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# Coordinate-space approach to the bound-electron self-energy

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The self-energy correction for an electron bound in an electrostatic potential is examined in coordinate space. The binding potential is assumed to be spherically symmetric and local but not necessarily Coulomb. Subtractions that remove infinite renormalization terms and lower-order terms are given as operators in coordinate space in order to facilitate numerical evaluations of the level shift. This approach is expected to be applicable to calculations of finite-nuclear-size corrections and electron-screening corrections to the self-energy, and to calculations of higher-order quantum-electrodynamic corrections where the self-energy diagram is part of a more complex external-field Feynman diagram.

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## I. INTRODUCTION

It is well known that quantum-electrodynamic (QED) corrections are an integral part of the theory of atomic energy levels. The largest QED effect in most atoms is the lowest-order self-energy correction, which corresponds to the virtual emission and reabsorption of a photon by the bound electron. Even in the simple case of an electron bound in a pure Coulomb field, the precise theoretical determination of this correction has required extensive numerical calculations. A number of methods of formulating the numerical calculation of the electron self-energy have been discussed [1–4], and numerical calculations based on these formulations have been done recently [5–7]. A necessary feature of any such work is the subtraction of the infinite mass renormalization in such a way that a numerical evaluation of the remainder is feasible. In this paper, we provide a formulation of the self-energy calculation for an arbitrary spherically symmetric local binding potential in which the infinities associated with mass renormalization are removed by subtractions made in coordinate space. This work has two objectives which have not been fully met by existing methods. One is to provide a basis, that includes the region of low nuclear charge $Z$, for precise calculations of the self-energy of an atomic electron bound in a field that is not a pure Coulomb field. The other objective is to provide a basis for calculations of the self-energy when it is embedded in a higher-order Feynman diagram. The latter application has been made with a preliminary version of this method in a calculation of the electron screening correction to the self-energy, where the effect on the self-energy from a correction to the Coulomb potential is evaluated in first-order perturbation theory [8].

In a previous paper, the QED expression for the self-energy correction, $\Delta E_{\rm SE}$, has been written as the sum $\Delta E_{\rm SE} = \Delta E_L + \Delta E_H$ of a low-energy part $\Delta E_L$ and a high-energy part $\Delta E_H$[3], where (in units in which $\hbar = c = m_e = 1$)

$$\Delta E_L = \frac{\alpha}{\pi}E_n - \frac{\alpha}{\pi}\mathrm{P}\int_0^{E_n} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha^l G(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^m\phi_n(\mathbf{x}_1)(\delta_{lm}\boldsymbol{\nabla}_2\cdot\boldsymbol{\nabla}_1 - \nabla_2^l\nabla_1^m)\frac{\sin[(E_n-z)x_{21}]}{(E_n-z)^2x_{21}} \quad (1)$$

and

$$\Delta E_H = \frac{\alpha}{2\pi i}\int_{C_H} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu G(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu\phi_n(\mathbf{x}_1)\frac{e^{-bx_{21}}}{x_{21}} - \delta m\int d\mathbf{x}\ \phi_n^\dagger(\mathbf{x})\beta\phi_n(\mathbf{x}), \quad (2)$$

and where $b = -i\left[(E_n-z)^2 + i\delta\right]^{1/2}$, $\mathrm{Re}(b) > 0$, and $\mathbf{x}_{21} = \mathbf{x}_2 - \mathbf{x}_1$. In these expressions, $\phi_n$ and $E_n$ are the eigenfunction and eigenvalue of the Dirac equation for the bound state $n$, and $G$ is the Green's function for the Dirac equation corresponding to the operator $G = (H-z)^{-1}$, where $H = \boldsymbol{\alpha}\cdot\mathbf{p} + V + \beta$ is the Dirac Hamiltonian. The indices $l$ and $m$ are summed from 1 to 3, and the index $\mu$ is summed from 0 to 3. The contour $C_H$ extends from $-i\infty$ to $0 - i\epsilon$ and from $0 + i\epsilon$ to $+i\infty$, with the appropriate branch of $b$ chosen in each case. Notational details are defined in Appendix A.

The expressions in (1) and (2) contain no assumptions concerning the external electrostatic potential except that the spectrum of the Dirac Hamiltonian resembles the Coulomb spectrum in a way that is evident from the derivation in Ref. [3]. We shall assume in addition that the orders of magnitude of the various Dirac operators for bound states of the external field are comparable to their counterparts in a Coulomb field to the extent that the identification of lower-order and higher-order terms made in the following discussion has validity.

The low-energy part in (1) is finite, so that subtractions are not necessary. However, it contains a finite part of the renormalization, and the physical level shift is smaller by a factor of order $(Z\alpha)^4$. In order to identify the physically relevant part of (1), we explicitly calculate the lower-order terms in Sec. II.

The main focus of this paper is on the high-energy part, for which we describe a method of isolating the divergent terms and carrying out the mass renormalization in coordinate space. A subtraction function is formulated that allows the removal of the lower-order terms and the infinities associated with mass renormalization pointwise, prior to carrying out the numerical integrations. Pointwise subtraction is not necessary to obtain a finite result, i.e., the subtraction could be carried out at a later stage of the calculation, but it is found that early removal of the problematic terms significantly improves the convergence of the numerical integrations. This approach can be extended to renormalize the self-energy diagram when it is embedded in a higher-order bound-state Feynman diagram, and it makes calculation of the Fourier transform of the wave functions unnecessary.

As a test case, this formulation has been applied to the calculation of the high-energy part of the Coulomb self energy. That work is planned to be described in a separate paper [9].

## II. LOW-ENERGY PART

The low-energy part of the self-energy is finite and can be calculated to sufficient accuracy that it is not necessary to subtract the parts that are lower order than the physical result prior to integration. Methods of evaluation of the complete low-energy part are described in Refs. [3, 10, 7]. Those calculations are applied to the Coulomb field case, but the formulation in terms of the radial Green's functions is applicable to a broad range of spherically symmetric external fields. In particular, the general expression for the real part of the low-energy part is [3]

$$\Delta E_L = \frac{\alpha}{\pi}E_n - \frac{\alpha}{\pi}\mathrm{P}\int_0^{E_n} dz \int_0^\infty dx_2 x_2^2 \int_0^\infty dx_1 x_1^2 \sum_\kappa \sum_{i,j=1}^{2} f_{\bar{i}}(x_2) G_\kappa^{ij}(x_2,x_1,z) f_{\bar{j}}(x_1) A_\kappa^{ij}(x_2,x_1), \tag{3}$$

where $f_i$ are the components of the radial wave function, $\bar{i} = 3 - i$, $G_\kappa^{ij}$ are the components of the radial Green's functions, and $A_\kappa^{ij}$ are functions that arise from the photon propagator. Detailed definitions of the notation are given in Ref. [3]. The explicit low-order parts given in Ref. [3] apply to a Coulomb field, and the corresponding generalization is derived in this section. It is of interest to identify the lower-order terms not only to isolate the physical part of the correction, but also to verify that these terms cancel the corresponding terms in the high-energy part. The identification of the lower-order terms made here is based on orders of magnitude that are valid for an electron in a Coulomb field, but the calculations are done for an arbitrary external field. Some remarks on Coulomb orders of magnitude are made in Appendix B.

To calculate the terms of order lower than $(Z\alpha)^4$, we write the low-energy part in terms of operators as [3]

$$\Delta E_L = \frac{\alpha}{\pi}E_n - \frac{\alpha}{4\pi^2}\mathrm{P}\int_{k<E_n} d\mathbf{k}\,\frac{1}{k}\left(\delta_{lm} - \frac{k^l k^m}{k^2}\right)\left\langle \alpha^l \frac{1}{\boldsymbol{\alpha}\cdot\mathbf{p} - \boldsymbol{\alpha}\cdot\mathbf{k} + V + \beta - E_n + k - i\delta}\alpha^m \right\rangle \tag{4}$$

and expand the right-hand side of (4), neglecting terms that are higher order than first in $V$ and $1 - E_n$, or higher order than second in $\boldsymbol{\alpha}\cdot\mathbf{p}$

$$\begin{aligned}\frac{1}{\boldsymbol{\alpha}\cdot\mathbf{p} - \boldsymbol{\alpha}\cdot\mathbf{k} + V + \beta - E_n + k - i\delta} &= -\left(\frac{1}{2E_nk} - \frac{1-E_n^2}{4k^2}\right)(\boldsymbol{\alpha}\cdot\mathbf{k} - \beta - E_n + k)\\ &-\frac{1}{4k^2}(\boldsymbol{\alpha}\cdot\mathbf{k} - \beta - E_n + k)(\boldsymbol{\alpha}\cdot\mathbf{p} + V)(\boldsymbol{\alpha}\cdot\mathbf{k} - \beta - E_n + k)\\ &-\frac{1}{8k^3}(\boldsymbol{\alpha}\cdot\mathbf{k} - \beta - E_n + k)\boldsymbol{\alpha}\cdot\mathbf{p}\,(\boldsymbol{\alpha}\cdot\mathbf{k} - \beta - E_n + k)\boldsymbol{\alpha}\cdot\mathbf{p}\,(\boldsymbol{\alpha}\cdot\mathbf{k} - \beta - E_n + k) + \cdots .\end{aligned} \tag{5}$$

