The two-loop self-energy: diagrams in the coordinate-momentum representation

Vladimir A. Yerokhin
Center for Advanced Studies, St. Petersburg State Polytechnical University, Polytekhnichestkaya 29, St. Petersburg 195251, Russia

The paper reports a technique of evaluation of Feynman diagrams in the mixed coordinate-momentum representation. The technique is employed for a recalculation of the two-loop self-energy correction for the ground state of hydrogen-like ions with the nuclear charge numbers \( Z = 10 − 30 \). The numerical accuracy is considerably improved as compared to the previous calculations. The higher-order (in \( Z \alpha \)) remainder function is inferred from the numerical results and extrapolated towards \( Z = 0 \) and 1. The extrapolated value for hydrogen is consistent (but still not in perfect agreement) with the analytical result obtained within the perturbative approach.

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I. INTRODUCTION

Investigations of the Lamb shift in atomic systems provide one of the most stringent tests of quantum electrodynamics (QED). They are also used for the determination of fundamental physical constants [1]. The main factors limiting the present theoretical understanding of the Lamb shift are the binding two-loop QED effects and, first of all, the two-loop self-energy correction.

Theoretical investigations of QED effects in light atoms traditionally rely on the perturbative expansion in the binding-strength parameter \( Z \alpha \) (\( Z \) is the nuclear charge and \( \alpha \) is the fine structure constant). The state of the art of such calculations is the evaluation of the dominant part of the two-loop correction to order \( m \alpha^2(Z\alpha)^6 \) [2–5]. The main problem of the \( Z\alpha \)-expansion approach is the difficulty of estimation of uncalculated higher-order effects. In the case of the two-loop self-energy correction, the higher-order binding effects are above the experimental error both for the light systems (particularly, for the hydrogen atom [6]) and for the heavy ions [7–10].

In the present investigation, we use the all-order approach which is nonperturbative in the parameter \( Z \alpha \). The nonperturbative calculations started with the pioneering works of Wichmann and Kroll [11] and P. J. Mohr [12, 13]. For heavy ions, the all-order approach is the only alternative as the parameter of \( Z \alpha \) is of order of unity. For light systems, this method is complementary to the \( Z\alpha \)-expansion approach and can provide results for the high-order remainder beyond the known \( Z\alpha \)-expansion terms.

The all-order calculation of the two-loop self-energy correction depicted on Fig. 1 was a long and difficult project accomplished in a series of papers [14–19]. The numerical results obtained in these studies agreed well with the first terms of the \( Z\alpha \) expansion calculated within the perturbative approach. However, a significant disagreement was reported [18] for the contribution to order \( m\alpha^2(Z\alpha)^6 \) (the so-called \( B_{60} \) coefficient). A reliable determination of this contribution from the all-order results requires a high numerical accuracy to be achieved for the low values of \( Z \), which is a challenging task. In our recent investigation [20], we briefly reported a new calculational technique for the evaluation of Feynman diagrams in the mixed coordinate-momentum representation. This technique significantly improved the numerical accuracy of the two-loop self-energy calculation and to a large extent removed the disagreement with the analytical approach.

In the present paper, we present a detailed description of this calculational technique. The relativistic units (\( m = \hbar = c = 1 \)) and the Heavinside charge units (\( \alpha = e^2/4\pi, e < 0 \)) will be used throughout the paper.

II. TWO-LOOP SELF-ENERGY

The Feynman diagrams representing the two-loop self-energy correction are shown in Fig. 1. The contribution of the first diagram [Fig. 1(a)] is conveniently divided into two parts, the irreducible and the reducible one. The reducible part is induced by the virtual states with the energy \( \varepsilon_n = \varepsilon_a \) in the middle electron propagator (\( \varepsilon_a \) is the energy of the reference state), and the irreducible part is the remainder. The irreducible part (often referred to as the loop-after-loop correction) can be interpreted as a second-order perturbation induced by the one-loop self-energy operator. The corresponding expression reads

\[
\Delta E_{LAL} = \left< \gamma_0 \tilde{\Sigma}(\varepsilon_a) G^\text{red} \gamma_0 \tilde{\Sigma}(\varepsilon_a) \right>,
\]

where \( \tilde{\Sigma}(\varepsilon_a) = \Sigma(\varepsilon_a) - \delta m \), \( \Sigma(\epsilon) \) is the one-loop self-energy operator [17], \( \delta m \) is the corresponding mass counterterm, and \( G^\text{red} \) is the reduced Dirac-Coulomb Green function. The irreducible part is finite and can be calculated separately by generalizing various methods developed for the one-loop self-energy.

The reducible part is given by

\[
\Delta E_{\text{red}} = \Delta E_{\text{SE}} \left< \gamma_0 \frac{\partial}{\partial \varepsilon} \tilde{\Sigma}(\varepsilon) \right>_{\varepsilon = \varepsilon_a},
\]

where \( \Delta E_{\text{SE}} = \left< \gamma_0 \tilde{\Sigma}(\varepsilon_a) \right> \) is the one-loop self-energy correction.
where δm will be referred to as the nucleus.

The contribution induced by the diagram in Fig. 1(b) will be referred to as the overlapping term. It is given by

\[ \Delta E_O = 2i\alpha \int_{-\infty}^{\infty} d\omega_1 \int d\mathbf{x}_1 \cdots d\mathbf{x}_4 D(\omega_1, x_{12}) \psi_{a}^{\dagger}(\mathbf{x}_1) \times \alpha_{\mu} G(\varepsilon_a - \omega_1) \gamma^\mu \Lambda^\mu(\varepsilon_a - \omega_1, \varepsilon_a) \psi_a(\mathbf{x}_4) - \delta m_O, \tag{3} \]

where δmO is the mass counterterm, D(ω, x_{12}) is the radial part of the photon propagator in the Feynman gauge,

\[ D(\omega, x_{12}) = \frac{\exp(i \sqrt{\omega^2 + 20} x_{12})}{4\pi x_{12}}, \tag{4} \]

G(ε) is the Dirac-Coulomb Green function defined by G(ε) = [ε - \mathcal{H}(1-i0)]^{-1}, with \mathcal{H} being the Dirac Coulomb Hamiltonian, and x_{12} = |x_1 - x_2|. The vertex function \Lambda^\mu is defined as

\[ \Lambda^\mu(\varepsilon_a - \omega_1, \varepsilon_a) = 2i\alpha \gamma^0 \int_{-\infty}^{\infty} d\omega_2 D(\omega_2, x_{24}) \alpha_\nu \times G(\varepsilon_a - \omega_1 - \omega_2) \alpha^\mu G(\varepsilon_a - \omega_2) \alpha^\nu. \tag{5} \]

The contribution induced by the diagram in Fig. 1(c) will be referred to as the nested term. It reads

\[ \Delta E_N = 2i\alpha \int_{-\infty}^{\infty} d\omega_1 \int d\mathbf{x}_1 \cdots d\mathbf{x}_4 D(\omega_1, x_{14}) \psi_{a}^{\dagger}(\mathbf{x}_1) \times \alpha_{\mu} G(\varepsilon_a - \omega_1) \gamma^\mu \Sigma(\varepsilon_a - \omega_1) G(\varepsilon_a - \omega_1) \alpha^\mu \psi_a(\mathbf{x}_4) - \delta m_N, \tag{6} \]

where δm_N denotes the mass counterterm.

The general analysis [17] shows that the sum of the reducible, the overlapping, and the nested terms is finite. However, the individual contributions are divergent both in the ultraviolet and the infrared regions of virtual photon energies. In order to make all contributions explicitly finite and suitable for a numerical evaluation, a careful rearrangement of individual parts is required. This rearrangement is discussed in detail in Ref. [17] and will not be repeated here. The general idea is that the bound electron propagators in the loops are expanded in terms of the interaction with the binding field and the resulting contributions are grouped together into three large classes: (i) the part calculated in the coordinate space, conventionally termed as the M term and denoted by ΔE_M, (ii) the part calculated in the momentum space (the F term ΔE_F), and (iii) the part calculated in the

mixed coordinate-momentum representation (the P term ΔE_P),

\[ \Delta E_{red} + \Delta E_O + \Delta E_N = \Delta E_M + \Delta E_F + \Delta E_P. \tag{7} \]

All the three terms can be made explicitly finite and calculated separately. The calculational technique is completely different for each term. In the present investigation, we concentrate on the P term, as the scheme of evaluation of the other two was described in detail in Ref. [17] and has not been changed significantly since that work.

