

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

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A 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 the other methods reported in the literature.

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I. 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. For several high- Z ions, a successful evaluation of this correction was performed by Desiderio and Johnson [1] using the method proposed by Brown, Langer, and Schaefer [2]. A 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. 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 (~ 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) and (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 by extensions of the potential-expansion method up to now.

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

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

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

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

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.

A 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 yields the fastest convergence of the partial-wave expansion among the methods reported so far in the literature.

II. 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

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

where $\alpha_\mu = (1, \boldsymbol{\alpha})$, $\boldsymbol{\alpha}$, and β are the Dirac matrices, $G(\omega, \mathbf{x}_1, \mathbf{x}_2) = [\omega - \mathcal{H}(1-i0)]^{-1}$, $\mathcal{H} = \mathcal{H}_0 + V(x)$, $\mathcal{H}_0 = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta$ 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

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

where $x_{12} = |\mathbf{x}_{12}| = |\mathbf{x}_1 - \mathbf{x}_2|$, and the branch of the square root is fixed by the condition $\text{Im}(\sqrt{\omega^2 + i0}) > 0$. 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 ,

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

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

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

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]:

$$\Delta E = \Delta E_{\text{zero}} + \Delta E_{\text{one}} + \Delta E_{\text{many}}, \quad (7)$$

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

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

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

where $\mathbf{q} = \mathbf{p}_1 - \mathbf{p}_2$, $\bar{\psi}_a(\mathbf{p}) = \psi_a^\dagger(\mathbf{p}) \gamma^0$, 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:

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

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 Ref. [19].) The high-energy part of the contour is $C_H = (\varepsilon_0 - i\infty, \varepsilon_0 - i0) + [\varepsilon_0 + i0, \varepsilon_0 + i\infty)$. 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 ΔE_{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,

$$G(E, \mathbf{x}_1, \mathbf{x}_2) = G^{(0)}(E, \mathbf{x}_1, \mathbf{x}_2) + \int d\mathbf{z} G^{(0)}(E, \mathbf{x}_1, \mathbf{z}) V(\mathbf{z}) \times G^{(0)}(E, \mathbf{z}, \mathbf{x}_2) + \int d\mathbf{z}_1 d\mathbf{z}_2 G^{(0)}(E, \mathbf{x}_1, \mathbf{z}_1) V(\mathbf{z}_1) \times G^{(0)}(E, \mathbf{z}_1, \mathbf{z}_2) V(\mathbf{z}_2) G^{(0)}(E, \mathbf{z}_2, \mathbf{x}_2) + \dots \quad (11)$$

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, $\mathbf{x}_1 \approx \mathbf{x}_2$. 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]. In this region the commutators of the potential V with the free Green function $G^{(0)}$ are small and can be neglected, which corresponds to expanding $V(\mathbf{z})$ in a Taylor series around $\mathbf{z} = \mathbf{x}_1$ (or \mathbf{x}_2) and keeping only the first term. Commuting V out to the left in Eq. (11) and repeatedly employing the identity

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

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

$$G_a(E, \mathbf{x}_1, \mathbf{x}_2) = G^{(0)}(E, \mathbf{x}_1, \mathbf{x}_2) - V(x_1) \frac{\partial}{\partial E} G^{(0)}(E, \mathbf{x}_1, \mathbf{x}_2) + V^2(x_1) \frac{\partial^2}{\partial E^2} G^{(0)}(E, \mathbf{x}_1, \mathbf{x}_2) + \dots \quad (13)$$

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

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

where $\Omega = -V(x_1) = Z\alpha/x_1$. Commuting V out to the right in Eq. (11), we obtain the same representation for G_a but with $\Omega = Z\alpha/x_2$.

It should be noted that the idea of commuting the potential V outside in the one-potential term was originally 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 $\mathbf{x}_1 \approx \mathbf{x}_2$ 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 power-series expansion of the potential V and the reference-state wave functions ψ_a around the point $\mathbf{x}_1 = \mathbf{x}_2$.

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]

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

($c = \sqrt{1 - E^2}$), we can employ this expression for the evaluation of G_a .