Neglected terms in this expansion contribute corrections of order $(Z\alpha)^4\ln(Z\alpha)^{-2}$ or higher. By dropping terms that are odd in $\mathbf{k}$, and taking into account the fact that

$$\begin{aligned}(E_n + \beta)\alpha^l|n\rangle &= \alpha^l(E_n - \beta)|n\rangle\\ &= \alpha^l(\boldsymbol{\alpha}\cdot\mathbf{p} + V)|n\rangle\end{aligned} \tag{6}$$

in estimating orders of magnitude, we find that the right-hand side of (5) has the same leading terms as

$$\frac{1}{2E_nk}(\beta + E_n - k) + \frac{1-E_n^2}{4k} - \frac{1}{4k^2}[2\boldsymbol{\alpha}\cdot\mathbf{k}\;\mathbf{p}\cdot\mathbf{k} - 2k\boldsymbol{\alpha}\cdot\mathbf{p} + 2k^2V + 2(\mathbf{p}\cdot\mathbf{k})^2 - kp^2] + \cdots . \tag{7}$$

Substitution of (7) into (4) and integration over $\mathbf{k}$ yields

$$\Delta E_L = \frac{\alpha}{\pi}[\ \tfrac{1}{2}E_n + \langle\beta\rangle - \tfrac{1}{2}(1-E_n^2) + \tfrac{1}{6}\langle\boldsymbol{\alpha}\cdot\mathbf{p}\rangle + \tfrac{1}{2}\langle V\rangle - \tfrac{1}{3}\langle p^2\rangle + \mathcal{O}((Z\alpha)^4\ln(Z\alpha)^{-2})]. \tag{8}$$

The replacements, based on the Dirac equation (see Appendix B),

$$\begin{aligned} 1-E_n^2 &\to \langle\beta\rangle - E_n - \langle V\rangle + \mathcal{O}((Z\alpha)^4),\\ \langle\boldsymbol{\alpha}\cdot\mathbf{p}\rangle &\to E_n - \langle\beta\rangle - \langle V\rangle,\\ \langle p^2\rangle &\to \langle\boldsymbol{\alpha}\cdot\mathbf{p}\rangle + \mathcal{O}((Z\alpha)^4), \end{aligned} \tag{9}$$

in (8) give

$$\Delta E_L = \frac{\alpha}{\pi}[\tfrac{5}{6}E_n + \tfrac{2}{3}\langle\beta\rangle + \tfrac{7}{6}\langle V\rangle + \mathcal{O}((Z\alpha)^4\ln(Z\alpha)^{-2})]. \tag{10}$$

The physical part of the low-energy part is thus isolated in a function $f_L(Z\alpha)$ defined by

$$\Delta E_L = \frac{\alpha}{\pi}\left(\tfrac{5}{6}E_n + \tfrac{2}{3}\langle\beta\rangle + \tfrac{7}{6}\langle V\rangle + \frac{(Z\alpha)^4}{n^3}f_L(Z\alpha)\right). \tag{11}$$

In a pure Coulomb field $E_n = \langle\beta\rangle$, and this result coincides with the earlier result specialized to that case [3].

The fact that this direct expansion procedure correctly isolates the lower-order terms is related to the fact that the low-energy part is written in the form of the Coulomb gauge. It was recognized in early work by Kroll and Lamb [11] that such an expansion can be employed in the Coulomb gauge to obtain the lowest-order Lamb shift. The analogous procedure in the Feynman gauge leads to an expansion that does not converge due to infrared photon contributions. Fried and Yennie encountered this problem and identified an alternative gauge in which spurious low-order terms vanish [12].

The numerically significant part of the low-energy part of the self-energy is calculated by evaluating the complete expression for $\Delta E_L$ in (3) and numerically solving (11) to obtain $f_L(Z\alpha)$. In the cases where $Z$ is small, this procedure entails substantial numerical cancellation, but it has been demonstrated that such an approach is feasible.

## III. REGULARIZATION

The high-energy part in (2) is only formal, in the sense that each of the two terms is infinite, and the difference is finite. To make the terms separately finite, a scheme such as dimensional regularization, Pauli-Villars regularization, etc., is needed. In this work, the Pauli-Villars method is employed [13]. It is implemented by making the replacement

$$\frac{1}{q^2+i\delta} \to \frac{1}{q^2+i\delta} - \frac{1}{q^2-\Lambda^2+i\delta} \tag{12}$$

in the momentum-space expression for the photon propagator. In coordinate space, this corresponds to the replacement

$$\frac{e^{-bx_{21}}}{x_{21}} \to \frac{e^{-bx_{21}}}{x_{21}} - \frac{e^{-b'x_{21}}}{x_{21}}, \tag{13}$$

where

$$b' = -i\left[(E_n - z)^2 - \Lambda^2 + i\delta\right]^{1/2}, \quad \mathrm{Re}(b') > 0. \tag{14}$$

In this case, the mass renormalization term $\delta m$ is given by the corresponding term calculated with the regularized photon propagator with the result

$$\delta m \to \delta m(\Lambda) = \frac{\alpha}{\pi}[\tfrac{3}{4}\ln(\Lambda^2) + \tfrac{3}{8}]. \tag{15}$$

The full regularized expression is then

$$\Delta E_H = \lim_{\Lambda\to\infty}\left[\frac{\alpha}{2\pi i}\int_{C_H} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu G(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu\phi_n(\mathbf{x}_1) \times\left(\frac{e^{-bx_{21}}}{x_{21}} - \frac{e^{-b'x_{21}}}{x_{21}}\right) - \delta m(\Lambda)\int d\mathbf{x}\ \phi_n^\dagger(\mathbf{x})\beta\phi_n(\mathbf{x})\right], \tag{16}$$

which, added to the low-energy part $\Delta E_L$, yields the finite physical result.

## IV. SINGULAR TERMS

Although the integration over $z$ in (16) is exponentially damped at large $|z|$ when $x_{21} \neq 0$, the unregulated integral is infinite, because the point $x_{21} = 0$ is included in the range of the coordinate-space integration. To isolate the divergent terms, we examine the integrand in the immediate vicinity of $x_{21} = 0$, and consider various expansions about this point. In particular, we employ three expansions. First, the Dirac Green's function in (16) is expanded in powers of the external potential $V$:

$$G(\mathbf{x}_2,\mathbf{x}_1,z) = F(\mathbf{x}_2,\mathbf{x}_1,z) - \int d\mathbf{x}_3 F(\mathbf{x}_2,\mathbf{x}_3,z)V(\mathbf{x}_3)F(\mathbf{x}_3,\mathbf{x}_1,z) + \cdots, \tag{17}$$

where $F(\mathbf{x}_2,\mathbf{x}_1,z)$ is the free-electron Dirac Green's function. Terms not included in the expansion in (17), when substituted into (16), give a finite contribution that is of order $(Z\alpha)^4$. The second expansion is the power-series expansion of the wave function in (16):

$$\phi_n(\mathbf{x}_1) = \phi_n(\mathbf{x}_2) + (\mathbf{x}_1 - \mathbf{x}_2)\cdot\boldsymbol{\nabla}_2\,\phi_n(\mathbf{x}_2) + \tfrac{1}{2}(x_1^l - x_2^l)(x_1^m - x_2^m)\frac{\partial}{\partial x_2^l}\frac{\partial}{\partial x_2^m}\phi_n(\mathbf{x}_2) + \cdots, \tag{18}$$

where the indices $l, m$ are summed from 1 to 3. This expansion is made to take into account the fact that the dominant contribution to the function at large $|z|$ comes from the region where $x_{21} \approx 0$. A series expansion of the wave function to isolate the renormalization terms has been employed in a calculation of the electromagnetic self-energy of quarks in a cavity [14, 15]; special features of the cavity potential considerably simplified that calculation, and a coordinate-space subtraction was not made. The series in (18) corresponds to an asymptotic expansion in $|z|^{-1}$ for the integrand of the integral over $z$ in (16), as suggested by the example given in Appendix C. It also corresponds to an expansion in powers of $\mathbf{p}$, and to a certain extent, powers of $Z\alpha$. The third expansion is

$$V(\mathbf{x}_3) = V(\mathbf{x}_2) + \cdots \tag{19}$$

in the second term on the right-hand side of (17). Higher-order terms in (19) correspond to commutators of $V$ and $F$. In the present approach, we isolate the terms corresponding to the first term in (17) and three terms in (18), together with the second term in (17), the first term in (18), and the term in (19). This group of four terms contains all the divergences, and in the Coulomb case, all the parts of order lower than $(Z\alpha)^4$ in (16). One of the terms isolated here is finite, i.e., the first term of (17) taken with the third term of (18), but it is of order $p^2 \sim (Z\alpha)^2$, and is removed to improve the numerical accuracy at low $Z$. The terms listed above are calculated exactly for an arbitrary spherically symmetric potential in terms of expectation values of simple operators in the following section.