### III. P TERM: BASIC FORMULAS

The Feynman diagrams contributing to the P term are shown in Fig. 2. They arise from the diagrams in Fig. 1 when the bound-electron propagators in the loops are expanded in terms of the interaction with the binding field. The characteristic feature of the diagrams on Fig. 2 is that the ultraviolet divergences in them originate from the one-loop subgraphs only. The divergent subgraphs are covariantly regularized and calculated in the momentum space, whereas the remaining part of the diagrams does not need any regularization and is evaluated in the coordinate space.

It should be mentioned that the necessity of calculation of Feynman diagrams in the mixed coordinate-momentum representation is a distinctive feature of the two-loop effects treated to all orders in the parameter Zα. Because of this, the P term has no analog neither in the one-loop calculations nor, to the best of our knowledge, in any other previous calculations. (All other two-loop effects evaluated to all orders in Zα were effectively reduced to one-loop contributions, see Ref. [21] and references therein.) For the first time the P term was calculated in Ref. [15] with help of a finite basis set representation of the spectrum of the Dirac equation. In the present investigation we report a different technique based on the analytical representation of the Green function in terms of the Whittaker functions.
As shown in Fig. 2, the \( P \) term is represented by a sum of five terms,

\[
\Delta E_P = \Delta E_{P,a} + \Delta E_{P,b} + \Delta E_{P,c} + \Delta E_{P,d} + \Delta E_{P,e},
\]

(8)
each of which refers to the corresponding diagram. In order to make the individual terms finite, we assume that the one-loop subgraphs are represented by the renormalized operators and that the infrared reference-state singularities are removed by the minimal subtractions. It can be explicitly checked that such definition of the \( P \) term is equivalent to the definition of Ref. [17], so that the present numerical results are directly comparable with those of the previous work.

The contribution of the diagram in Fig. 2(a) is given by

\[
\Delta E_{P,a} = 2i\alpha \int_{-\infty}^{\infty} d\omega \int \frac{dp}{(2\pi)^3} \int dx_1 dx_2 D(\omega, x_{12}) \\
\times \psi_{\mu}^{\dagger}(x_1) \alpha_{\mu} \left[ G_{V}(E, x_1, p) S_{1}(E, p) G_{V}(E, p, x_2) \\
- G_{V}^{(a)}(E, x_1, p) S_{1}(\varepsilon, p) G_{V}^{(a)}(E, p, x_2) \right] \alpha^\mu \psi_\varepsilon(x_2),
\]

(9)
where \( E = \varepsilon_a - \omega \),

\[
S_{1}(\varepsilon, p) = \frac{1}{\gamma^{0}\varepsilon - \gamma \cdot p - m} \Sigma^{(0)}_{\varepsilon}(\varepsilon, p) \frac{1}{\gamma^{0}\varepsilon - \gamma \cdot p - m}.
\]

(10)
\( \Sigma^{(0)}_{\varepsilon} \) is the renormalized free self-energy operator (see Ref. [17] for its definition and explicit representations), and the function \( G_{V} \) is the Fourier transform of the product of the Green function \( G \) and the Coulomb potential \( V_{C}(x) = -Z\alpha/x \),

\[
G_{V}(\varepsilon, x_1, p) = \int dx_2 e^{ip \cdot x_2} G(\varepsilon, x_1, x_2) V_{C}(x_2),
\]

(11)

\[
G_{V}(\varepsilon, p, x_2) = \int dx_1 e^{-ip \cdot x_1} V_{C}(x_1) G(\varepsilon, x_1, x_2).
\]

(12)
The second term in the brackets of Eq. (9) removes the reference-state singularity present in the first term. The definition of the function \( G_{V}^{(a)} \) is obtained from Eqs. (11) and (12) by the substitution \( G \rightarrow G^{(a)} \), where \( G^{(a)} \) is the reference-state part of the electron propagator defined by

\[
G^{(a)}(\varepsilon, x_1, x_2) = \sum_{\mu, \nu} \frac{\psi_{\mu}(x_1) \psi_{\nu}^{\dagger}(x_2)}{\varepsilon - \varepsilon_a + i\delta}. \]

(13)
Here, \( \psi_{\mu} \) denotes the virtual electron state of the same energy and of the same parity as the reference state and \( \mu_{\nu} \) is its momentum projection.

The contribution of the diagram in Fig. 2(b) is given by (with the combinatorial factor of 2)

\[
\Delta E_{P,b} = 4i\alpha \int_{-\infty}^{\infty} d\omega \int \frac{dp_1}{(2\pi)^3} \int \frac{dp_2}{(2\pi)^3} \int dx_1 dx_2 D(\omega, x_{12}) \\
\times \psi_{\mu}^{\dagger}(x_1) \alpha_{\mu} \left[ G_{V}(E, x_1, p) - G_{V}^{(0)}(E, x_1, p) \right] \\
\times S_{2}(E, p) G^{(0)}(E, p, x_2) \alpha^\mu \psi_\varepsilon(x_2),
\]

(14)
where

\[
S_{2}(\varepsilon, p) = \frac{1}{\gamma^{0}\varepsilon - \gamma \cdot p - m} \Sigma^{(0)}_{\varepsilon}(\varepsilon, p),
\]

(15)
\( G^{(0)} \) is the free Dirac Green function, and the function \( G_{V}^{(0)} \) is defined by Eqs. (11) and (12) after the substitution \( G \rightarrow G^{(0)} \).

The contribution of the diagram in Fig. 2(c) is

\[
\Delta E_{P,c} = 2i\alpha \int_{-\infty}^{\infty} d\omega \int \frac{dp_1}{(2\pi)^3} \int \frac{dp_2}{(2\pi)^3} \int dx_1 dx_2 \\
\times D(\omega, x_{12}) V_{C}(q) \psi_{\mu}^{\dagger}(x_1) \alpha_{\mu} \\
\times \left[ G_{V}(E, x_1, p_1) G_{1}(E, p_1, p_2) G_{V}(E, p_2, x_2) \\
- G_{V}^{(a)}(E, x_1, p_1) G_{1}(\varepsilon, p_1, p_2) G_{V}^{(a)}(E, p_2, x_2) \right] \\
\times \alpha^\mu \psi_\varepsilon(x_2),
\]

(16)
where \( V_{C}(q) = -4\pi Z\alpha/q^2 \) is the Coulomb potential in momentum space.

\[
G_{1}(\varepsilon, p_1, p_2) = \frac{1}{\gamma^{0}\varepsilon - \gamma \cdot p_1 - m} \\
\times \Gamma^{\mu}_{R}(\varepsilon, p_1; \varepsilon, p_2) \frac{1}{\gamma^{0}\varepsilon - \gamma \cdot p_2 - m},
\]

(17)
and \( \Gamma^{\mu}_{R} \) is the time component of the renormalized free vertex operator \( \Gamma^{\mu}_{R} \) (its explicit representation can be found in Ref. [17]).

