert\kappa\rvert=1$	$1410.715\,203$	$1429.146\,6$	$339.733\,982$	$346.798\,4$	$3.548\,480$	$3.796\,632$
2	$16.099\,356$	$20.342\,3$	$6.979\,535$	$8.564\,2$	$0.228\,968$	$0.201\,262$
3	$3.688\,342$	$5.475\,2$	$1.722\,985$	$2.395\,0$	$0.073\,832$	$0.078\,764$
4	$1.379\,780$	$2.581\,8$	$0.646\,882$	$1.119\,1$	$0.023\,291$	$0.034\,477$
5	$0.563\,792$	$1.502\,8$	$0.263\,506$	$0.643\,3$	$0.007\,670$	$0.017\,634$
6	$0.233\,686$	$0.979\,1$	$0.108\,871$	$0.414\,0$	$0.002\,586$	$0.010\,043$
7	$0.096\,744$	$0.685\,1$	$0.044\,967$	$0.286\,3$	$0.000\,889$	$0.006\,184$
8	$0.039\,919$	$0.503\,9$	$0.018\,535$	$0.208\,1$	$0.000\,312$	$0.004\,042$
9	$0.016\,454$	$0.384\,5$	$0.007\,645$	$0.157\,1$	$0.000\,114$	$0.002\,770$
10	$0.006\,808$	$0.301\,9$	$0.003\,174$	$0.122\,0$	$0.000\,044$	$0.001\,972$
11	$0.002\,852$	$0.242\,5$	$0.001\,340$	$0.096\,9$	$0.000\,018$	$0.001\,449$
12	$0.001\,228$	$0.198\,5$	$0.000\,585$	$0.078\,5$	$0.000\,008$	$0.001\,094$
13	$0.000\,555$	$0.165\,0$	$0.000\,270$	$0.064\,5$	$0.000\,004$	$0.000\,845$
14	$0.000\,271$	$0.139\,0$	$0.000\,136$	$0.053\,8$	$0.000\,003$	$0.000\,665$
15	$0.000\,147$	$0.118\,4$	$0.000\,076$	$0.045\,3$	$0.000\,002$	$0.000\,533$
$\sum_{\lvert\kappa\rvert=16}^{35}$	$0.000\,400$	$0.839\,6$	$0.000\,207$	$0.297\,8$	$0.000\,005$	$0.002\,851$
$\sum_{\lvert\kappa\rvert=36}^{\infty}$ (extr.)	$0.000\,036(10)$	$0.35(8)$	$0.000\,011(7)$	$0.082(10)$	$0.000\,000$	$0.000\,62(3)$
Total	$6.484\,865(10)$	$6.54(8)$	$4.894\,417(7)$	$4.898(10)$	$2.199\,494$	$2.199\,49(3)$
Ref. [6]	$6.484\,8(2)$		$4.894\,45(6)$		$2.199\,493\,8(3)$	
Behavior	$5/\lvert\kappa\rvert^4$	$100/\lvert\kappa\rvert^{2.5}$	$10/\lvert\kappa\rvert^{4.5}$	$40/\lvert\kappa\rvert^{2.5}$	$10/\lvert\kappa\rvert^5$	$2/\lvert\kappa\rvert^3$

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TABLE III: The same as Table I, but for the $2p_{1/2}$ state.