The direct expansion of the high-energy part described above correctly calculates the power series in $(Z\alpha)$ up to order $(Z\alpha)^4$, despite the fact that the expression is written in the Feynman gauge. The spurious low-order terms that appear in the expansion of the complete self-energy in this gauge are not present, because the soft-photon contributions that give rise to these terms are isolated in the low-energy part.

## V. CALCULATION OF THE SINGULAR TERMS

The singular terms defined in the preceding section are denoted by $\Delta E_H^{(i,j)}$, where $i$ indicates the order in $V$, and $j$ indicates the order in the power series in (18).

The leading term is

$$\Delta E_H^{(0,0)} = \frac{\alpha}{2\pi i}\int_{C_H} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1\, \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu F(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu\phi_n(\mathbf{x}_2)\left(\frac{e^{-bx_{21}}}{x_{21}} - \frac{e^{-b'x_{21}}}{x_{21}}\right), \tag{20}$$

where the free Green's function

$$F(\mathbf{x}_2,\mathbf{x}_1,z) = \lim_{Z\alpha\to 0} G(\mathbf{x}_2,\mathbf{x}_1,z) \tag{21}$$

is given explicitly by

$$F(\mathbf{x}_2,\mathbf{x}_1,z) = \left[\left(\frac{c}{x_{21}} + \frac{1}{x_{21}^2}\right) i\boldsymbol{\alpha}\cdot\mathbf{x}_{21} + \beta + z\right]\frac{e^{-cx_{21}}}{4\pi x_{21}}, \tag{22}$$

with $c = (1 - z^2)^{1/2}$, $\mathrm{Re}(c) > 0$. In (20), integration over $\mathbf{x}_1$ is elementary,

$$\int d\mathbf{x}_1\, F(\mathbf{x}_2,\mathbf{x}_1,z)\left(\frac{e^{-bx_{21}}}{x_{21}} - \frac{e^{-b'x_{21}}}{x_{21}}\right) = (\beta + z)\left(\frac{1}{b+c} - \frac{1}{b'+c}\right), \tag{23}$$

so that

$$\Delta E_H^{(0,0)} = \frac{\alpha}{\pi i}\int_{C_H} dz\, \langle 2\beta - z\rangle\left(\frac{1}{b+c} - \frac{1}{b'+c}\right). \tag{24}$$

Integration over $z$ yields (see Appendix D)

$$\Delta E_H^{(0,0)} = \frac{\alpha}{\pi}\left[\langle\beta\rangle\left(\ln(\Lambda^2) - 1 + \frac{1-E_n^2}{E_n^2}\ln\left(1+E_n^2\right)\right) - E_n\left(\tfrac{1}{4}\ln(\Lambda^2) + \frac{3E_n^2 - 2}{8E_n^2} + \frac{1-E_n^4}{4E_n^4}\ln\left(1+E_n^2\right)\right) + \mathcal{O}(\Lambda^{-1})\right]. \tag{25}$$

The second term is

$$\Delta E_H^{(0,1)} = \frac{\alpha}{2\pi i}\int_{C_H} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu F(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu(\mathbf{x}_1-\mathbf{x}_2)\cdot\boldsymbol{\nabla}\ \phi_n(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_2}\left(\frac{e^{-bx_{21}}}{x_{21}}-\frac{e^{-b'x_{21}}}{x_{21}}\right). \tag{26}$$

Integration over $\mathbf{x}_1$ yields

$$\int d\mathbf{x}_1\ F(\mathbf{x}_2,\mathbf{x}_1,z)(\mathbf{x}_1-\mathbf{x}_2)\left(\frac{e^{-bx_{21}}}{x_{21}}-\frac{e^{-b'x_{21}}}{x_{21}}\right) = -\frac{i}{3}\boldsymbol{\alpha}\left(\frac{1}{b+c}-\frac{1}{b'+c}+\frac{c}{(b+c)^2}-\frac{c}{(b'+c)^2}\right). \tag{27}$$

Hence

$$\Delta E_H^{(0,1)} = \frac{\alpha}{\pi i}\int_{C_H} dz\ \tfrac{1}{3}\langle\boldsymbol{\alpha}\cdot\mathbf{p}\,\rangle\left(\frac{1}{b+c}-\frac{1}{b'+c}+\frac{c}{(b+c)^2}-\frac{c}{(b'+c)^2}\right), \tag{28}$$

and

$$\Delta E_H^{(0,1)} = \frac{\alpha}{\pi}\langle\boldsymbol{\alpha}\cdot\mathbf{p}\,\rangle\left(\tfrac{1}{4}\ln(\Lambda^2)-\frac{6-3E_n^2+7E_n^4}{24E_n^2(1+E_n^2)}+\frac{1-E_n^4}{4E_n^4}\ln\left(1+E_n^2\right)+\mathcal{O}(\Lambda^{-1})\right). \tag{29}$$

The next term

$$\Delta E_H^{(0,2)} = \frac{\alpha}{2\pi i}\int_{C_H} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu F(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu$$
$$\times\tfrac{1}{2}(x_1^l-x_2^l)(x_1^m-x_2^m)\frac{\partial}{\partial x^l}\frac{\partial}{\partial x^m}\phi_n(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_2}\left(\frac{e^{-bx_{21}}}{x_{21}}-\frac{e^{-b'x_{21}}}{x_{21}}\right) \tag{30}$$

is evaluated with the aid of

$$\int d\mathbf{x}_1\ F(\mathbf{x}_2,\mathbf{x}_1,z)(x_1^l-x_2^l)(x_1^m-x_2^m)\left(\frac{e^{-bx_{21}}}{x_{21}}-\frac{e^{-b'x_{21}}}{x_{21}}\right) = \tfrac{2}{3}\delta_{lm}(\beta+z)\left(\frac{1}{(b+c)^3}-\frac{1}{(b'+c)^3}\right), \tag{31}$$

to give

$$\Delta E_H^{(0,2)} = -\frac{\alpha}{\pi i}\int_{C_H} dz\ \tfrac{1}{3}\left\langle(2\beta-z)p^2\right\rangle\left(\frac{1}{(b+c)^3}-\frac{1}{(b'+c)^3}\right), \tag{32}$$

with the result

$$\Delta E_H^{(0,2)} = \frac{\alpha}{\pi}\Bigg[\left\langle\beta p^2\right\rangle\left(-\frac{3+6E_n^2-E_n^4}{3E_n^2(1+E_n^2)^2}+\frac{1}{E_n^4}\ln\left(1+E_n^2\right)\right)$$
$$+\left\langle E_n p^2\right\rangle\left(\frac{6+3E_n^2+E_n^4}{12E_n^4(1+E_n^2)}-\frac{1}{2E_n^6}\ln\left(1+E_n^2\right)\right)+\mathcal{O}(\Lambda^{-1})\Bigg]. \tag{33}$$

The last term is the correction linear in $V$,

$$\Delta E_H^{(1,0)} = -\frac{\alpha}{2\pi i}\int_{C_H} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu \int d\mathbf{x}_3 F(\mathbf{x}_2,\mathbf{x}_3,z)$$
$$\times V(\mathbf{x}_2)F(\mathbf{x}_3,\mathbf{x}_1,z)\alpha^\mu\phi_n(\mathbf{x}_2)\left(\frac{e^{-bx_{21}}}{x_{21}}-\frac{e^{-b'x_{21}}}{x_{21}}\right). \tag{34}$$