The contribution of the diagram in Fig. 2(d) is given by (with the combinatorial factor of 2)

\[
\Delta E_{P,d} = 4i\alpha \int_{-\infty}^{\infty} d\omega \int \frac{dp_1}{(2\pi)^3} \int \frac{dp_2}{(2\pi)^3} \int dx_1 dx_2 \\
\times D(\omega, x_{12}) V_{C}(q) \psi_{\mu}^{\dagger}(x_1) \alpha_{\mu} G_{V}(E, x_1, p_1) \\
\times S_{2}(E, p_1) G^{(0)}(E, p_2, x_2) \alpha^\mu \psi_\varepsilon(x_2),
\]

(18)
where

\[
S_{2}(\varepsilon, p_1) = \frac{1}{\gamma^{0}\varepsilon - \gamma \cdot p_1 - m} \Gamma^{\mu}_{R}(\varepsilon, p_1; \varepsilon, p_2). \]

(19)
The contribution of the diagram in Fig. 2(e) can be
written as (with the combinatorial factor of 2)
\[ \Delta E_{P,\alpha} = -4i\alpha \int_{-\infty}^{\infty} d\omega \int \frac{dp_1}{(2\pi)^3} \frac{dp_2}{(2\pi)^3} \int dz \]
\[ \times \frac{\exp(-i\mathbf{q} \cdot \mathbf{z})}{\omega^2 - \mathbf{q}^2 + i\eta} \psi_1^\dagger(z) \alpha_{\mu} \psi_1(z) \]
\[ \times \left[ G_V(E, \mathbf{z}, \mathbf{p}_1) - G_V^{(0)}(E, \mathbf{z}, \mathbf{p}_1) \right] \]
\[ \times \frac{1}{\gamma^0 E - \gamma \cdot \mathbf{p}_1 - m} \Gamma^\mu_R(E, \mathbf{p}_1; \varepsilon_\alpha, \mathbf{p}_2) \psi_\alpha(\mathbf{p}_2). \]

\[ (20) \]

**IV. Calculation**

The main problem of the evaluation of the \( P \) term is connected with the fact that the regularization of ultraviolet divergences in the one-loop subgraphs is carried out in the momentum space, while the bound-electron propagators are most easily evaluated in the coordinate space. As a result, the expressions listed in the previous section contain the Fourier transform of the product of the Dirac Coulomb Green functions \( G \) with the Coulomb potential \( V_C \) over one of the radial arguments, see Eqs. (11) and (12). Since we were not able to find a satisfactory analytical representation for such an object, the only possible way was to evaluate the Fourier transform numerically. This way entails numerous numerical integrations of rapidly oscillating functions, which may make the computations prohibitively expensive, unless care is taken in choosing the optimal calculational approach.

In the previous investigations \([15–17]\), the \( P \) term was calculated with the help of a finite basis set for the Dirac equation. The advantage of the basis-set methods is that they represent the Dirac Green function as a continuous function of the radial arguments (for any finite size of the basis), whereas the exact Green function is discontinuous when the two radial arguments are equal. The usage of a finite basis set allows one to perform the Fourier transform of the Green function over one radial variable independently of the other. However, the convergence with respect to the size of the basis appears to be the limiting factor for the accuracy of the calculations. In the present investigation, we set up a different calculational approach based on the analytical representation of the Green function. Technical details of evaluation of the Dirac Coulomb Green function in the mixed coordinate-momentum representation are described in Appendix A. The corresponding formulas for the free Dirac Green function are summarized in Appendix B.

**A. Nested diagrams**

In this subsection, we address the diagrams in Figs. 2(a)–(d) and outline the major steps required to make the basic formulas suitable for a numerical evaluation.

The integrations over the angular variables \([\hat{x}_1, \hat{x}_2, \text{and } \hat{p}_1, \text{and } \hat{p}_2] \) in Eqs. (9) and (14) and \([\hat{x}_1, \hat{x}_2, \text{and } \hat{p}_1, \text{and } \hat{p}_2] \) in Eqs. (16) and (18), where \( \hat{x} = x/|x| \) are relatively simple. We employ the fact that the matrix elements of the operators \( S_{1,2} \) and \( G_{1,2} \) with the Dirac wave functions are (i) diagonal with respect to the angular momentum quantum number \( \kappa \) and the momentum projection \( \mu \) and (ii) do not depend on \( \mu \):
\[ \langle \kappa\mu|S_i|\kappa'\mu' \rangle = \delta_{\kappa,\kappa'} \delta_{\mu,\mu'} \langle \kappa|S_i|\kappa \rangle, \]
\[ \langle \kappa\mu|G_i|\kappa'\mu' \rangle = \delta_{\kappa,\kappa'} \delta_{\mu,\mu'} \langle \kappa|G_i|\kappa \rangle. \]

As a result, the integrations over \( \hat{p} \) in Eqs. (9) and (14) and \( \hat{p}_1 \) and \( \hat{p}_2 \) in Eqs. (16) and (18) are exactly the same as for the zero- and one-potential parts of the one-loop self-energy correction, see Ref. [22] for details. The integrations over \( \hat{x}_1 \) and \( \hat{x}_2 \) are the same as for the many-potential part of the one-loop self-energy correction.

As illustrated in Ref. [22], the integrations over \( \hat{p}_1 \) and \( \hat{p}_2 \) in Eqs. (16) and (18) can be easily reduced to a single integral over \( \xi = \hat{p}_1 \cdot \hat{p}_2 \), which needs to be evaluated numerically. The calculation is complicated by the presence of an integrable Coulomb singularity \((\sim 1/q^2, q = |\hat{p}_1 - \hat{p}_2|)\). This singularity is removed in two steps. First, the change of the integration variable \( \xi \rightarrow q \) weakens it to \( \sim 1/q \). The remaining singularity is removed by subtraction of the vertex function with the equal arguments,
\[ \Gamma^0_R(p_1, p_2) \rightarrow \Gamma^0_R(p_1, p_2) - \frac{1}{2} \left[ \Gamma^0_R(p_1, p_1) + \Gamma^0_R(p_2, p_2) \right]. \]

The vertex operator with two equal arguments is related to the free self-energy operator by the Ward identity:
\[ \Gamma^0_R(p, p) = -\frac{\partial}{\partial p^0} \Sigma^0_R(p). \]

In the subtracted terms, the Coulomb singularity is easily integrated out by using identities obtained from the definition of the Dirac Coulomb Green function, as, e.g.,
\[ \int \frac{dp_2}{(2\pi)^3} V_C(q) \gamma^0 \frac{1}{E - \gamma \cdot p_2 - m} G_V(E, p_2, x_2) = G_V(E, p_1, x_2) - G_V^{(0)}(E, p_1, x_2). \]

Finally, we change the contour of the integration over the virtual photon energy \( \omega \) in Eqs. (9), (14), (16), and (18) from \((-\infty, \infty)\) to a new contour \( C_{LH} \), whose main part is parallel to the imaginary axis. The contour \( C_{LH} \) consists of the low-energy \( C_L \) and the high-energy \( C_H \) parts. The low-energy part extends over \((\Delta - i0, -i0)\) on the lower bank of the cut of the photon propagator and over \((i0, \Delta + i0)\) on the upper bank of the cut, with the parameter \( \Delta \) fixed by \( \Delta = Z_0 \varepsilon_a \). The high-energy part consists of two intervals, \((\Delta + i0, \Delta + i\infty)\) and \((\Delta - i0, \Delta - i\infty)\). The contour \( C_{LH} \) differs from the one used by P. J. Mohr [12] only by the choice of the breaking point \( \Delta \) (the value \( \Delta = \varepsilon_a \) was employed in that work).
In our previous calculations we used the contour that extended along the imaginary axis (which corresponds to the choice of $\Delta = 0$). The contour $C_{LH}$ is more convenient for the numerical evaluation. Firstly, there is no pole contributions originating from the reference-state part of the electron propagators. Secondly and more importantly, the photon propagator on the low-energy part of the contour involves $\sin(\omega x_{12})$, which suppresses small denominators due to the virtual bound states and leads to a smooth behaviour of the integrand for small $\omega$.

In the present investigation, we are concerned with the reference state being the ground state only. In this case, no pole contributions appears for the contour $C_{LH}$. For the excited reference states, however, there are single and double poles on the low-energy part of the contour, which arise from the intermediate states bounded more deeply than the reference state. These poles require a separate treatment or a deformation of the integration contour into the complex plane.

**B. Overlapping diagram**

In this subsection we address the overlapping diagram shown in Fig. 2(e), whose expression is given by Eq. (20). The angular integration in this expression is rather involved and will be considered in detail.

