Coulomb-gauge self-energy calculation for high-Z hydrogenic ions

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We present results from numerical calculations in the Coulomb gauge of the first-order self-energy shift of bound hydrogenic states in highly stripped ions. We apply the expressions for the renormalized free-electron self-energy and vertex operators obtained by G. S. Adkins [Phys. Rev. D **27**, 1814 (1983); **34**, 2489 (1986)] to the evaluation of the zero- and one-potential terms. It is found that in this gauge the contribution from the many-potential term, which limits the overall accuracy, is significantly smaller than in the covariant Feynman gauge. This enables us to improve the accuracy of the self-energy prediction considerably compared to that obtained in the corresponding Feynman-gauge calculations.

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I. INTRODUCTION

Today, experimentalists are performing extremely precise measurements on static and dynamic properties of highly stripped ions [1]. These simple systems provide an excellent opportunity for testing the validity of quantum electrodynamics (QED) in strong electromagnetic fields. Radiative effects such as self-energy, vacuum polarization, and vertex correction constitute a significant part of the binding energy of an electron in a few-electron ion of high nuclear charge Z, and in order to interpret the experimental results, equally precise calculations of these contributions have to be performed.

For systems involving more than one electron, the combined effect of electron correlation and QED requires a theoretical treatment where these two effects are treated simultaneously in order to obtain high accuracy [2]. By expressing the electromagnetic field in the noncovariant Coulomb gauge, much of the interelectronic interaction can be treated in an instantaneous manner; this is due to the explicit appearance of the instantaneous Coulomb and Breit interaction terms in this gauge. It is of interest then to also be able to calculate radiative corrections in the Coulomb gauge, and in this article we will focus on one of these corrections—the self-energy of an electron in a high-Z hydrogenlike ion.

A standard way of evaluating the self-energy of an electron in a high-Z ion, originally due to Brown, Langer, and Schaefer [3] and improved by Blundell and Snyderman [4], involves a potential expansion whereby the energy shift is partly expressed in terms of expectation values of free-QED operators. Adkins [5,6] obtained expressions for the relevant Coulomb-gauge operators already in 1983 and 1986. However, to our knowledge there have been no publications demonstrating the applicability of his results to the bound, atomic case. It is the purpose of the present paper to provide such a demonstration. We use units such that $\hbar = c = 1$ throughout.

II. THE BOUND SELF-ENERGY SHIFT

The bound self-energy shift is obtained from Sucher's level-shift formula [7] as the expectation value of the renormalized bound self-energy operator with respect to the bound state $|a\rangle$:

$$\Delta E_a^{\mathrm{SE}} = \langle a|\Sigma_{\mathrm{bou}}|a\rangle - \langle a|\delta m|a\rangle. \tag{1}$$

Σ_{bou} involves the bound electron propagator which can be rewritten using a potential expansion as shown in Fig. 1. The self-energy shift then decomposes into three terms: a zero-potential, one-potential, and many-potential term. The zero- and one-potential terms contain divergent parts which cancel due to renormalization constraints, and the many-potential term is finite in itself. Thus, after this cancellation the total self-energy shift is given by the sum of three finite terms:

$$\Delta E_a^{\mathrm{SE}} = \Delta E_a^{\mathrm{ZP}} + \Delta E_a^{\mathrm{OP}} + \Delta E_a^{\mathrm{MP}}. \tag{2}$$

The zero-potential term is the expectation value of the free, renormalized self-energy operator:

$$\Delta E_a^{\mathrm{ZP}} = \langle a|\Sigma_{\mathrm{free}}^{\mathrm{ren.}}|a\rangle. \tag{3}$$

The one-potential term is the expectation value of the free, renormalized vertex correction to the interaction with the nuclear potential $A^\mu = (V_{\mathrm{nuc}}, \mathbf{0})$:

$$\Delta E_a^{\mathrm{OP}} = -e\langle a|\Lambda_{\mathrm{ren.}}^{\mu} A_\mu|a\rangle = -e\langle a|\Lambda_{\mathrm{ren.}}^{0} V_{\mathrm{nuc}}|a\rangle. \tag{4}$$

We compute these two terms in the momentum-space representation.

By expanding the photon propagator in terms of partial waves, the many-potential term can be expressed as a sum over the angular momentum l of the photon:

$$\Delta E^{\mathrm{MP}} = \sum_{l=0}^{\infty} \Delta E_l^{\mathrm{MP}}. \tag{5}$$

Each l term can be obtained using the subtraction scheme (see Fig. 1):

$$\Delta E_{a,l}^{\mathrm{MP}} = \langle a|\Sigma_{\mathrm{bou}}|a\rangle_l - \langle a|\Sigma_{\mathrm{free}}|a\rangle_l - \langle a|(-e)\Lambda^0 V_{\mathrm{nuc}}|a\rangle_l, \tag{6}$$

where the terms on the right-hand side involve the *unrenormalized* operators. We compute these terms in position space.