In view of the operator identity

$$\frac{1}{H_0-z}\,\frac{1}{H_0-z} = \left(\frac{\partial}{\partial\epsilon}\frac{1}{H_0-z-\epsilon}\right)_{\epsilon=0}, \tag{35}$$

the integral over the product of $F$'s is

$$\int d\mathbf{x}_3\ F(\mathbf{x}_2,\mathbf{x}_3,z)F(\mathbf{x}_3,\mathbf{x}_1,z) = \left(\frac{\partial}{\partial\epsilon}F(\mathbf{x}_2,\mathbf{x}_1,z+\epsilon)\right)_{\epsilon=0}, \tag{36}$$

and so

$$\Delta E_H^{(1,0)} = -\frac{\alpha}{2\pi i}\int_{C_H} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu V(\mathbf{x}_2)\left(\frac{\partial}{\partial\epsilon}F(\mathbf{x}_2,\mathbf{x}_1,z+\epsilon)\right)_{\epsilon=0}\alpha^\mu\phi_n(\mathbf{x}_2)\left(\frac{e^{-bx_{21}}}{x_{21}}-\frac{e^{-b'x_{21}}}{x_{21}}\right). \tag{37}$$

Integration over $\mathbf{x}_1$ according to (23), and differentiation with respect to $\epsilon$ yields

$$\Delta E_H^{(1,0)} = \frac{\alpha}{\pi i}\int_{C_H} dz\left[\langle V\rangle\left(\frac{1}{b+c}-\frac{1}{b'+c}\right)-\langle V(2\beta-z)\rangle\frac{z}{c}\left(\frac{1}{(b+c)^2}-\frac{1}{(b'+c)^2}\right)\right], \tag{38}$$

and

$$\Delta E_H^{(1,0)} = \frac{\alpha}{\pi}\left[\langle V\rangle\left(\tfrac{1}{4}\ln(\Lambda^2)+\frac{6-E_n^2}{8E_n^2}-\frac{3+E_n^4}{4E_n^4}\ln\left(1+E_n^2\right)\right)-\left\langle\frac{\beta}{E_n}V\right\rangle\left(2-\frac{2}{E_n^2}\ln\left(1+E_n^2\right)\right)+\mathcal{O}(\Lambda^{-1})\right]. \tag{39}$$

The above terms are combined into a high-energy analytic part $\Delta E_A$, defined by

$$\Delta E_A = \lim_{\Lambda\to\infty}\left[\Delta E_H^{(0,0)}+\Delta E_H^{(0,1)}+\Delta E_H^{(0,2)}+\Delta E_H^{(1,0)}-\delta m(\Lambda)\langle\beta\rangle\right], \tag{40}$$

where the last term is the renormalization term from (2). Taking advantage of the Dirac equation to replace $\langle\boldsymbol{\alpha}\cdot\mathbf{p}\rangle$ by $E_n-\langle\beta\rangle-\langle V\rangle$, we have

$$\begin{aligned}\Delta E_A = \frac{\alpha}{\pi}\Bigg[& E_n\left(-\frac{2E_n^2}{3(1+E_n^2)}\right)+\langle\beta\rangle\left(\frac{3-18E_n^2-13E_n^4}{12E_n^2(1+E_n^2)}-\frac{(1-E_n^2)(1-3E_n^2)}{4E_n^4}\ln\left(1+E_n^2\right)\right)\\ &+\langle V\rangle\left(\frac{6+3E_n^2+E_n^4}{6E_n^2(1+E_n^2)}-\frac{1}{E_n^4}\ln\left(1+E_n^2\right)\right)+\left\langle\frac{\beta}{E_n}V\right\rangle\left(-2+\frac{2}{E_n^2}\ln\left(1+E_n^2\right)\right)\\ &+\left\langle E_np^2\right\rangle\left(\frac{6+3E_n^2+E_n^4}{12E_n^4(1+E_n^2)}-\frac{1}{2E_n^6}\ln\left(1+E_n^2\right)\right)+\left\langle\beta p^2\right\rangle\left(-\frac{3+6E_n^2-E_n^4}{3E_n^2(1+E_n^2)^2}+\frac{1}{E_n^4}\ln\left(1+E_n^2\right)\right)\Bigg].\end{aligned} \tag{41}$$

The divergent terms vanish in the sum (41) as expected. The terms containing $p^2$ can be eliminated with the aid of the Dirac equation identities (see Appendix B):

$$\begin{aligned}\left\langle E_np^2\right\rangle &= E_n(E_n^2-1)-2E_n^2\langle V\rangle+\left\langle E_nV^2\right\rangle,\\ \left\langle\beta p^2\right\rangle &= \langle\beta\rangle(E_n^2-1)-2\langle V\rangle-\left\langle\beta V^2\right\rangle,\end{aligned} \tag{42}$$

to give

$$\begin{aligned}\Delta E_A = \frac{\alpha}{\pi}\Bigg[& E_n\left(-\frac{6-9E_n^2+7E_n^4}{12E_n^4}+\frac{1-E_n^2}{2E_n^6}\ln\left(1+E_n^2\right)\right)\\ &+\langle\beta\rangle\left(\frac{(5+9E_n^2)(3-6E_n^2-E_n^4)}{12E_n^2(1+E_n^2)^2}-\frac{(1-E_n^2)(5-3E_n^2)}{4E_n^4}\ln\left(1+E_n^2\right)\right)\\ &+\langle V\rangle\left(2\frac{3+6E_n^2-E_n^4}{3E_n^2(1+E_n^2)^2}-\frac{2}{E_n^4}\ln\left(1+E_n^2\right)\right)+\left\langle\frac{\beta}{E_n}V\right\rangle\left(-2+\frac{2}{E_n^2}\ln\left(1+E_n^2\right)\right)\\ &+\left\langle E_nV^2\right\rangle\left(\frac{6+3E_n^2+E_n^4}{12E_n^4(1+E_n^2)}-\frac{1}{2E_n^6}\ln\left(1+E_n^2\right)\right)+\left\langle\beta V^2\right\rangle\left(\frac{3+6E_n^2-E_n^4}{3E_n^2(1+E_n^2)^2}-\frac{1}{E_n^4}\ln\left(1+E_n^2\right)\right)\Bigg].\end{aligned} \tag{43}$$

With Coulomb orders of magnitude as a guide, but not assuming the Coulomb identity $\langle\beta\rangle = E_n$, we identify the parts of $\Delta E_A$ that are of order lower than $(Z\alpha)^4$ by expanding in powers of $1-E_n^2$:

$$\begin{aligned}\Delta E_A = \frac{\alpha}{\pi}\Bigg[& E_n\left(-\tfrac{1}{3}+\frac{2\ln 2-1}{4}\left(1-E_n^2\right)\right)+\langle\beta\rangle\left(-\tfrac{7}{6}+\frac{3-2\ln 2}{4}\left(1-E_n^2\right)\right)\\ &+\langle V\rangle\left(\tfrac{4}{3}-2\ln 2\right)+\left\langle\frac{\beta}{E_n}V\right\rangle(2\ln 2-2)+\mathcal{O}((Z\alpha)^4)\Bigg].\end{aligned} \tag{44}$$

This expression is simplified by taking advantage of the facts that (see Appendix B)

$$E_n(1-E_n^2) = \langle\beta\rangle - E_n - \langle V\rangle + \mathcal{O}((Z\alpha)^4),$$
$$\langle\beta\rangle(1-E_n^2) = \langle\beta\rangle - E_n - \langle V\rangle + \mathcal{O}((Z\alpha)^4), \tag{45}$$
$$\left\langle \frac{\beta}{E_n}V\right\rangle = \langle V\rangle + \mathcal{O}((Z\alpha)^4),$$

to obtain

$$\Delta E_A = \frac{\alpha}{\pi}[-\tfrac{5}{6}E_n - \tfrac{2}{3}\langle\beta\rangle - \tfrac{7}{6}\langle V\rangle + \mathcal{O}((Z\alpha)^4)]. \tag{46}$$

We note that the leading terms cancel the corresponding terms in the low-energy part.