In order to perform the integration over $\bar{z}$, we expand the exponent into the spherical waves,

$$ e^{-i\mathbf{q}\cdot \bar{z}} = 4\pi \sum_{LM} j_L(q\bar{z}) Y_{LM}(\hat{q}) Y^*_{LM}(\hat{z}), $$

where $j_L$ is the spherical Bessel function and $Y_{LM}$ is the spherical harmonics. The time component ($\mu = 0$) of the $\bar{z}$ integration is immediately evaluated in terms of the basic integrals of the form

$$ \int d\bar{z} \chi^\dagger_{\kappa a \mu a}(\bar{z}) Y_{LM}(\bar{z}) \chi_{\kappa a \mu a}(\bar{z}) = s_{LM}^{\kappa a} \langle \kappa a || C^{(L)} || \kappa a \rangle, $$

with $C_{J_{1j_2m_1j_2m_2}}$ being the Clebsch-Gordan coefficient. The vector components ($\mu = 1, 2, 3$) of the $\bar{z}$ integration are calculated after expanding the integrand in terms of the vector spherical harmonics $Y_{JLM}$ [24, 25],

$$ \chi^\dagger_{\kappa a \mu a}(\bar{z}) \sigma \chi_{\kappa a \mu a}(\bar{z}) = \sum_{JLM} s_{JLM}^{a} S_{Jlm}(\kappa a, \kappa a) Y_{JLM}(\bar{z}), $$

where $\sigma$ is a vector incorporating Pauli matrices. The coefficients $S_{JL}$ are given by

$$ S_{J+1}(\kappa a, \kappa b) = \sqrt{J+1} \frac{(-1)^{J+a}}{2J+1} \left(\frac{1 + \kappa a + \kappa b}{J+1}\right) \times \langle -\kappa b || C^{(J)} || \kappa a \rangle, $$

$$ S_{J}(\kappa a, \kappa b) = \frac{-\kappa a - \kappa b}{\sqrt{J(J+1)}} \langle \kappa b || C^{(J)} || \kappa a \rangle, $$

$$ S_{J-1}(\kappa a, \kappa b) = \sqrt{J+1} \frac{(-1)^{J+a}}{2J+1} \left(1 - \frac{\kappa a + \kappa b}{J}\right) \times \langle -\kappa b || C^{(J)} || \kappa a \rangle. $$

For $J = 0$, the only nonvanishing coefficient is $S_{01}$.

We now turn to the evaluation of the integrals over $\hat{p}_1$ and $\hat{p}_2$ in Eq. (20). The aim is to integrate out all angular variables except $\xi = \hat{p}_1 \cdot \hat{p}_2$. To this end, we examine the angular structures encountered in the integrand. The time component of the vertex operator sandwiched between the Dirac wave functions involves two independent angular structures, which are identified by

$$ \psi_n^\dagger(p_1) \frac{1}{\gamma^0 E - \gamma \cdot p_1 - m} \Gamma_R(E, p_1; \varepsilon_n, p_2) \psi_n(p_2) $$

$$ = \frac{\alpha}{4\pi} \frac{i^{\lambda_n - \lambda_a}}{m} \left\{ \left[ g_n R_{1g} + f_n R_{1f} \right] \chi^\dagger_{\kappa a \mu a}(\hat{p}_1) \chi_{\kappa a \mu a}(\hat{p}_2) \right\} $$

$$ + \left[ g_n R_{2g} + f_n R_{2f} \right] \chi^\dagger_{\kappa a \mu a}(\hat{p}_1) \chi_{\kappa a \mu a}(\hat{p}_2), $$

where $g_n \equiv g_n(p_1)$ and $f_n \equiv f_n(p_1)$ are the upper and the lower radial components of the Dirac wave function $\psi_n$ and $F_1$ are scalar functions $F_i \equiv F_i(E, \varepsilon_n, p_1, p_2, q)$, with $p_1 = |p_1|$, $p_2 = |p_2|$, and $q = |q|$. The vector part of the vertex operator induces six angular structures,

$$ \psi_n^\dagger(p_1) \frac{1}{\gamma^0 E - \gamma \cdot p_1 - m} \Gamma_R(E, p_1; \varepsilon_n, p_2) \psi_n(p_2) $$

$$ = \frac{\alpha}{4\pi} \frac{i^{\lambda_n - \lambda_a}}{m} \left\{ \left[ g_n R_{1g} + f_n R_{1f} \right] \chi^\dagger_{\kappa a \mu a}(\hat{p}_1) \sigma \chi_{\kappa a \mu a}(\hat{p}_2) \right\} $$

$$ + \left[ g_n R_{2g} + f_n R_{2f} \right] \chi^\dagger_{\kappa a \mu a}(\hat{p}_1) \chi_{\kappa a \mu a}(\hat{p}_2) $$

$$ + \left[ g_n R_{3g} + f_n R_{3f} \right] \chi^\dagger_{\kappa a \mu a}(\hat{p}_1) \chi_{\kappa a \mu a}(\hat{p}_2) $$

$$ + \left[ g_n R_{4g} + f_n R_{4f} \right] p_2 \chi^\dagger_{\kappa a \mu a}(\hat{p}_1) \chi_{\kappa a \mu a}(\hat{p}_2) $$

$$ + \left[ g_n R_{5g} + f_n R_{5f} \right] p_1 \chi^\dagger_{\kappa a \mu a}(\hat{p}_1) \chi_{\kappa a \mu a}(\hat{p}_2) $$

$$ + \left[ g_n R_{6g} + f_n R_{6f} \right] p_2 \chi^\dagger_{\kappa a \mu a}(\hat{p}_1) \chi_{\kappa a \mu a}(\hat{p}_2), $$

where $R_i \equiv R_i(E, \varepsilon_n, p_1, p_2, q)$. The functions $F_i$ and $R_i$ can be straightforwardly obtained from formulas in Appendix A of Ref. [26].

Using Eqs. (33) and (34), it is possible to parameterize the angular structure of the integrand of Eq. (20) by four basic angular factors $t_{\kappa a, \kappa b}$, $t_{\kappa a, \kappa b}^\sigma$, $S_{\kappa a, \kappa b}^p$, and $S_{\kappa a, \kappa b}^q$ defined as

$$ t_{\kappa a, \kappa b}(J) = \sum_{\mu \kappa \mu \kappa} s_{JLM}^{a} \chi^\dagger_{\kappa a \mu a}(\hat{p}_1) Y_{JLM}(\hat{q}) \chi_{\kappa a \mu a}(\hat{p}_2), $$

(35)
\[ s_{\kappa_n,\kappa_n}(JL) = \sum_{\mu,M} s_{\jmath M}^{\gamma a} \chi_{\kappa_n,\mu\kappa_n}(\hat{p}_1) \cdot \textbf{Y}_{JLM}(\hat{q}) \chi_{\kappa_n,\mu\kappa_n}(\hat{p}_2), \]

(36)

\[ s_{\kappa_n,\kappa_n}^{\phi}(JL) = \sum_{\mu,M} s_{\jmath M}^{\gamma a} \chi_{\kappa_n,\mu\kappa_n}(\hat{p}_1) \cdot \textbf{Y}_{JLM}(\hat{q}) \chi_{\kappa_n,\mu\kappa_n}(\hat{p}_2). \]

(37)

By an explicit evaluation with help of formulas from Ref. [25], one can show that the above angular factors are the functions of \( p_1, p_2, \) and \( q \) only (or, in other words, that they depend on the angular variables only through \( \xi \)). This statement allows us to integrate out all angles in Eq. (20) except \( \xi \). The calculation of angular factors is described in Appendix C.

For a numerical evaluation of Eq. (20), we need to deform the contour of the \( \omega \) integration. In this case (in contrast to the nested contributions), we find it convenient just to rotate the integration contour to the imaginary axis, \( \omega \rightarrow i\omega \). This leads to appearance of the pole contribution. So,

\[ \Delta E_{P,e} = \Delta E_{P,e}^{\text{im}} + \Delta E_{P,e}^{\text{pole}}, \]

(38)

where \( \Delta E_{P,e}^{\text{im}} \) is the contribution of the integral along the imaginary axis and \( \Delta E_{P,e}^{\text{pole}} \) is the pole contribution.