An analogous to Eq. (14) approximation for the function $G^{(2+)}$ is obtained by subtracting the first two terms of the Taylor expansion from G_a ,

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

According to the derivation, the functions $G_a(E, \mathbf{x}_1, \mathbf{x}_2)$ and $G_a^{(2+)}(E, \mathbf{x}_1, \mathbf{x}_2)$ approximate, correspondingly, $G(E, \mathbf{x}_1, \mathbf{x}_2)$ and $G^{(2+)}(E, \mathbf{x}_1, \mathbf{x}_2)$ in the region where $\mathbf{x}_1 \approx \mathbf{x}_2$. 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:

$$\Omega = \frac{2Z\alpha}{x_1 + x_2}, \quad (17)$$

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 is thus written as a sum of the subtraction and the remainder term,

$$\Delta E_{\text{many}} = \Delta E_{\text{many}}^{\text{sub}} + \Delta E_{\text{many}}^{\text{remd}}. \quad (18)$$

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

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

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

Calculational formulas for the remainder term $\Delta E_{\text{many}}^{\text{remd}}$ 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 obtain the subtraction term in a form suitable for the numerical evaluation, one has first to perform the angular part of integrations over $\mathbf{x}_1, \mathbf{x}_2$ 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 \mathbf{x}_{12} only. Their product can be written as

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

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

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

where

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

and $P_l(\xi)$ is a Legendre polynomial.

Substituting Eq. (21) into Eq. (19) and performing simple angular-momentum algebraic manipulations, we obtain

$$\begin{aligned} \Delta E_{\text{many}}^{\text{sub}} = & 2i\alpha \int_{C_H} d\omega \int_0^\infty dx_1 dx_2 \int_{-1}^1 d\xi (x_1 x_2)^2 \{ \mathcal{F}_1(\omega, x_1, x_2, \xi) \\ & \times g_a(x_1) f_a(x_2) [x_1 P_{\bar{l}_a}(\xi) - x_2 P_{l_a}(\xi)] \\ & + \mathcal{F}_1(\omega, x_1, x_2, \xi) f_a(x_1) g_a(x_2) [x_2 P_{\bar{l}_a}(\xi) \\ & - x_1 P_{l_a}(\xi)] + 2\mathcal{F}_2(\omega, x_1, x_2, \xi) [g_a(x_1) g_a(x_2) P_{l_a}(\xi) \\ & - f_a(x_1) f_a(x_2) P_{\bar{l}_a}(\xi)] - \mathcal{F}_3(\omega, x_1, x_2, \xi) \\ & \times [g_a(x_1) g_a(x_2) P_{l_a}(\xi) + f_a(x_1) f_a(x_2) P_{\bar{l}_a}(\xi)] \}, \end{aligned} \quad (23)$$

where $l_a = |\kappa_a + 1/2| - 1/2$, $\bar{l}_a = 2j_a - l_a$, and $g_a(x)$ and $f_a(x)$ are the upper and the lower radial components of the reference-state wave function $\psi_a(\mathbf{x})$. The integration over ω in Eq. (23) can be carried out analytically in terms of the exponential integral function, as described in the Appendix, leaving a three-dimensional integration over the radial variables to be performed numerically.

III. 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 approach. Since the potential-expansion method is well documented (see, e.g., a detailed description in Ref. [19]), here we concentrate on distinct 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 $\Delta E_{\text{many}}^{\text{remd}}$ and (ii) the many-potential subtraction term $\Delta E_{\text{many}}^{\text{sub}}$.

The radial integrations over x_1 and x_2 in the remainder term $\Delta E_{\text{many}}^{\text{remd}}$ are performed after the change of variables $(x_1, x_2) \rightarrow (r, y)$ [4]:

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

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

$$E + \Omega = \varepsilon_a - \varepsilon_0 - i\omega + \frac{2Z\alpha}{x_1 + x_2}. \quad (25)$$

For certain values of x_1 and x_2 , $\text{Re}(E + \Omega) = 1$. When ω is small, a fast change of the phase of the square root