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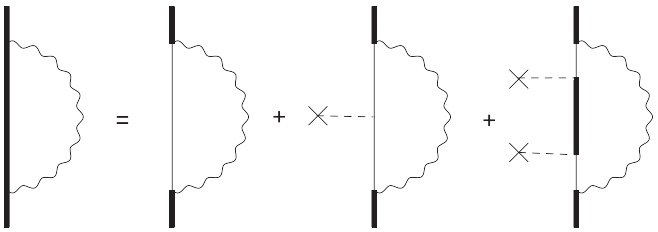

FIG. 1. Expansion of the bound self-energy operator in terms of a free particle scattered in the nuclear potential. The heavy lines represent bound states. The dashed lines corresponds to the scalar Coulomb interaction.

III. NUMERICAL METHOD

Let us now turn to a brief description of the numerical implementation. To represent our states we use a numerical spectrum obtained by solving the radial Dirac equation on a discretized space in the presence of a spherically symmetric binding potential $V(r)$ (see Ref. [8]). This allows us to take into account the finite size of the nuclear charge distribution, and by setting $V(r) = 0$ we obtain a complete set of free states. The spin-angular parts are treated analytically.

In evaluating the zero-potential term, we use Malenfant's [9] modified form

$$\Sigma^{\text{ren.}}_{\text{free}} = A(\not{p} - m) + B\gamma\cdot\mathbf{p} + Cm \tag{7}$$

of Adkins' renormalized self-energy function where the Feynman parameter integrations have been carried out. The expectation value of this operator is obtained as a three-dimensional momentum-space integral. After performing the angular integrations we end up with a one-dimensional integral over $p = |\mathbf{p}|$:

$$\Delta E^{\text{ZP}}_a = \int_0^\infty dp\ p^2\big\{P_a^2[A(E_a - m) + Cm] + Q_a^2[A(E_a + m) - Cm] + 2pP_aQ_a(A - B)\big\}, \tag{8}$$

where P_a and Q_a are the Fourier-transformed large and small components of the radial wave function, respectively, and E_a is the energy of the state $|a\rangle$. We evaluate this integral using Gauss-Legendre quadrature.

For the one-potential term we separate the tensor structure of Adkins' result for Λ^0 as

$$\Lambda^0_{\text{ren.}}(\mathbf{p},\mathbf{q}) = \frac{\alpha}{4\pi}[\gamma^0 h_1 + (\gamma\cdot\mathbf{p}\gamma^0\gamma\cdot\mathbf{q})h_2 + (m\gamma\cdot\mathbf{p}\gamma^0)h_3 + (m\gamma^0\gamma\cdot\mathbf{q})h_4 + (\gamma\cdot\mathbf{p})h_5 + (\gamma\cdot\mathbf{q})h_6 + mh_7]. \tag{9}$$

Here, the h_i are functions of $|\mathbf{p}|$, $|\mathbf{q}|$, and $\cos\vartheta$, where ϑ is the angle between $\mathbf{p}$ and $\mathbf{q}$. The h_i functions also contain integrals over up to three Feynman parameters. Performing some of these integrations analytically, we are left with just two Feynman parameters. After treating the spin-angular parts analytically, we end up with the following expression for the one-potential term:

$$\begin{aligned}\Delta E^{\text{OP}}_a = -e\frac{\alpha}{2}\int_0^\infty dp\ p^2\int_0^\infty dq\ q^2\int_{-1}^1 d(\cos\vartheta)\ V_{\text{nuc}}(p,q,\cos\vartheta)\{&\mathcal{P}_{|\kappa+1/2|-1/2}(\cos\vartheta)[h_1P_pP_q + h_2pqQ_pQ_q \\ &- h_3mpQ_pP_q - h_4mqP_pQ_q - h_5pQ_pP_q - h_6qP_pQ_q + h_7mP_pP_q] + \mathcal{P}_{|-\kappa+1/2|-1/2}(\cos\vartheta)[h_1Q_pQ_q \\ &+ h_2pqP_pP_q + h_3mpP_pQ_q + h_4mqQ_pP_q - h_5pP_pQ_q - h_6qQ_pP_q - h_7mQ_pQ_q]\},\end{aligned} \tag{10}$$

where $p = |\mathbf{p}|$, $q = |\mathbf{q}|$, and $\mathcal{P}_l(\cos\vartheta)$ is the lth Legendre polynomial in $\cos\vartheta$, and where $P_p = P_a(p)$, $Q_q = Q_a(q)$, and so on. The spin-angular quantum number κ is equal to $(-1)^{j+l+\frac{1}{2}}(j+\frac{1}{2})$. All of the integrations in (10), including those implicit in the h_i functions, are performed using Gauss-Legendre quadrature. The integrand has an integrable Coulomb singularity at $p = q$ which is handled with the variable substitutions suggested by Blundell [10]. A detailed treatment of the one-potential term in the Coulomb gauge, including explicit expressions for the h_i functions, is given in [11].