The final result after the angular integrations and the rotation of the contour is

\[
\Delta E_{P,e}^{\text{im}} = \frac{\alpha^2}{\pi^2} \sum_{\kappa_n} \int_0^\infty d\omega \int_0^\infty dp_1 \, dp_2 \frac{q \, p_1 p_2}{-\omega^2 - q^2} \int_0^\infty d\tilde{z} \tilde{z}^2 \\
\times \left\{ -\sum_j (-1)^{k_1} j_j(qz) \langle \kappa_n | \mathbf{C}^{(j)}(\kappa_n) \rangle \left[ (g_a \tilde{G}_{V_{\kappa_n}}^{a11} + f_a \tilde{G}_{V_{\kappa_n}}^{1a1}) \mathbf{F}_g + \left( g_a \tilde{G}_{V_{\kappa_n}}^{a12} + f_a \tilde{G}_{V_{\kappa_n}}^{1a2} \right) \mathbf{F}_f \right] \\
- \sum_{JL} (-1)^{k_2} j_L(qz) \left[ (g_a \tilde{G}_{V_{\kappa_n}}^{2a1} S_{JL}(\kappa_n, -\kappa_n) - f_a \tilde{G}_{V_{\kappa_n}}^{1a2} S_{JL}(-\kappa_n, \kappa_n) \right] \mathbf{R}_q \\
+ \left[ g_a \tilde{G}_{V_{\kappa_n}}^{2a2} S_{JL}(\kappa_n, -\kappa_n) - f_a \tilde{G}_{V_{\kappa_n}}^{1a1} S_{JL}(-\kappa_n, \kappa_n) \right] \mathbf{R}_f \right\},
\]

(39)

where \( k_1 = (J - l_n + l_n)/2, k_2 = (L - l_n + l_n - 1)/2, l_n = |\kappa_n + 1/2| - 1/2, g_a \equiv g_a(z) \) and \( f_a \equiv f_a(z) \) are the radial components of the reference-state wave function, and \( \tilde{G}_{V_{\kappa_n}}^{ij} \) stand for the difference of the radial components of the Coulomb Green function (times \( V_C \)) and the free Green function (times \( V_C \)),

\[ \tilde{G}_{V_{\kappa_n}}^{ij} \equiv G_{V_{\kappa_n}}^{ij}(\varepsilon_a - i\omega, z, p_1) - G_{V_{\kappa_n}}^{(0)ij}(\varepsilon_a - i\omega, z, p_1). \]

The angular functions in Eq. (39) are defined by

\[ \mathbf{F}_g = \mathbf{F}_{1g} t_{\kappa_n,\kappa_n}(J) + \mathbf{F}_{2g} t_{-\kappa_n,\kappa_n}(J), \]

(40)

\[ \mathbf{R}_g = \mathbf{R}_{1g} s_{\kappa_n,\kappa_n}^{\gamma}(JL) + \mathbf{R}_{2g} s_{-\kappa_n,\kappa_n}^{\gamma}(JL) + p_1 \mathbf{R}_{3g} s_{\kappa_n,\kappa_n}^{\gamma a}(JL) + p_2 \mathbf{R}_{4g} s_{\kappa_n,\kappa_n}^{\gamma a}(JL) + p_1 \mathbf{R}_{5g} s_{-\kappa_n,\kappa_n}^{\gamma a}(JL) + p_2 \mathbf{R}_{6g} s_{-\kappa_n,\kappa_n}^{\gamma a}(JL), \]

(41)

and the same for the \( \mathbf{F}_f \) and \( \mathbf{R}_f \) functions.

The pole contribution \( \Delta E_{P,e}^{\text{pole}} \) is obtained from Eq. (39) by the following substitution (valid for \( a \) being the ground state),

\[ \tilde{G}_{V_{\kappa_n}}^{ij} \rightarrow -\frac{\pi}{2} \delta(\omega) \phi_a^i(z) \phi_a^j(p_1), \]

(42)

where \( \phi_a^i(z) = g_a(z), \phi_a^2(z) = f_a(z), \) and \( \phi_{V_a}(p) \) is the Fourier transform of the product \( \phi_a^i(x) V_C(x) \).

A useful check of the angular-momentum algebra consists in making the substitution \( \Gamma^\mu_{P,e}(E, p_1; \varepsilon_a, p_2) \rightarrow \gamma^\mu \) in Eq. (20). The result is an one-loop self-energy contribution which can be calculated independently in the coordinate representation.

C. Numerical evaluation

We start our discussion of the numerical evaluation of the \( P \) term with \( \Delta E_{P,a} \) and \( \Delta E_{P,b} \) given by Eqs. (9) and (14), respectively. These are the two simplest contributions. After carrying out integrations over the angular variables as described in Sec. IV A, five integrations remain to be calculated numerically, namely those over \( \omega, p, x_1, \) and \( x_2 \) and the Bessel transform integral implicitly present in the Green function.

The radial integrations over \( x_1 \) and \( x_2 \) have to be organized in such a way as to avoid unnecessary recalculation of the Bessel transform integrals, as discussed in Appendix A. To this end, we set up a radial grid \( \{x_{i,j,k}\} \).
as follows. The first-level elements \(x_{i,0,0}\) are given by

\[
x_{i,0,0} = \rho_0 \frac{1-t_i^2}{t_i^2},
\]

where \(\rho_0\) is a parameter adjusted empirically, the variable \(t_i\) is uniformly distributed over the interval \((t_{\text{min}},1)\), and a small value of \(t_{\text{min}} > 0\) cuts off the radial integrations at large distances. The second-level elements \(x_{i,j,0}\) represent the Gauss-Legendre quadratures on the interval \((x_{i,0,0},x_{i,j+1,0})\). The third-level elements \(x_{i,j,k}\) represent the Gauss-Legendre quadratures on the interval \((x_{i,j,0},x_{i,j+1,0})\). In the result, we obtain an ordered three-level radial grid. To perform the radial integrations over \(x_1\) and \(x_2\), it is sufficient to know the integrand on this grid only.

The general scheme of the evaluation of \(\Delta E_{P,a}\) looks as follows. For fixed values of \(\kappa\), \(\omega\), and \(p\), we set up the radial grid \(\{x_{i,j,k}\}\). On this radial grid, we store the components of the Dirac Green function \(\phi^0(E,x)\) and \(\phi^\kappa(E,x)\) [see Eqs. (A3) and (A4)], the Bessel transform functions \(\psi^0(E,p;x)\) and \(\psi^\kappa(E,p;x)\) [see Eqs. (A9) and (A10)], and the other functions required for the evaluation of the integrand (the radial part of the photon propagator, the reference-state wave function, etc.). After that, the radial integrations are performed simply by summing up the stored numerical values. Next, we perform the integration over \(p\), then the one over \(\omega\), and finally, the summation over \(\kappa\).

The most expensive part of the calculation is the evaluation of the Bessel transform integrals. In order to control the accuracy of numerical integrations, one needs an efficient procedure for calculating the transforms for various momenta, including ones as large as \(10^6\). In our calculations, we used the Gauss-Legendre integration quadratures in the region where the argument of the Bessel function is of about unity or smaller. Outside this region, the spherical Bessel function was expressed as a combination of the sine and cosine functions. The numerical evaluation of the sine and cosine transform was performed with help of routines of the NAG Fortran library.

The scheme described above works well for the \(\Delta E_{P,a}\) contribution but turns out to be not sufficiently effective for \(\Delta E_{P,b}\), leading to a slow convergence of the radial integrations with respect to the number of integration points. This is because the free Green function \(G^{(0)}(\varepsilon,\mathbf{x},\mathbf{p})\) contains a Bessel function [see Eq. (B5)], which oscillates rapidly in the high-momenta region. This problem was solved by observing that the integral over \(x_2\) in Eq. (14) has a structure similar to \(\psi^0(E,p;x_1)\), i.e., it is essentially a Bessel transform over the intervals \((0,x_1)\) and \((x_1,\infty)\). We thus perform the integration over \(x_2\) in Eq. (14) by means of the same approach as used in the evaluation of the Bessel transform functions \(\psi^\kappa(E,p;x_1)\). This approach improves the convergence of the radial integrals drastically.