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	-767.728001	-767.7280	-184.021481	-184.02148	-0.171545	-0.171545
Subtraction	30.582424		11.527613		0.290350	
$ \kappa =1$	739.691981	759.8308	175.775040	183.50551	1.371144	1.632207
2	3.435185	8.8559	1.260600	3.33931	-0.001514	0.012042
3	0.227353	2.2995	0.094384	0.86390	0.001728	0.008313
4	0.029960	1.0284	0.012972	0.36777	0.000469	0.003806
5	0.007001	0.5682	0.002982	0.19345	0.000155	0.001988
6	0.002592	0.3520	0.001033	0.11457	0.000062	0.001158
7	0.001246	0.2347	0.000457	0.07333	0.000029	0.000731
8	0.000682	0.1648	0.000231	0.04960	0.000015	0.000490
9	0.000403	0.1202	0.000127	0.03499	0.000008	0.000344
10	0.000250	0.0904	0.000073	0.02552	0.000005	0.000251
11	0.000162	0.0697	0.000044	0.01912	0.000003	0.000188
12	0.000108	0.0548	0.000028	0.01465	0.000002	0.000145
13	0.000074	0.0438	0.000018	0.01144	0.000001	0.000114
14	0.000052	0.0355	0.000012	0.00908	0.000001	0.000091
15	0.000037	0.0292	0.000008	0.00732	0.000001	0.000074
$\sum_{ \kappa =16}^{35}$	0.000115	0.1678	0.000020	0.03882	0.000002	0.000420
$\sum_{ \kappa =36}^{\infty}$ (extr.)	0.000003(2)	0.034(3)	0.000001(1)	0.0072(4)	0.000000	0.000099(3)
Total	6.251627(2)	6.252(3)	4.654162(1)	4.6541(4)	1.490916	1.490916(3)
Ref. [6]	6.251627(8)		4.6541622(2)		1.4909160(3)	
Behavior	$30/ \kappa ^5$	$100/ \kappa ^3$	$100/ \kappa ^6$	$25/ \kappa ^3$	$0.5/ \kappa ^5$	$0.25/ \kappa ^3$

$\sqrt{1-(E+\Omega)^2}$ 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 $\text{Re}(E+\Omega)=1$ and employing a larger number of integration points in this region.

The numerical evaluation of the subtraction term $\Delta E_{\text{many}}^{\text{sub}}$ consists of a three-dimensional integration over the radial variables, which has a structure of the standard two-electron integral,

$$J = \int_0^{\infty} dx_1 dx_2 \int_{-1}^1 d\xi \frac{(x_1 x_2)^2}{x_{12}} f(x_1, x_2, \xi), \quad (26)$$

where the function f has a finite limit for $x_{12} \rightarrow 0$. The integrable singularity in this expression is removed by employing the *perimetric* coordinates [38],

$$u = x_1 + x_2 - x_{12}, \quad (27a)$$

$$v = x_1 - x_2 + x_{12}, \quad (27b)$$

$$w = -x_1 + x_2 + x_{12}. \quad (27c)$$

In the new variables, the integral J is

$$J = \frac{1}{4} \int_0^{\infty} du dv dw x_1 x_2 f(x_1, x_2, \xi). \quad (28)$$

Performing the integrations in this expression numerically, one should have in mind that the function f contains a square root, whose argument changes its sign for certain combinations of the radial variables, similarly to the case described for the remainder term $\Delta E_{\text{many}}^{\text{remd}}$. The point at which the argument of the square root vanishes is

$$\varepsilon_a - \varepsilon_0 + \frac{2Z\alpha}{x_1 + x_2} = 1. \quad (29)$$

This feature was taken into account by breaking the integration intervals at the singular point and by employing a larger number of integration points in its vicinity.

IV. RESULTS AND DISCUSSION

In Tables I–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”

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	-1457.418809	-1457.4188	-356.528846	-356.5288	-1.962337	-1.962337
Subtraction	31.058101		11.890558		0.275605	
$ \kappa =1$	1410.715203	1429.1466	339.733982	346.7984	3.548480	3.796632
2	16.099356	20.3423	6.979535	8.5642	0.228968	0.201262
3	3.688342	5.4752	1.722985	2.3950	0.073832	0.078764
4	1.379780	2.5818	0.646882	1.1191	0.023291	0.034477
5	0.563792	1.5028	0.263506	0.6433	0.007670	0.017634
6	0.233686	0.9791	0.108871	0.4140	0.002586	0.010043
7	0.096744	0.6851	0.044967	0.2863	0.000889	0.006184
8	0.039919	0.5039	0.018535	0.2081	0.000312	0.004042
9	0.016454	0.3845	0.007645	0.1571	0.000114	0.002770
10	0.006808	0.3019	0.003174	0.1220	0.000044	0.001972
11	0.002852	0.2425	0.001340	0.0969	0.000018	0.001449
12	0.001228	0.1985	0.000585	0.0785	0.000008	0.001094
13	0.000555	0.1650	0.000270	0.0645	0.000004	0.000845
14	0.000271	0.1390	0.000136	0.0538	0.000003	0.000665
15	0.000147	0.1184	0.000076	0.0453	0.000002	0.000533
$\sum_{ \kappa =16}^{35}$	0.000400	0.8396	0.000207	0.2978	0.000005	0.002851
$\sum_{ \kappa =36}^{\infty}$ (extr.)	0.000036(10)	0.35(8)	0.000011(7)	0.082(10)	0.000000	0.00062(3)
Total	6.484865(10)	6.54(8)	4.894417(7)	4.898(10)	2.199494	2.19949(3)
Ref. [6]	6.4848(2)		4.89445(6)		2.1994938(3)	
Behavior	$5/ \kappa ^4$	$100/ \kappa ^{2.5}$	$10/ \kappa ^{4.5}$	$40/ \kappa ^{2.5}$	$10/ \kappa ^5$	$2/ \kappa ^3$