In view of this relation, and the fact that the leading terms cancel in the total self-energy, it is convenient to isolate the remainder of the analytic part in terms of a function $f_A(Z\alpha)$ by writing

$$\Delta E_A = \frac{\alpha}{\pi}\left(-\tfrac{5}{6}E_n - \tfrac{2}{3}\langle\beta\rangle - \tfrac{7}{6}\langle V\rangle + \frac{(Z\alpha)^4}{n^3}f_A(Z\alpha)\right). \tag{47}$$

It follows from (43) that

$$\begin{aligned}\frac{(Z\alpha)^4}{n^3}f_A(Z\alpha) = {} & \tfrac{1}{2}\langle E_n-\beta\rangle + E_n(1-E_n^2)\left(-\frac{2-E_n^2}{4E_n^4} + \frac{1}{2E_n^6}\ln(1+E_n^2)\right)\\ & + \langle\beta\rangle(1-E_n^2)\left(\frac{15+26E_n^2-5E_n^4}{12E_n^2(1+E_n^2)^2} - \frac{5-3E_n^2}{4E_n^4}\ln(1+E_n^2)\right)\\ & + \langle V\rangle\left(\frac{(3+7E_n^2)(4+E_n^2+E_n^4)}{6E_n^2(1+E_n^2)^2} - \frac{2}{E_n^4}\ln(1+E_n^2)\right) + \left\langle\frac{\beta}{E_n}V\right\rangle\left(-2+\frac{2}{E_n^2}\ln(1+E_n^2)\right)\\ & + \langle E_nV^2\rangle\left(\frac{6+3E_n^2+E_n^4}{12E_n^4(1+E_n^2)} - \frac{1}{2E_n^6}\ln(1+E_n^2)\right) + \langle\beta V^2\rangle\left(\frac{3+6E_n^2-E_n^4}{3E_n^2(1+E_n^2)^2} - \frac{1}{E_n^4}\ln(1+E_n^2)\right).\end{aligned} \tag{48}$$

The first term on the right-hand side is isolated to minimize numerical cancellations for small $Z\alpha$.

## VI. CALCULATION OF THE SUBTRACTION FUNCTIONS

The singular terms identified in the preceding section are examined further in this section to obtain the corresponding expressions as functions of $z$, $x_2$, and $x_1$. This is done so that the numerical subtraction can be made pointwise before integration over these variables, in order to minimize the loss of accuracy associated with the removal of these terms. In particular, we calculate a remainder $\Delta E_B$ by pointwise subtraction of the singular terms from the complete high-energy part

$$\Delta E_B = \Delta E_H - \Delta E_A. \tag{49}$$

The main consideration is that the same numerical integration formula be applied to both terms, so that the dominant integration errors in the complete term and the subtraction term are equal and opposite and largely cancel. In addition, the integral of the difference is finite, so the regulator subtraction is unnecessary and will not be included in this part of the calculation. The functions $K^{(i,j)}(x_2,x_1,z)$ give pointwise values of the integrands of the singular terms:

$$\Delta E_H^{(i,j)} = \frac{\alpha}{2\pi i}\int_{C_H}dz\int_0^\infty dx_2\,x_2^2\int_0^\infty dx_1\,x_1^2\,K^{(i,j)}(x_2,x_1,z). \tag{50}$$

The first term, (20), corresponds to

$$K^{(0,0)}(x_2,x_1,z) = \int d\Omega_2\int d\Omega_1\,\phi_n^\dagger(\mathbf{x}_2)\alpha_\mu F(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu\phi_n(\mathbf{x}_2)\frac{e^{-bx_{21}}}{x_{21}}. \tag{51}$$

The integral over $\Omega_1$ is (see Appendix E)

$$\int d\Omega_1\,\alpha_\mu F(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu\frac{e^{-bx_{21}}}{x_{21}} = \int_{-1}^{1}d\xi\,\frac{e^{-(b+c)R}}{R^2}\left[\left(\frac{c}{R}+\frac{1}{R^2}\right)i\boldsymbol{\alpha}\cdot\hat{\mathbf{x}}_2(x_2-\xi x_1)+2\beta-z\right], \tag{52}$$

where

$$R = (x_2^2 - 2x_2x_1\xi + x_1^2)^{1/2}. \tag{53}$$

In view of the fact that

$$\phi_n^\dagger(\mathbf{x})\boldsymbol{\alpha}\cdot\hat{\mathbf{x}}\phi_n(\mathbf{x}) = 0, \tag{54}$$

we have

$$K^{(0,0)}(x_2,x_1,z) = \int d\Omega_2\ \phi_n^\dagger(\mathbf{x}_2)\int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R^2}(2\beta - z)\phi_n(\mathbf{x}_2), \tag{55}$$

and hence

$$K^{(0,0)}(x_2,x_1,z) = F_n^T(x_2)\int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R^2}(2\beta - z)F_n(x_2), \tag{56}$$

where the notation is defined in Appendix A.

The second term is

$$K^{(0,1)}(x_2,x_1,z) = \int d\Omega_2 \int d\Omega_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu F(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu(\mathbf{x}_1-\mathbf{x}_2)\cdot\boldsymbol{\nabla}\ \phi_n(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_2}\frac{e^{-bx_{21}}}{x_{21}}, \tag{57}$$

with the corresponding angle integral (see Appendix E)

$$\int d\Omega_1\ \alpha_\mu F(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu(x_1^m - x_2^m)\frac{e^{-bx_{21}}}{x_{21}}$$

$$= -\int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R^2}\left[\left(\frac{c}{R}+\frac{1}{R^2}\right)i\alpha^l\left[R^2\hat{x}_2^l\hat{x}_2^m + \tfrac{1}{2}(1-\xi^2)x_1^2(\delta_{lm} - 3\hat{x}_2^l\hat{x}_2^m)\right] + (2\beta - z)(x_2 - \xi x_1)\hat{x}_2^m\right]. \tag{58}$$

With the aid of the identities (see Appendix A)

$$\begin{aligned}
&\int d\Omega\ \phi_n^\dagger(\mathbf{x})i(\boldsymbol{\alpha}\cdot\hat{\mathbf{x}})(\hat{\mathbf{x}}\cdot\boldsymbol{\nabla})\phi_n(\mathbf{x}) = -F_n^T(x)\alpha\beta\frac{\partial}{\partial x}F_n(x),\\
&\int d\Omega\ \phi_n^\dagger(\mathbf{x})i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\phi_n(\mathbf{x}) = -F_n^T(x)\alpha\beta\left(\frac{\partial}{\partial x}+\beta\frac{\kappa}{x}\right)F_n(x),\\
&\int d\Omega\ \phi_n^\dagger(\mathbf{x})(2\beta - z)\hat{\mathbf{x}}\cdot\boldsymbol{\nabla}\phi_n(\mathbf{x}) = F_n^T(x)(2\beta - z)\frac{\partial}{\partial x}F_n(x),
\end{aligned} \tag{59}$$

we obtain

$$\begin{aligned}
K^{(0,1)}(x_2,x_1,z) = F_n^T(x_2)\int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R^2}\Bigg[&(cR+1)\,\alpha\beta\frac{\partial}{\partial x_2} - \left(\frac{c}{R}+\frac{1}{R^2}\right)(1-\xi^2)x_1^2\alpha\beta\left(\frac{\partial}{\partial x_2} - \beta\frac{\kappa}{2x_2}\right)\\
&-(x_2 - \xi x_1)(2\beta - z)\frac{\partial}{\partial x_2}\Bigg]F_n(x_2).
\end{aligned} \tag{60}$$

The next term is

$$K^{(0,2)}(x_2,x_1,z) = \int d\Omega_2 \int d\Omega_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu F(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu\tfrac{1}{2}(x_1^l - x_2^l)(x_1^m - x_2^m)\frac{\partial}{\partial x^l}\frac{\partial}{\partial x^m}\phi_n(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_2}\frac{e^{-bx_{21}}}{x_{21}}. \tag{61}$$

We retain only the diagonal part of this term,

$$K_D^{(0,2)}(x_2,x_1,z) = \int d\Omega_2 \int d\Omega_1\ \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu F_D(\mathbf{x}_2,\mathbf{x}_1,z)\alpha^\mu\tfrac{1}{2}(x_1^l - x_2^l)(x_1^m - x_2^m)\frac{\partial}{\partial x^l}\frac{\partial}{\partial x^m}\phi_n(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_2}\frac{e^{-bx_{21}}}{x_{21}}, \tag{62}$$

corresponding to the diagonal part of the free Green's function,

$$F_D(\mathbf{x}_2,\mathbf{x}_1,z) = (\beta + z)\frac{e^{-cx_{21}}}{4\pi x_{21}}. \tag{63}$$

The off-diagonal term is not necessary for the calculation, and it gives no contribution to the final result, i.e.,

$$\int_0^\infty dx_1\ x_1^2\left[K^{(0,2)}(x_2,x_1,z) - K_D^{(0,2)}(x_2,x_1,z)\right] = 0. \tag{64}$$