The evaluation of the two remaining nested contributions, \(\Delta E_{P,c}\) and \(\Delta E_{P,d}\), was performed in the full analogy with the discussed above. However, it turned out to be much more time consuming due to a larger number of integrations. Indeed, in place of an integration over \(p\) in \(\Delta E_{P,a}\) and \(\Delta E_{P,b}\), there are now four integrations (those over \(p_1, p_2\), and \(q\) and the Feynman-parameter integration implicitly present in the vertex operator). Fortunately, the integrations over \(q\) and over the Feynman parameter can be carried out independently of the integrations over \(x_1\) and \(x_2\) and thus do not significantly influence the total calculational time. The two integrations over \(p_1\) and \(p_2\), however, lead to a considerable increase of the computational expense (this being about a week of the processor time for each value of \(Z\)).

For the overlapping contribution \(\Delta E_{P,e}\), there are seven integrations to be performed numerically. Five of them are explicitly written in Eq. (39), one over the Feynman parameter is implicitly present in the vertex operator, and the last one is the Bessel transform integral in the Green function. The number of nested integrations can be reduced by observing that the integrations over \(p_2\) and over the Feynman parameter can be carried out independently of the integration over \(z\). The calculation is complicated by the fact that the integral over \(z\) contains a Bessel function, thus being essentially a Bessel transform. In order to get a stable result for the \(z\) integration in the region of large values of \(qz\), we had to interpolate the part of the integrand that multiplies the Bessel function and evaluate the Bessel transform analytically.

V. RESULTS AND DISCUSSION

The results of our calculation of the \(P\) term for the ground state of hydrogen-like ions with \(Z \geq 10\) are listed in Table I. The individual contributions are presented in a way that allows a detailed comparison with the previous calculations. Specifically, the first four columns of Table I are directly comparable to the four columns of Table 2 in Ref. [17]. The previous results listed in the fifth column of Table I were obtained in Ref. [18] for \(Z \leq 60\) and in Ref. [17] for the other \(Z\). The agreement with the previous calculations is very good in most cases, but the present numerical accuracy is significantly higher. A small deviation in the high-\(Z\) region is probably due to a difference in the treatment of the nucleus. (In the present work, the point nuclear model is used, whereas the previous investigations [17, 18] were conducted with a partial inclusion of the finite nuclear size effect in the \(P\) term.)

The uncertainty of the present results is mainly due to the termination of the partial-wave expansion. In our calculation, we included typically 20-30 partial waves and estimated the omitted tail by fitting the data obtained as a function of the cutoff parameter. Perspectives for improving the present accuracy further (which is required if one is to perform a calculation for lower values of \(Z\)) seem to be questionable. The main problem is that the high partial waves become increasingly difficult to control numerically. At the same time, the extrapolation of
The main motivation of the present investigation was to improve the numerical accuracy of the total two-loop self-energy correction in the region of medium values of $Z$, in order to get a more reliable extrapolation towards $Z = 0$. To this end, a new approach was developed for the evaluation of the $P$ term, as described above. Besides that, the other parts of the two-loop self-energy correction were reevaluated to a higher accuracy. This was accomplished by the methods described in Ref. [17], with the increased number of partial waves included and with denser integration grids. The results were first presented in Ref. [20].

Table II summarizes our results for the total two-loop self-energy correction for the ground state of hydrogen-like ions with the nuclear charge $Z = 10–30$. We observe that the calculational errors of the $P$ term do not influence significantly the errors of the total results, as the main uncertainty is now delivered by the $M$ term. This uncertainty originates both from the dependence of the results on the number of integration points and from the termination of the partial-wave expansions. Since there are two independent partial-wave expansion parameters in the $M$ term (see Ref. [17] for details), the number of expansion terms grows drastically as the cutoff parameter is increased. Because of this, significant extension of the partial-wave summations looks prohibitively expensive at present.

The two-loop self-energy correction for the ground state of hydrogen-like atoms can be conveniently represented in the following form, separating out the known terms of the $Z\alpha$ expansion,

$$\Delta E = m \left( \frac{\alpha}{\pi} \right)^2 (Z\alpha)^4 \left[ B_{40} + (Z\alpha) G_{50}(Z) \right], \quad (44)$$

and

$$G_{50}(Z) = B_{50} + (Z\alpha) \left\{ \ln^3[(Z\alpha)^{-2}] B_{63} + \ln^2[(Z\alpha)^{-2}] B_{62} + \ln[(Z\alpha)^{-2}] B_{61} + G_{60}(Z) \right\}, \quad (45)$$

where $B_{ij}$ are the expansion coefficients with the first index corresponding to the power of $Z\alpha$ and the second index, to the power of logarithm, and $G_{ij}(Z)$ are the functions incorporating the corresponding $B_{ij}$ and all higher orders in $Z\alpha$, $G_{ij}(Z) = B_{ij} + Z\alpha(\ldots)$. The results for the expansion coefficients (see Refs. [1–5] and references therein) are: $B_{40} = 1.409244$, $B_{50} = -24.2668(31)$, $B_{63} = -8/27$, $B_{62} = 16/27 - (16/9)\ln 2$, $B_{61} = 48.388913$, and $B_{60} = -61.69(2)$.

The functions $G_{ij}(Z)$ inferred from our numerical data are plotted in Fig. 3. The visual agreement of our results with the analytical values of the expansion coefficients is very good for $B_{40}$ and $B_{50}$, but not exactly satisfactory for $B_{60}$. In order to produce a clearer statement, we need to extrapolate our data towards low values of $Z$. For this we use a variant of the procedure first employed in Ref. [27]. The extrapolation towards the required value of $Z = Z_0$ ($= 0$ and 1 in our case) is performed in two steps. First, we apply an (exact) linear fit to each pair of two consecutive points from our data set and store the resulting values at $Z = Z_0$. Second, we perform a global polynomial least-squares fit to the set of data obtained on the first step and take the fitted value at $Z = Z_0$ as a final result. Similar procedure applied to the function $G_{50}$ reproduces the analytical result for the coefficient $B_{50}$ with the accuracy of about 1%. For comparison, a global polynomial fit yields a result accurate within 5% only.

When applied to the remainder function $G_{60}(Z)$, the

Table I: The $P$ term for the ground state of hydrogen-like ions, in units of $\Delta E/[\alpha^2(Z\alpha)^4/\pi^2]$. 

| $Z$ | Figs. (a,b) | Figs. (c,d) | Fig. (e) | Total | Previous [17, 18] |
|-----|-----------|-----------|---------|------|-----------------|
| 10  | $-855.4289(20)$ | $1265.4550(50)$ | $-1131.3372(22)$ | $-721.3111(58)$ | $-721.34(12)$ |
| 12  | $-486.0740(20)$ | $744.6950(50)$ | $-907.6064(17)$ | $-439.0654(56)$ | $-439.06(28)$ |
| 15  | $-239.2533(15)$ | $384.3590(30)$ | $-380.3170(12)$ | $-235.2113(36)$ | $-235.205(70)$ |
| 17  | $-159.4480(15)$ | $263.5625(20)$ | $-268.3945(12)$ | $-164.2800(28)$ | $-164.28(28)$ |
| 20  | $-93.3597(7)$ | $160.3551(20)$ | $-160.0247(10)$ | $-102.0293(23)$ | $-102.026(55)$ |
| 25  | $-44.1992(7)$ | $79.9950(15)$ | $-87.7882(10)$ | $-51.9824(19)$ | $-51.98(19)$ |
| 30  | $-23.8155(7)$ | $44.8102(27)$ | $-50.4083(10)$ | $-29.4135(30)$ | $-29.41(30)$ |
| 40  | $-9.0138(4)$ | $17.6601(2)$ | $-20.1713(6)$ | $-11.5790(7)$ | $-11.575(30)$ |
| 50  | $-4.3931(5)$ | $8.4020(4)$ | $-9.5506(4)$ | $-5.4877(7)$ | $-5.48(26)$ |
| 60  | $-2.4455(3)$ | $4.5451(4)$ | $-5.0660(2)$ | $-2.9664(5)$ | $-2.97(18)$ |
| 70  | $-1.5203(2)$ | $2.6716(1)$ | $-2.9354(2)$ | $-1.7841(3)$ | $-1.75(25)$ |
| 83  | $-0.8655(2)$ | $1.4268(1)$ | $-1.6307(1)$ | $-1.0693(2)$ | $-1.06(13)$ |
| 92  | $-0.5545(1)$ | $0.9091(1)$ | $-1.1902(1)$ | $-0.8356(2)$ | $-0.82(10)$ |
| 100 | $-0.2990(2)$ | $0.5426(1)$ | $-0.9792(4)$ | $-0.7356(5)$ | $-0.72(3)$ |
First, the analytical result for the 