stands for the many-potential subtraction term $\Delta E_{\text{many}}^{\text{sub}}$ (absent in the standard approach), whereas the individual partial-wave expansion contributions correspond to the many-potential remainder term $\Delta E_{\text{many}}^{\text{remd}}$ and to the many-potential term ΔE_{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 properties of the partial-wave expansion in all the cases studied. It also indicates that this 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 canceled numerically in order to obtain the physical contri-

bution to order $\alpha(Z\alpha)^4$. In our approach, the numerical integrations can be relatively easily performed up to a sufficient accuracy, so that the numerical cancellations do not pose any serious problems. Even in the most difficult case, $Z=1$, the present numerical scheme yields a result with a reasonable accuracy, $F_{1s}(1\alpha)=10.31685(10)$, which is in a good agreement with the most precise value by Jentschura *et al.* [11], $F_{1s}(1\alpha)=10.316793650(1)$.

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 1 h on a modern personal computer. This feature makes the present 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

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	-1520.728283	-1520.7283	-377.853426	-377.8534	-3.966890	-3.966890
Subtraction	14.376901		6.031862		0.094695	
$ \kappa =1$	1481.688696	1483.5248	361.003647	361.8092	3.886215	3.910643
2	18.863382	21.1676	8.100485	9.1216	0.219596	0.221754
3	3.816241	5.8808	1.740929	2.6519	0.058070	0.074793
4	1.186255	2.8327	0.546763	1.2671	0.017578	0.032082
5	0.417922	1.6746	0.193629	0.7373	0.005943	0.016268
6	0.155297	1.1039	0.072407	0.4774	0.002214	0.009235
7	0.059471	0.7794	0.028021	0.3309	0.000913	0.005686
8	0.023323	0.5772	0.011192	0.2405	0.000420	0.003724
9	0.009401	0.4427	0.004654	0.1811	0.000215	0.002560
10	0.003945	0.3489	0.002053	0.1402	0.000122	0.001830
11	0.001764	0.2811	0.000985	0.1109	0.000074	0.001350
12	0.000866	0.2304	0.000528	0.0893	0.000048	0.001024
13	0.000479	0.1917	0.000318	0.0730	0.000033	0.000794
14	0.000300	0.1615	0.000212	0.0605	0.000023	0.000628
15	0.000209	0.1375	0.000153	0.0507	0.000016	0.000505
$\sum_{ \kappa =16}^{35}$	0.000928	0.9610	0.000668	0.3203	0.000054	0.002747
$\sum_{ \kappa =36}^{\infty}$ (extr.)	0.00013(3)	0.32(8)	0.00008(2)	0.079(10)	0.000002	0.00061(3)
Total	-0.12277(3)	-0.11(8)	-0.11484(2)	-0.113(10)	0.319341	0.31934(3)
Ref. [6]	-0.1228(2)		-0.11483(4)		0.3193408(4)	
Behavior	$2/ \kappa ^{3.5}$	$130/ \kappa ^{2.5}$	$7/ \kappa ^4$	$200/ \kappa ^3$	$10/ \kappa ^5$	$2/ \kappa ^3$

allow one to 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 and could be also applied for higher-order self-energy corrections.

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APPENDIX: INTEGRALS OVER THE VIRTUAL PHOTON ENERGY IN THE SUBTRACTION TERM

The integral over ω in Eq. (23) can be expressed as a linear combination of the basic integrals J_i ,