The relevant angle integral is

$$\int d\Omega_1 \alpha_\mu F_D(\mathbf{x}_2, \mathbf{x}_1, z)\alpha^\mu (x_1^l - x_2^l)(x_1^m - x_2^m)\,\frac{e^{-bx_{21}}}{x_{21}}$$

$$= \int_{-1}^{1} d\xi\, \frac{e^{-(b+c)R}}{R^2}(2\beta - z)\left[R^2 \hat{x}_2^l \hat{x}_2^m + \tfrac{1}{2}(1-\xi^2)x_1^2(\delta_{lm} - 3\hat{x}_2^l\hat{x}_2^m)\right], \tag{65}$$

which together with (see Appendix A)

$$\int d\Omega\, \phi_n^\dagger(\mathbf{x})(2\beta - z)(\hat{\mathbf{x}}\cdot\boldsymbol{\nabla})^2\phi_n(\mathbf{x}) = F_n^T(x)(2\beta - z)\frac{\partial^2}{\partial x^2}F_n(x),$$

$$\int d\Omega\, \phi_n^\dagger(\mathbf{x})(2\beta - z)\nabla^2\phi_n(\mathbf{x}) = F_n^T(x)(2\beta - z)\left(\frac{1}{x}\frac{\partial^2}{\partial x^2}x - \frac{\kappa(\kappa+\beta)}{x^2}\right)F_n(x), \tag{66}$$

yields

$$K_D^{(0,2)}(x_2, x_1, z) = F_n^T(x_2)\int_{-1}^{1} d\xi\, \frac{e^{-(b+c)R}}{2R^2}(2\beta - z)\left[R^2\frac{\partial^2}{\partial x_2^2} - (1-\xi^2)x_1^2\left(\frac{\partial^2}{\partial x_2^2} - \frac{1}{x_2}\frac{\partial}{\partial x_2} + \frac{\kappa(\kappa+\beta)}{2x_2^2}\right)\right]F_n(x_2). \tag{67}$$

The term proportional to $V$ is

$$K^{(1,0)}(x_2, x_1, z) = -\int d\Omega_2 \int d\Omega_1\, \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu \int d\mathbf{x}_3 F(\mathbf{x}_2, \mathbf{x}_3, z)V(\mathbf{x}_2)F(\mathbf{x}_3, \mathbf{x}_1, z)\alpha^\mu\phi_n(\mathbf{x}_2)\frac{e^{-bx_{21}}}{x_{21}}$$

$$= -\int d\Omega_2 \int d\Omega_1\, \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu V(\mathbf{x}_2)\left(\frac{\partial}{\partial\epsilon}F(\mathbf{x}_2, \mathbf{x}_1, z+\epsilon)\right)_{\epsilon=0}\alpha^\mu\phi_n(\mathbf{x}_2)\frac{e^{-bx_{21}}}{x_{21}}. \tag{68}$$

Following (51) through (56), and differentiating with respect to $\epsilon$, we obtain

$$K^{(1,0)}(x_2, x_1, z) = F_n^T(x_2)\int_{-1}^{1} d\xi\, \frac{e^{-(b+c)R}}{R^2}V(x_2)\left(1 - (2\beta - z)R\frac{z}{c}\right)F_n(x_2), \tag{69}$$

where the spherical symmetry of $V(\mathbf{x})$ has been taken into account.

The complete subtraction function $K_A(x_2, x_1, z)$ is the sum

$$K_A(x_2, x_1, z) = K^{(0,0)}(x_2, x_1, z) + K^{(0,1)}(x_2, x_1, z) + K_D^{(0,2)}(x_2, x_1, z) + K^{(1,0)}(x_2, x_1, z) \tag{70}$$

of the individual terms that are obtained above and summarized below:

$$K^{(0,0)}(x_2, x_1, z) = F_n^T(x_2)Q_1(x_2, x_1, z)(2\beta - z)F_n(x_2), \tag{71}$$

$$K^{(0,1)}(x_2, x_1, z) = F_n^T(x_2)\Bigg[Q_2(x_2, x_1, z)\alpha\beta\frac{\partial}{\partial x_2} - Q_3(x_2, x_1, z)x_1^2\alpha\beta\left(\frac{\partial}{\partial x_2} - \beta\frac{\kappa}{2x_2}\right) - Q_4(x_2, x_1, z)(2\beta - z)\frac{\partial}{\partial x_2}\Bigg]F_n(x_2), \tag{72}$$

$$K_D^{(0,2)}(x_2, x_1, z) = F_n^T(x_2)\left(\beta - \frac{z}{2}\right)\left[Q_5(x_2, x_1, z)\frac{\partial^2}{\partial x_2^2} - Q_6(x_2, x_1, z)x_1^2\left(\frac{\partial^2}{\partial x_2^2} - \frac{1}{x_2}\frac{\partial}{\partial x_2} + \frac{\kappa(\kappa+\beta)}{2x_2^2}\right)\right]F_n(x_2), \tag{73}$$

$$K^{(1,0)}(x_2, x_1, z) = F_n^T(x_2)V(x_2)\left(Q_1(x_2, x_1, z) - (2\beta - z)\frac{z}{c}Q_7(x_2, x_1, z)\right)F_n(x_2). \tag{74}$$

The derivatives of the radial wave function can be eliminated from (72) and (73) with the aid of the radial differential equation, which gives

$$\frac{\partial}{\partial x}F_n(x) = \left(\alpha(1-\beta E_n) - (1+\beta\kappa)\frac{1}{x} + \alpha\beta V(x)\right)F_n(x) \tag{75}$$

and

$$\frac{\partial^2}{\partial x^2}F_n(x) = \left(\alpha(1-\beta E_n) - (1+\beta\kappa)\frac{1}{x} + \alpha\beta V(x)\right)\frac{\partial}{\partial x}F_n(x) + \left((1+\beta\kappa)\frac{1}{x^2} + \alpha\beta\frac{\partial V(x)}{\partial x}\right)F_n(x). \tag{76}$$

The functions $Q_i$ are given by

$$Q_1(x_2,x_1,z) = \int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R^2} = P_{-2}, \tag{77}$$

$$Q_2(x_2,x_1,z) = \int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R^2}(cR+1) = cP_{-1} + P_{-2}, \tag{78}$$

$$Q_3(x_2,x_1,z) = \int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R^4}(cR+1)(1-\xi^2)$$
$$= \frac{1}{(2x_2x_1)^2}\left[2(x_2^2+x_1^2)(cP_{-1}+P_{-2}) - (cP_1+P_0) - (x_2^2-x_1^2)^2(cP_{-3}+P_{-4})\right], \tag{79}$$

$$Q_4(x_2,x_1,z) = \int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R^2}(x_2-\xi x_1)$$
$$= \frac{1}{2x_2}\left[P_0 + (x_2^2-x_1^2)P_{-2}\right], \tag{80}$$

$$Q_5(x_2,x_1,z) = \int_{-1}^{1} d\xi\ e^{-(b+c)R} = P_0, \tag{81}$$

$$Q_6(x_2,x_1,z) = \int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R^2}(1-\xi^2)$$
$$= \frac{1}{(2x_2x_1)^2}\left[2(x_2^2+x_1^2)P_0 - P_2 - (x_2^2-x_1^2)^2P_{-2}\right], \tag{82}$$

$$Q_7(x_2,x_1,z) = \int_{-1}^{1} d\xi\ \frac{e^{-(b+c)R}}{R} = P_{-1}. \tag{83}$$

In the above equations, the functions $Q_i$ are expressed in terms of a set of integrals $P_i$ defined by

$$P_i = \int_{-1}^{1} d\xi\ R^i e^{-(b+c)R} = \frac{1}{x_2x_1}\int_{|x_2-x_1|}^{x_2+x_1} dR\ R^{(i+1)}e^{-(b+c)R}. \tag{84}$$

Integration over $R$ is relatively convenient for analytic or numerical evaluation.

In terms of the function $K_A(x_2,x_1,z)$ in (70), we write the modified high-energy part as

$$\Delta E_B = \frac{\alpha}{2\pi i}\int_{C_H} dz \int_0^\infty dx_2\ x_2^2 \int_0^\infty dx_1\ x_1^2 \left(\sum_\kappa \sum_{i,j=1}^{2}\left[\ f_i(x_2)G_\kappa^{ij}(x_2,x_1,z)f_j(x_1)A_\kappa(x_2,x_1)\right.\right.$$
$$\left.\left. - f_{\bar{i}}(x_2)G_\kappa^{ij}(x_2,x_1,z)f_{\bar{j}}(x_1)A_\kappa^{ij}(x_2,x_1)\right] - K_A(x_2,x_1,z)\right), \tag{85}$$

where the notation of Eq. (3) is employed, with the exception that the functions $A_\kappa^{ij}$ are defined differently here, as described in Ref. [3]. A corresponding numerical function $f_B(Z\alpha)$ is defined by

$$\Delta E_B = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}f_B(Z\alpha). \tag{86}$$

The total high-energy part is the sum

$$f_H(Z\alpha) = f_A(Z\alpha) + f_B(Z\alpha), \tag{87}$$

with $f_A(Z\alpha)$ given by (48) and $f_B(Z\alpha)$ given by (85) together with (86).