The shift of the central value is due to two reasons. marginally consistent with the 2005 result of 
The extrapolated value for \( Z_c \) significantly reduced the disagreement with the analytical cal-

Eq. (47) with the corresponding contribution induced 
two-loop self-energy correction obtained in this work 

\[ \delta B \] (nonlogarithmic) contribution to order \( m \alpha^2(Z \alpha)^4/\pi^2 \)

So, our estimate of the total two-

For the ground state of hydrogen is

\[ G_{60}(Z = 1, \text{total}) = -86 (15) - 15 (2) = -101 (15) \quad (48) \]

The numerical contribution of this effect is

\(-10.2 (1.5) \quad \text{kHz}, \quad \text{which is much larger than the error of the experimental determination of the} \quad 1S - 2S \]

transition frequency in hydrogen [6] (34 Hz) and comparable with the experimental errors for the \( 2S - 12D \)

transitions [28] (7 kHz).

To conclude, in the present investigation, we described in detail the technique of evaluation of Feynman diagrams in the mixed coordinate-momentum representation based on the analytical representation of the bound electron propagators in terms of the Whittaker functions. This technique allowed us to significantly improve the accuracy of the numerical evaluation of the part of the two-loop self-energy correction conventionally termed as the \( P \) term. The all-order (in the parameter \( Z \alpha \)) results are reported for the two-loop self-energy correction for the ground state of hydrogen-like ions with with the nuclear charge number \( Z = 10 - 30 \). The higher-order (in \( Z \alpha \)) remainder function is inferred from the numerical results and extrapolated towards \( Z = 0 \) and 1. The extrapolated value is in marginal agreement with the analytical result obtained within the perturbative approach.

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Appendix A: Dirac Coulomb Green function in the coordinate-momentum representation

The Dirac Coulomb Green function is commonly written in coordinate space as an expansion in the relativistic angular momentum parameter \( \kappa \) [11, 12, 29],

\[
G(E, x_1, x_2) = \sum_{\kappa \mu} \left( G^{11}_\kappa(E, x_1, x_2) \chi_{\kappa\mu}(\hat{x}_1) \chi^{\dagger}_{\kappa\mu}(\hat{x}_2) G^{21}_\kappa(E, x_1, x_2) i\chi_{-\kappa\mu}(\hat{x}_1) \chi^{\dagger}_{-\kappa\mu}(\hat{x}_2) G^{12}_\kappa(E, x_1, x_2) (-i) \chi_{\kappa\mu}(\hat{x}_1) \chi^{\dagger}_{-\kappa\mu}(\hat{x}_2) G^{22}_\kappa(E, x_1, x_2) \chi_{-\kappa\mu}(\hat{x}_1) \chi^{\dagger}_{-\kappa\mu}(\hat{x}_2) \right), \tag{A1}
\]

where \( \chi_{\kappa\mu}(\hat{x}) \) are the Dirac spin-angular spinors [23] and \( \hat{x} = x/|x| \). The \( 2 \times 2 \) matrix of the radial components \( G^{ij}_\kappa \) is referred to as the radial Green function and denoted as \( G_\kappa \). The radial Green function can be expressed in terms of the two-component solutions of the radial Dirac equation regular at the origin \( (\phi^0_\kappa) \) and the infinity \( (\phi^\infty_\kappa) \) as follows

\[
G_\kappa(E, x_1, x_2) = -\phi^\infty_\kappa(E, x_1) \phi^0_\kappa(E, x_2) \theta(x_1 - x_2) - \phi^0_\kappa(E, x_1) \phi^\infty_\kappa(E, x_2) \theta(x_2 - x_1). \tag{A2}
\]

The upper and the lower components of the functions \( \phi^0_\kappa \) and \( \phi^\infty_\kappa \) will be denoted by subscripts "+" and "-", respectively. They are given by

\[
\phi^\pm_\kappa(E, x) = \Delta_\kappa^{-1/2} \frac{\sqrt{1 \pm E}}{\sqrt{x/2}} \left[ (\lambda - \nu) M_{\nu \mp \lambda} (2cx) \right], \tag{A3}
\]

\[
\phi^\infty_\kappa(E, x) = \Delta_\kappa^{-1/2} \frac{\sqrt{1 \pm E}}{\sqrt{x/2}} \left[ (\lambda + \nu) W_{\nu \pm \lambda} (2cx) \right], \tag{A4}
\]

\[
\Delta_\kappa = \frac{\kappa}{c} - \frac{\alpha Z}{c^2}.
\]
where $\Delta_n = 4c^2 \Gamma(1+2\lambda)/\Gamma(\lambda-\nu)$, $c = \sqrt{1-E^2}$ defined so that $\Re(c) > 0$, $\lambda = \sqrt{k^2 - (Z\alpha)^2}$, $\nu = Z\alpha E/c$, and $M_{n,\beta}$ and $W_{n,\beta}$ are the Whittaker functions of the first and the second kind, respectively.

The Dirac Coulomb Green function in the coordinate-momentum representation is obtained from the above formulas by the Fourier transform over one of the radial arguments. Let us consider the transform over, e.g., the second radial argument,

$$G(E, x_1, p_2) = \int dx_2 e^{ip_2 \cdot x_2} G(E, x_1, x_2).$$  \hspace{1cm} (A5)

Its partial-wave expansion takes the form

$$\psi^\infty (E, p; x_1) = -\phi^\infty_k (E, x_1) \psi^\infty_k (E, p_2; x_1)$$  \hspace{1cm} (A8)

with the radial part given by the following matrix

$$G_k (E, x_1, p_2) = 4\pi \int_0^\infty dx_2 x_2^2 \left( j_l (p_2 x_2) G_{11} (E, x_1, x_2) - \frac{\alpha}{|\kappa|} j_{l'} (p_2 x_2) G_{12} (E, x_1, x_2) \right),$$  \hspace{1cm} (A7)

where $l = |\kappa + 1/2| - 1/2$ and $l' = |\kappa - 1/2| - 1/2$. Using Eq. (A2), we obtain the following representation for the radial Green function in the mixed coordinate-momentum representation

$$G_k (E, x_1, p_2) = -\phi^\infty_k (E, x_1) \psi^\infty_k (E, p_2; x_1)$$  \hspace{1cm} (A8)

where

$$\psi^0_k (E, p; x_1) = 4\pi \int_0^{x_1} dx_2 x_2^2 \left( j_l (p x_2) \phi^0_k (E, x_2) - \frac{\alpha}{|\kappa|} j_{l'} (p x_2) \phi^0_k (E, x_2) \right),$$  \hspace{1cm} (A9)

and

$$\psi^\infty_k (E, p; x_1) = 4\pi \int_{x_1}^\infty dx_2 x_2^2 \left( j_l (p x_2) \phi^\infty_k (E, x_2) - \frac{\alpha}{|\kappa|} j_{l'} (p x_2) \phi^\infty_k (E, x_2) \right).$$  \hspace{1cm} (A10)

The integration over $x_2$ in the functions $\psi^0_k$ and $\psi^\infty_k$ has to be performed numerically. The problems here are that (i) the integration interval depends on $x_1$ and (ii) the integrand contains the spherical Bessel function which oscillates rapidly in the high-momenta region. Clearly, a straightforward use of Eqs. (A9) and (A10) in our calculations would lead to a re-evaluation of the integral for each new value of $x_1$, making the computation prohibitively expensive. One can observe, however, that if the function $\psi_k (E, p; x)$ is known for a particular set of $E$, $p$, and $x$, then the evaluation of $\psi_k (E, p; x')$ can be done by computing the Bessel transform integral over the interval $(x, x')$ only. So, introducing an ordered radial grid $\{x_i\}$, one can store the whole set of values $\{\psi_k (E, p; x_i)\}$ by performing just one Bessel transform over the interval $(0, \infty)$. This shows that for a fixed values of $E$ and $p$, the integrations of the type $\int_0^\infty dx \psi_k (E, p; x)$ can be performed without a recalculation of the Bessel transform integral.