	$Z=5$		$Z=10$		$Z=92$	
	A	B	A	B	A	B
Free	$-1520.728\,283$	$-1520.728\,3$	$-377.853\,426$	$-377.853\,4$	$-3.966\,890$	$-3.966\,890$
Subtraction	$14.376\,901$		$6.031\,862$		$0.094\,695$	
$\|\kappa\|=1$	$1481.688\,696$	$1483.524\,8$	$361.003\,647$	$361.809\,2$	$3.886\,215$	$3.910\,643$
2	$18.863\,382$	$21.167\,6$	$8.100\,485$	$9.121\,6$	$0.219\,596$	$0.221\,754$
3	$3.816\,241$	$5.880\,8$	$1.740\,929$	$2.651\,9$	$0.058\,070$	$0.074\,793$
4	$1.186\,255$	$2.832\,7$	$0.546\,763$	$1.267\,1$	$0.017\,578$	$0.032\,082$
5	$0.417\,922$	$1.674\,6$	$0.193\,629$	$0.737\,3$	$0.005\,943$	$0.016\,268$
6	$0.155\,297$	$1.103\,9$	$0.072\,407$	$0.477\,4$	$0.002\,214$	$0.009\,235$
7	$0.059\,471$	$0.779\,4$	$0.028\,021$	$0.330\,9$	$0.000\,913$	$0.005\,686$
8	$0.023\,323$	$0.577\,2$	$0.011\,192$	$0.240\,5$	$0.000\,420$	$0.003\,724$
9	$0.009\,401$	$0.442\,7$	$0.004\,654$	$0.181\,1$	$0.000\,215$	$0.002\,560$
10	$0.003\,945$	$0.348\,9$	$0.002\,053$	$0.140\,2$	$0.000\,122$	$0.001\,830$
11	$0.001\,764$	$0.281\,1$	$0.000\,985$	$0.110\,9$	$0.000\,074$	$0.001\,350$
12	$0.000\,866$	$0.230\,4$	$0.000\,528$	$0.089\,3$	$0.000\,048$	$0.001\,024$
13	$0.000\,479$	$0.191\,7$	$0.000\,318$	$0.073\,0$	$0.000\,033$	$0.000\,794$
14	$0.000\,300$	$0.161\,5$	$0.000\,212$	$0.060\,5$	$0.000\,023$	$0.000\,628$
15	$0.000\,209$	$0.137\,5$	$0.000\,153$	$0.050\,7$	$0.000\,016$	$0.000\,505$
$\sum_{\|\kappa\|=16}^{35}$	$0.000\,928$	$0.961\,0$	$0.000\,668$	$0.320\,3$	$0.000\,054$	$0.002\,747$
$\sum_{\|\kappa\|=36}^{\infty}$ (extr.)	$0.000\,13(3)$	$0.32(8)$	$0.000\,08(2)$	$0.079(10)$	$0.000\,002$	$0.000\,61(3)$
Total	$-0.122\,77(3)$	$-0.11(8)$	$-0.114\,84(2)$	$-0.113(10)$	$0.319\,341$	$0.319\,34(3)$
Ref. [6]	$-0.122\,8(2)$		$-0.114\,83(4)$		$0.319\,340\,8(4)$	
Behavior	$2/\|\kappa\|^{3.5}$	$130/\|\kappa\|^{2.5}$	$7/\|\kappa\|^4$	$200/\|\kappa\|^3$	$10/\|\kappa\|^5$	$2/\|\kappa\|^3$

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TABLE IV: One-loop self-energy correction, in terms of $F(Z\alpha)$.

	$1s$	$2s$	$2p_{1/2}$	$2p_{3/2}$	Ref.
5	$6.251\,627(2)$	$6.484\,865(10)$	$-0.122\,77(3)$	$0.125\,64(4)$	
	$6.251\,627(8)$	$6.484\,8(2)$	$-0.122\,8(2)$	$0.125\,6(1)$	[6]
	$6.251\,6270\,78(1)$	$6.484\,860\,42(1)$	$-0.122\,774\,94(1)$	$0.125\,623\,30(1)$	[11]
	$6.251\,620(3)$				[14]
6	$5.817\,887(1)$	$6.052\,312(10)$	$-0.121\,43(3)$	$0.126\,43(4)$	
7	$5.458\,026\,1(8)$	$5.693\,756(10)$	$-0.119\,95(3)$	$0.127\,31(3)$	
8	$5.152\,029\,1(8)$	$5.389\,169(9)$	$-0.118\,35(3)$	$0.128\,27(3)$	
9	$4.887\,004\,2(8)$	$5.125\,656(8)$	$-0.116\,65(2)$	$0.129\,29(4)$	
10	$4.654\,162\,4(8)$	$4.894\,417(7)$	$-0.114\,84(2)$	$0.130\,36(4)$	
	$4.654\,162\,2(2)$	$4.894\,45(6)$	$-0.114\,83(4)$	$0.130\,36(2)$	[6]
	$4.654\,161\,9(1)$	$4.894\,444\,4(6)$	$-0.114\,852(2)$	$0.130\,350\,7(3)$	[14]

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