## VII. RESULTS AND CONCLUSION

The total self-energy is given by

$$\Delta E_n = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}F(Z\alpha)m_e c^2, \tag{88}$$

where

$$F(Z\alpha) = f_L(Z\alpha) + f_H(Z\alpha) \tag{89}$$

from (11) and (87).

The foregoing discussion provides a prescription for removing the renormalization terms from the bound-state self-energy diagram in such a way that a complete numerical evaluation is feasible for a broad class of external potentials. The renormalization subtraction is carried out before numerical integration over the two radial coordinates or integration over the intermediate-state energy parameter, so numerical integration errors are not amplified by the subtraction process. The fact that the subtraction term is relatively simple is particularly beneficial in the case where the self-energy diagram is embedded in a more complex Feynman diagram. On the other hand, the subtraction term does not cancel term by term in the summation over intermediate angular momentum in (85), so the slow convergence of that sum is not improved by the subtraction. This factor can be compensated in the numerical evaluation by the introduction of a high-order asymptotic expansion in the sum to carry out an analytic summation of the leading orders [9].

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## APPENDIX A

Some known background material and definitions of notation are given here. The Dirac equation is

$$[-i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + V(\mathbf{x}) + \beta - E_n]\phi_n(\mathbf{x}) = 0, \tag{A1}$$

where the $4\times 4$ matrices $\boldsymbol{\alpha}$ and $\beta$ are given by

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}; \tag{A2}$$

the components of $\boldsymbol{\sigma}$ are the Pauli spin matrices, and $I$ is the $2\times 2$ identity matrix. Since we are dealing only with spherically symmetric potentials, the wave function is written as [16]

$$\phi_n(\mathbf{x}) = \begin{pmatrix} f_1(x)\chi_\kappa^\mu(\hat{\mathbf{x}}) \\ if_2(x)\chi_{-\kappa}^\mu(\hat{\mathbf{x}}) \end{pmatrix}, \tag{A3}$$

where $\chi_\kappa^\mu(\hat{\mathbf{x}})$ is a two-component eigenfunction of total angular momentum with the properties that

$$(\boldsymbol{\sigma}\cdot\mathbf{L} + 1)\,\chi_\kappa^\mu(\hat{\mathbf{x}}) = -\kappa\chi_\kappa^\mu(\hat{\mathbf{x}}) \tag{A4}$$

and

$$\boldsymbol{\sigma}\cdot\hat{\mathbf{x}}\;\chi_\kappa^\mu(\hat{\mathbf{x}}) = -\chi_{-\kappa}^\mu(\hat{\mathbf{x}}). \tag{A5}$$

In view of the spherical symmetry assumed in this work, it is useful to make the separation

$$\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} = \boldsymbol{\alpha}\cdot\hat{\mathbf{x}}\left(\frac{1}{x}\frac{\partial}{\partial x}x - \beta\frac{K}{x}\right) \tag{A6}$$

in the gradient term in the Dirac equation, where

$$K = \beta(\boldsymbol{\sigma}\cdot\mathbf{L} + 1) \tag{A7}$$

is the Dirac angular momentum operator. The operator $K$ gives

$$K\phi_n(\mathbf{x}) = -\kappa\phi_n(\mathbf{x}) \tag{A8}$$

and

$$K\boldsymbol{\alpha}\cdot\hat{\mathbf{x}}\phi_n(\mathbf{x}) = -\kappa\boldsymbol{\alpha}\cdot\hat{\mathbf{x}}\phi_n(\mathbf{x}). \tag{A9}$$

The range of $\kappa$ is all nonzero integers. It immediately follows that

$$\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\phi_n(\mathbf{x}) = \boldsymbol{\alpha}\cdot\hat{\mathbf{x}}\left(\frac{1}{x}\frac{\partial}{\partial x}x + \beta\frac{\kappa}{x}\right)\phi_n(\mathbf{x}), \tag{A10}$$

and

$$\begin{aligned}\nabla^2\phi_n(\mathbf{x}) &= \left[\boldsymbol{\alpha}\cdot\hat{\mathbf{x}}\left(\frac{1}{x}\frac{\partial}{\partial x}x - \beta\frac{K}{x}\right)\right]^2\phi_n(\mathbf{x}) \\ &= \boldsymbol{\alpha}\cdot\hat{\mathbf{x}}\left(\frac{1}{x}\frac{\partial}{\partial x}x + \beta\frac{\kappa}{x}\right) \\ &\quad\times\boldsymbol{\alpha}\cdot\hat{\mathbf{x}}\left(\frac{1}{x}\frac{\partial}{\partial x}x + \beta\frac{\kappa}{x}\right)\phi_n(\mathbf{x}) \\ &= \left(\frac{1}{x}\frac{\partial^2}{\partial x^2}x - \frac{\kappa(\kappa+\beta)}{x^2}\right)\phi_n(\mathbf{x}).\end{aligned} \tag{A11}$$

Substitution of the identity in (A6) into the full Dirac equation in (A1) yields the two-component radial Dirac equation

$$\left(\alpha\beta\frac{1}{x}\frac{\partial}{\partial x}x + \alpha\frac{\kappa}{x} + V(x) + \beta - E_n\right)F_n(x) = 0, \tag{A12}$$

where

$$F_n(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} \tag{A13}$$

is the radial wave function. The matrices in (A12) are

$$\alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{A14}$$

In this paper, in expressions containing the full wave function $\phi_n(\mathbf{x})$, $\boldsymbol{\alpha}$, and $\beta$ refer to the $4\times 4$ Dirac matrices defined in (A2), and in expressions containing the radial wave function $F_n(x)$, $\alpha$ and $\beta$ denote the corresponding $2\times 2$ matrices defined in (A14).

## APPENDIX B

Some details in the derivation of Dirac expectation-value identities and order-of-magnitude arguments employed in this paper are supplied in this appendix.

The Dirac Hamiltonian

$$H = \boldsymbol{\alpha}\cdot\mathbf{p} + V + \beta \tag{B1}$$

satisfies the operator identity

$$\beta H + H\beta = 2\beta V + 2, \tag{B2}$$

since $\beta\boldsymbol{\alpha}+\boldsymbol{\alpha}\beta = 0$. Taking the expectation value of (B2) in the state $n$ yields

$$E_n\langle\beta\rangle = \langle\beta V\rangle + 1. \tag{B3}$$

Two additional exact identities are

$$\begin{aligned}\langle p^2\rangle &= \langle(\boldsymbol{\alpha}\cdot\mathbf{p})^2\rangle \\ &= \langle(E_n - V - \beta)^2\rangle \\ &= E_n^2 - 1 - 2E_n\langle V\rangle + \langle V^2\rangle,\end{aligned} \tag{B4}$$

and

$$\begin{aligned}\langle\beta p^2\rangle &= -\langle\boldsymbol{\alpha}\cdot\mathbf{p}\,\beta\,\boldsymbol{\alpha}\cdot\mathbf{p}\rangle \\ &= -\langle(E_n - V - \beta)\beta(E_n - V - \beta)\rangle \\ &= \langle\beta\rangle(E_n^2 - 1) - 2\langle V\rangle - \langle\beta V^2\rangle.\end{aligned} \tag{B5}$$

In both of the above equations, (B3) is taken into account to simplify the result.

Coulomb order-of-magnitude estimates are based on the fact that in a Coulomb bound state, the radial coordinate $x$ and momentum $\mathbf{p}$ have orders of magnitude given by

$$x \sim \frac{1}{Z\alpha} \tag{B6}$$

and

$$|\mathbf{p}| \sim Z\alpha. \tag{B7}$$

As a consequence, we have, for example,

$$\begin{aligned}\langle V\rangle &= \left\langle -\frac{Z\alpha}{x}\right\rangle = \mathcal{O}((Z\alpha)^2), \\ \langle p^2\rangle &= \mathcal{O}((Z\alpha)^2), \\ \langle V^2\rangle &= \mathcal{O}((Z\alpha)^4).\end{aligned} \tag{B8}$$

These estimates, together with the fact that the small components of the wave function are of order $(Z\alpha)$ relative to the large components, lead directly to

$$\begin{aligned}\langle\boldsymbol{\alpha}\cdot\mathbf{p}\rangle &= \mathcal{O}((Z\alpha)^2), \\ E_n &= 1 + \mathcal{O}((Z\alpha)^2), \\ \langle\beta V\rangle &= \langle V\rangle + \mathcal{O}((Z\alpha)^4), \\ \langle V\boldsymbol{\alpha}\cdot\mathbf{p}\rangle &= \mathcal{O}((Z\alpha)^4).\end{aligned} \tag{B9}$$