**Appendix B: Free Dirac Green function in the coordinate-momentum representation**

The free Dirac Green function $G^{(0)}$ is a much simpler object than the Dirac Coulomb Green function $G$ and is known in the closed analytical form as well as in the partial-wave expansion form (see, e.g., Ref. [12]). For the purposes of the present investigation, we employ the coordinate-momentum representation and put $G^{(0)}$ into the form analogous to Eqs. (A6) and (A7). The simplest way to achieve this is to start with the momentum representation of $G^{(0)}$, which has a particularly simple form,

$$G^{(0)} (E, p_1, p_2) = (2\pi)^3 \frac{\delta^3 (p_1 - p_2)}{\gamma^0 E - \gamma \cdot p_2 - m} \gamma^0$$

$$= (2\pi)^3 \frac{E + \alpha \cdot p_2 + m\gamma^0}{E^2 - p_2^2 - m^2} \delta^3 (p_1 - p_2),$$  \hspace{1cm} (B1)

where $\alpha = \gamma^0 \gamma$. Using the completeness of the angular-momentum spinors $\chi_{\kappa \mu}$,

$$\sum_{\kappa \mu} \chi_{\kappa \mu} (\hat{p}_1) \chi_{\kappa \mu}^\dagger (\hat{p}_2) = I \delta (\hat{p}_1 - \hat{p}_2),$$  \hspace{1cm} (B2)

and the identity $(\sigma \cdot \hat{p}) \chi_{\kappa \mu} (\hat{p}) = -\chi_{-\kappa \mu} (\hat{p})$, we cast Eq. (B1) into the partial-wave expansion form similar to that for the Dirac Coulomb Green function,
\[ G^{(0)}(E, \mathbf{p}_1, \mathbf{p}_2) = (2\pi)^3 \frac{1}{E^2 - p^2 - m^2} \sum_{\kappa \mu} \left( (E + m) \chi_{\kappa \mu}(\hat{\mathbf{p}}_1) \chi_{\kappa \mu}^\dagger(\hat{\mathbf{p}}_2) - p_2 \chi_{\kappa \mu}(\hat{\mathbf{p}}_1) \chi_{\kappa \mu}^\dagger(\hat{\mathbf{p}}_2) - p_1 \chi_{\kappa \mu}(\hat{\mathbf{p}}_1) \chi_{\kappa \mu}^\dagger(\hat{\mathbf{p}}_2) - p_1 \chi_{\kappa \mu}(\hat{\mathbf{p}}_2) \chi_{\kappa \mu}^\dagger(\hat{\mathbf{p}}_1) (E - m) \chi_{\kappa \mu}(\hat{\mathbf{p}}_1) \chi_{\kappa \mu}^\dagger(\hat{\mathbf{p}}_2) \right), \]  

(B3)

where \( p_i = |\mathbf{p}_i| \). The coordinate-momentum representation of \( G^{(0)} \) is obtained by the Fourier transform of the above expression over the first radial argument,

\[ G^{(0)}(E, x_1, \mathbf{p}_2) = \int \frac{dp_1}{(2\pi)^3} e^{ip_1 x_1} G^{(0)}(E, \mathbf{p}_1, \mathbf{p}_2). \]  

(B4)

After performing the integration over \( p_1 \), the free Dirac Green function is written in the form of Eq. (A6), with the radial part given by

\[ G^{(0)}(E, x_1, \mathbf{p}_2) = \frac{4\pi}{E^2 - p^2 - m^2} \left( (E + m) \frac{j_1(p_2x_1)}{|p_2|} - \frac{p_2 j_1(p_2x_1)}{|p_2|} - (E - m) \frac{j_1(p_2x_1)}{|p_2|} \right). \]  

(B5)

**Appendix C: Angular factors**

In this section we address the factors \( t_{\kappa_a, \kappa_a} \) and \( s^n_{\kappa_a, \kappa_a} \), which are defined by Eqs. (35)-(37). Inserting the explicit definitions of the angular-momentum spinors in these formulas, averaging over the momentum projections of the reference state, and calculating the sums of the Clebsch-Gordan coefficients, we arrive at the following results,

\[ t_{\kappa_a, \kappa_a}(J) = \frac{(-1)^{j_a + 1/2}}{\sqrt{4\pi} \Pi_{j_a} l_a} \left\{ \begin{array}{ccc} j_a & j_a & J \\ l_a & 1/2 \end{array} \right\} \times \sum_{M} (-1)^M Y_{JM}(\hat{\mathbf{q}}) Y_{l_a l_a}^{J-M}(\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2), \]  

(C1)

\[ s^n_{\kappa_a, \kappa_a}(JL) = (-1)^{j_a + L} \frac{\sqrt{6}}{4\pi} \frac{\Pi_{j_a} L}{\Pi_{j_a} L} \left\{ \begin{array}{ccc} j_a & j_n & J \\ 1/2 & 1/2 & 1 \\ l_n & l_a & L \end{array} \right\} \times \sum_{M} (-1)^M Y_{LM}(\hat{\mathbf{q}}) Y_{l_n l_a}^{L-M}(\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2), \]  

(C2)

\[ s^p_{\kappa_a, \kappa_a}(JL) = \frac{(-1)^{j_a + 1/2} \sqrt{3}}{\Pi_{j_a} \Pi_{j_a}} \left\{ \begin{array}{ccc} j_a & j_n & J \\ l_n & 1/2 \end{array} \right\} \times \sum_{M} (-1)^M Y_{LM}^{J-p}(\hat{\mathbf{q}}, \hat{\mathbf{p}}_1) Y_{l_n l_a}^{L-M}(\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2), \]  

(C3)

where \( \Pi_{j_1, j_2, \ldots} = \sqrt{(2j_1 + 1)(2j_2 + 1)\ldots} \) and \( Y_{LM}(\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2) \) are the bipolar spherical harmonics [25].

With help of formulas from the book [25], it is possible to obtain explicit results for the angular factors \( t_{\kappa_a, \kappa_a} \) and \( s^n_{\kappa_a, \kappa_a} \), which are functions of \( p_1 = |\mathbf{p}_1|, p_2 = |\mathbf{p}_2| \), and \( q = |\mathbf{p}_1 - \mathbf{p}_2| \) only. However, the resulting formulas turn out to be rather lengthy and not very convenient for numerical evaluation as they become numerically unstable for \( q \to 0 \). Because of this, we prefer to evaluate Eqs. (C1)-(C4) numerically, after some simplifications that exploit the fact that the result does not depend on any angles except for \( \hat{\mathbf{p}}_1 \cdot \hat{\mathbf{p}}_2 \). Namely, we set the azimuthal spherical coordinate of \( \hat{\mathbf{p}}_1 \) and \( \hat{\mathbf{p}}_2 \) to zero (\( \phi_1 = \phi_2 = 0 \)) and direct \( \hat{\mathbf{p}}_1 \) along the z axis (\( \theta_1 = 0 \)).