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

Z	1s	2s	$2p_{1/2}$	$2p_{3/2}$	Ref.
5	6.251627(2)	6.484865(10)	-0.12277(3)	0.12564(4)	
	6.251627(8)	6.4848(2)	-0.1228(2)	0.1256(1)	[6]
	6.251627078(1)	6.48486042(1)	-0.12277494(1)	0.12562330(1)	[11]
	6.251620(3)				[14]
6	5.817887(1)	6.052312(10)	-0.12143(3)	0.12643(4)	
7	5.4580261(8)	5.693756(10)	-0.11995(3)	0.12731(3)	
8	5.1520291(8)	5.389169(9)	-0.11835(3)	0.12827(3)	
9	4.8870042(8)	5.125656(8)	-0.11665(2)	0.12929(4)	
10	4.6541624(8)	4.894417(7)	-0.11484(2)	0.13036(4)	
	4.6541622(2)	4.89445(6)	-0.11483(4)	0.13036(2)	[6]
	4.6541619(1)	4.8944444(6)	-0.114852(2)	0.1303507(3)	[14]

$$J_i = i \int_{C_H} d\omega f_i(\omega) \exp[(i|\omega| - c)x_{12}], \quad (\text{A1})$$

where $c = \sqrt{1 - (\varepsilon - \omega)^2}$, $C_H = (\varepsilon_0 - i\infty, \varepsilon_0 - i0) + [\varepsilon_0 + i0, \varepsilon_0 + i\infty)$, $\varepsilon_0 > 0$ is the parameter of the contour, ε is either ε_a or $\varepsilon_a + \Omega$, and the functions f_i are

$$f_1(\omega) = 1, \quad (\text{A2})$$

$$f_2(\omega) = x_{12} \frac{\varepsilon - \omega}{c}, \quad (\text{A3})$$

$$f_3(\omega) = c, \quad (\text{A4})$$

$$f_4(\omega) = \varepsilon - \omega, \quad (\text{A5})$$

$$f_5(\omega) = x_{12} \frac{(\varepsilon - \omega)^2}{c}. \quad (\text{A6})$$

Let us evaluate, e.g., the integral J_1 . Introducing the new variable y by $\omega = \varepsilon_0 + iy$ ($\omega = \varepsilon_0 - iy$) in the upper (lower) part of the contour, we obtain

$$J_1 = -2 \operatorname{Re} \exp[i\varepsilon_0 x_{12}] \times \int_0^\infty dy \exp\{-[y + \sqrt{1 + (y + i\alpha)^2}]x_{12}\}, \quad (\text{A7})$$

where $\alpha = \varepsilon - \varepsilon_0$. This integral is evaluated by introducing the new variable

$$t = y + \sqrt{1 + (y + i\alpha)^2} - \sqrt{1 - \alpha^2}, \quad (\text{A8})$$

with the result

$$J_1 = -\operatorname{Re} \exp[(i\varepsilon_0 - a)x_{12}] \times \left[\frac{1}{x_{12}} + \frac{1}{z} - x_{12} \exp(zx_{12}) E_1(zx_{12}) \right], \quad (\text{A9})$$

where $a = \sqrt{1 - \alpha^2}$, $z = a + i\alpha$, and $E_1(z)$ is the exponential integral function. The results for other basic integrals are

$$J_2 = -\operatorname{Im} \exp[(i\varepsilon_0 - a)x_{12}] \times \left[1 - \frac{x_{12}}{z} + x_{12}^2 \exp(zx_{12}) E_1(zx_{12}) \right], \quad (\text{A10})$$

$$J_3 = -\frac{1}{2} \operatorname{Re} \exp[(i\varepsilon_0 - a)x_{12}] \left[\frac{1}{x_{12}^2} + \frac{z}{x_{12}} + \frac{1}{2z^2} - \frac{x_{12}}{2z} + \left(2 + \frac{x_{12}^2}{2} \right) \exp(zx_{12}) E_1(zx_{12}) \right], \quad (\text{A11})$$

$$J_4 = -\frac{1}{2} \operatorname{Im} \exp[(i\varepsilon_0 - a)x_{12}] \left[\frac{1}{x_{12}^2} + \frac{z}{x_{12}} - \frac{1}{2z^2} + \frac{x_{12}}{2z} - \frac{x_{12}^2}{2} \exp(zx_{12}) E_1(zx_{12}) \right], \quad (\text{A12})$$

$$J_5 = -\frac{1}{2} \operatorname{Re} \exp[(i\varepsilon_0 - a)x_{12}] \left[-4i\alpha - \frac{1}{x_{12}} - \frac{2}{z} + z - \frac{x_{12}}{2z^2} + \frac{x_{12}^2}{2z} + x_{12} \left(2 - \frac{x_{12}^2}{2} \right) \exp(zx_{12}) E_1(zx_{12}) \right]. \quad (\text{A13})$$

All the expressions for the integrals J_i can readily be evaluated numerically. A detailed description of an algorithm for the computation of the exponential integral function of a complex argument can be found in Ref. [14].

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