Hence,

$$\begin{aligned}1 - E_n^2 &= E_n(\langle\beta\rangle - E_n) - \langle\beta V\rangle \\ &= \langle\beta\rangle - E_n - \langle V\rangle + \mathcal{O}((Z\alpha)^4), \\ \langle p^2\rangle &= \langle(\boldsymbol{\alpha}\cdot\mathbf{p})^2\rangle \\ &= \tfrac{1}{2}\langle\boldsymbol{\alpha}\cdot\mathbf{p}\,(E_n - V - \beta) + (E_n - V - \beta)\boldsymbol{\alpha}\cdot\mathbf{p}\rangle \\ &= \langle\boldsymbol{\alpha}\cdot\mathbf{p}\rangle + \mathcal{O}((Z\alpha)^4).\end{aligned} \tag{B10}$$

## APPENDIX C

This appendix gives an example that indicates that the power-series expansion of the wave function discussed in Sec. IV leads to an asymptotic expansion for large values of $|z|$ of the integrand in Eq. (2). A simple expression with the essential features of (2) is

$$u(y) = \int d\mathbf{x}_2 \int d\mathbf{x}_1 f(\mathbf{x}_2)\,[a + y\mathbf{b}\cdot(\mathbf{x}_2 - \mathbf{x}_1)]\,\frac{e^{-y|\mathbf{x}_2-\mathbf{x}_1|}}{4\pi|\mathbf{x}_2 - \mathbf{x}_1|^2}\,g(\mathbf{x}_1). \tag{C1}$$

If $g(\mathbf{x}_1)$ is expanded about the point $\mathbf{x}_2$ we have

$$g(\mathbf{x}_1) = g(\mathbf{x}_2) + (\mathbf{x}_1 - \mathbf{x}_2)\cdot\boldsymbol{\nabla}_2\, g(\mathbf{x}_2) + \tfrac{1}{2}(x_1^l - x_2^l)(x_1^m - x_2^m)\frac{\partial}{\partial x_2^l}\frac{\partial}{\partial x_2^m}g(\mathbf{x}_2) + \cdots. \tag{C2}$$

Term by term integration over $\mathbf{x}_1$ in (C1) is elementary, and yields

$$u(y) = \frac{a}{y}\int d\mathbf{x} f(\mathbf{x})\,g(\mathbf{x}) - \frac{2}{3y^2}\int d\mathbf{x} f(\mathbf{x})\,\mathbf{b}\cdot\boldsymbol{\nabla}\,g(\mathbf{x}) + \frac{a}{3y^3}\int d\mathbf{x} f(\mathbf{x})\nabla^2 g(\mathbf{x}) + \cdots, \tag{C3}$$

where the three terms correspond to the three terms in (C2). Since gradients of the wave function are proportional to the momentum, the series depicted above is a power series in $\mathbf{p}$ or $Z\alpha$, as well as an asymptotic series in $y^{-1}$.

## APPENDIX D

In Sec. V, the result of integration over $z$ is given for a number of singular terms in the high-energy part. In this appendix, we indicate a method of evaluation of the integrals for one example:

$$I = \frac{1}{i}\int_{C_H} dz\, z\left(\frac{1}{b+c} - \frac{1}{b'+c}\right). \tag{D1}$$

Changes of variables $y = -iz$ on the positive imaginary axis and $y = iz$ on the negative imaginary axis lead to

$$I = 2\,\mathrm{Im}\int_0^\infty dy\, y\left(\frac{1}{y - iE_n + (1+y^2)^{1/2}} - \frac{1}{[\Lambda^2 + (y-iE_n)^2]^{1/2} + (1+y^2)^{1/2}}\right). \tag{D2}$$

In the second term in (D2), we make the replacement $(1+y^2)^{1/2} \to y$ with a resulting change in the integral of order $\Lambda^{-1}$. To integrate each of the two terms in (D2) separately, we introduce a temporary cutoff

$$I = 2\,\mathrm{Im}\lim_{Y\to\infty}\int_0^Y dy\, y\left(\frac{1}{y - iE_n + (1+y^2)^{1/2}} - \frac{1}{[\Lambda^2 + (y-iE_n)^2]^{1/2} + y}\right) + \mathcal{O}(\Lambda^{-1}), \tag{D3}$$

where the limit $Y \to \infty$ is taken before the limit $\Lambda \to \infty$. Each integral can be evaluated analytically, with the result for large $Y$ that

$$2\,\mathrm{Im}\int_0^Y dy\, \frac{y}{y - iE_n + (1+y^2)^{1/2}} = \frac{E_n}{4}\left(2\,\ln(2Y) - \frac{1}{E_n^2} + \frac{1-E_n^4}{E_n^4}\ln(1+E_n^2)\right) + \mathcal{O}(Y^{-1}) \tag{D4}$$

and

$$2\,\mathrm{Im}\int_0^Y dy\, \frac{y}{[\Lambda^2 + (y-iE_n)^2]^{1/2} + y} = \frac{E_n}{4}\left[2\,\ln(2Y) - \ln(\Lambda^2) - \frac{\Lambda^2}{E_n^2} - \left(\frac{\Lambda^2}{E_n^2} - 1\right)^2 \ln\left(1 - \frac{E_n^2}{\Lambda^2}\right)\right] + \mathcal{O}(Y^{-1}). \tag{D5}$$

Taking the difference for large $\Lambda$ yields

$$I = \frac{E_n}{4}\left(\ln(\Lambda^2) + \frac{3E_n^2 - 2}{2E_n^2} + \frac{1-E_n^4}{E_n^4}\ln\left(1+E_n^2\right)\right) + \mathcal{O}(\Lambda^{-1}). \tag{D6}$$

The remaining integrals in Sec. V can be evaluated in this way.

## APPENDIX E

Formulas pertaining to integration over $d\Omega_1$ in Sec. VI are given here. The calculation is facilitated by expressing the integral in terms of spherical angles $\theta$ and $\phi$ of $\mathbf{x}_1$ relative to the direction of $\mathbf{x}_2$. In particular, we write

$$\mathbf{x}_1 = x_1\cos\phi\sin\theta\;\hat{\mathbf{a}} + x_1\sin\phi\sin\theta\;\hat{\mathbf{b}} + x_1\cos\theta\;\hat{\mathbf{x}}_2, \tag{E1}$$

where $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ are orthogonal unit vectors in the plane perpendicular to $\hat{\mathbf{x}}_2$. For $\xi = \cos\theta$, $R = (x_2^2 - 2x_2x_1\xi + x_1^2)^{1/2}$, and $f$ a function of $R$, we have

$$\begin{aligned}\int d\Omega_1(\mathbf{x}_1 - \mathbf{x}_2)\, f(R) &= \int_{-1}^{1} d\xi \int_0^{2\pi} d\phi\, \left(x_1\cos\phi\sqrt{1-\xi^2}\;\hat{\mathbf{a}} + x_1\sin\phi\sqrt{1-\xi^2}\;\hat{\mathbf{b}} + x_1\xi\;\hat{\mathbf{x}}_2 - \mathbf{x}_2\right) f(R)\\ &= 2\pi\int_{-1}^{1} d\xi(\xi x_1 - x_2)\hat{\mathbf{x}}_2\, f(R)\end{aligned} \tag{E2}$$

and

$$\begin{aligned}\int d\Omega_1(x_1^l - x_2^l)(x_1^m - x_2^m)\, f(R) &= \int_{-1}^{1} d\xi \int_0^{2\pi} d\phi\, \left(x_1\cos\phi\sqrt{1-\xi^2}\;\hat{a}^l + x_1\sin\phi\sqrt{1-\xi^2}\;\hat{b}^l + x_1\xi\;\hat{x}_2^l - x_2^l\right)\\ &\quad\times\left(x_1\cos\phi\sqrt{1-\xi^2}\;\hat{a}^m + x_1\sin\phi\sqrt{1-\xi^2}\;\hat{b}^m + x_1\xi\;\hat{x}_2^m - x_2^m\right) f(R)\\ &= 2\pi\int_{-1}^{1} d\xi\left[x_1^2\tfrac{1}{2}(1-\xi^2)(\hat{a}^l\hat{a}^m + \hat{b}^l\hat{b}^m) + (x_1\xi - x_2)^2\hat{x}_2^l\hat{x}_2^m\right] f(R)\\ &= 2\pi\int_{-1}^{1} d\xi\left[R^2\hat{x}_2^l\hat{x}_2^m + \tfrac{1}{2}(1-\xi^2)x_1^2(\delta_{lm} - 3\hat{x}_2^l\hat{x}_2^m)\right] f(R).\end{aligned} \tag{E3}$$

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