The unrenormalized terms in the many-potential term, Eq. (6), are extracted from their corresponding Feynman diagrams using the bound-state QED Feynman rules. The general expression for first term, the unrenormalized bound self-energy, is

$$\langle a|\Sigma_{\text{bou}}|a\rangle = i\langle a|\int\frac{dz}{2\pi}S_{\text{F}}(z)I(z;\boldsymbol{x}_2,\boldsymbol{x}_1)|a\rangle, \tag{11}$$

where $S_{\text{F}}(z)$ is the bound electron propagator

$$S_{\text{F}}(z) = \sum_n \frac{|n\rangle\langle n|}{E_a - E_n - z + i\eta\ \text{sgn}(E_n)}. \tag{12}$$

The gauge dependence of Eq. (11) resides in the interaction term $I(z;\boldsymbol{x}_2,\boldsymbol{x}_1)$, which includes the photon propagator $D_{\mu\nu}(z;\boldsymbol{x}_2,\boldsymbol{x}_1)$:

$$I(z;\boldsymbol{x}_2,\boldsymbol{x}_1) = e^2\alpha^\mu\alpha^\nu D_{\mu\nu}(z;\boldsymbol{x}_2,\boldsymbol{x}_1). \tag{13}$$

In the Coulomb gauge the interaction term consists of the instantaneous Coulomb interaction

$$I_{\text{C}}(\boldsymbol{x}_2,\boldsymbol{x}_1) = e^2\int\frac{d^3k}{(2\pi)^3}\frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{x}_2-\boldsymbol{x}_1)}}{\boldsymbol{k}^2 + i\eta}, \tag{14}$$

and the Breit interaction

$$I_{\mathrm{B}}(z;\boldsymbol{x}_2,\boldsymbol{x}_1) = e^2 \int \frac{d^3k}{(2\pi)^3}\left(\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2 - \frac{(\boldsymbol{\alpha}\cdot\boldsymbol{\nabla})_1(\boldsymbol{\alpha}\cdot\boldsymbol{\nabla})_2}{\boldsymbol{k}^2}\right)\frac{\mathrm{e}^{i\boldsymbol{k}\cdot(\boldsymbol{x}_2-\boldsymbol{x}_1)}}{z^2-\boldsymbol{k}^2+i\eta}. \tag{15}$$

The unrenormalized Coulomb-gauge bound self-energy is then expressed as

$$\langle a|\Sigma_{\mathrm{bou}}|a\rangle_l = \int_0^\infty dk \sum_n \left(\mathrm{sgn}(E_n)\,\langle a|V_{\mathrm{C}}^l(kr_2)|n\rangle\cdot\langle n|V_{\mathrm{C}}^l(kr_1)|a\rangle + \frac{\langle a|V_{\mathrm{G}}^l(kr_2)|n\rangle\cdot\langle n|V_{\mathrm{G}}^l(kr_1)|a\rangle - \langle a|V_{\mathrm{SR}}^l(kr_2)|n\rangle\cdot\langle n|V_{\mathrm{SR}}^l(kr_1)|a\rangle}{E_a - E_n - k\,\mathrm{sgn}(E_n)}\right), \tag{16}$$

and it includes an integration over the radial part of the linear momentum of the photon, $k = |\boldsymbol{k}|$. For the bound self-energy the summation over the intermediate state $|n\rangle$ is performed over a complete numerical spectrum of single-electron states, of both positive and negative energy, obtained in the presence of the binding potential. The expression in Eq. (16) is also valid for the unrenormalized zero-potential term, if the summation over intermediate states is instead performed over a complete set of *free* single-electron states. In Eq. (16) V_{C}^l, V_{G}^l, and V_{SR}^l are single-vertex potentials for the three types of interactions that occur in the Coulomb gauge, the Coulomb interaction, the Gaunt interaction, and the scalar retardation. The expressions for V_{G}^l and V_{SR}^l are given in [12], and the potential $V_{\mathrm{C}}^l(kr)$ for the Coulomb interaction is

$$V_{\mathrm{C}}^l(kr) = \frac{e}{2\pi}\sqrt{(2l+1)}\; j_l(kr)\mathrm{C}^l, \tag{17}$$

where $j_l(kr)$ is the spherical Bessel function and C^l is the angular tensor.

The unrenormalized one-potential term is extracted with a similar procedure, and the expression we use in the calculation of the many-potential term is

$$-e\langle a|\Lambda^0 V_{\mathrm{nuc}}|a\rangle_l = -e\int_0^\infty dk \sum_{t,u}\left(\langle a|V_{\mathrm{C}}^l(kr_2)|u\rangle\langle u|V_{\mathrm{nuc}}|t\rangle\langle t|V_{\mathrm{C}}^l(kr_1)|a\rangle F + \frac{\langle a|V_{\mathrm{G}}^l(kr_2)|u\rangle\langle u|V_{\mathrm{nuc}}|t\rangle\langle t|V_{\mathrm{G}}^l(kr_1)|a\rangle - \langle a|V_{\mathrm{SR}}^l(kr_2)|u\rangle\langle u|V_{\mathrm{nuc}}|t\rangle\langle t|V_{\mathrm{SR}}^l(kr_1)|a\rangle}{[E_a - E_t - k\,\mathrm{sgn}(E_t)][E_a - E_u - k\,\mathrm{sgn}(E_u)]}G\right), \tag{18}$$

where

$$F = [\mathrm{sgn}(E_t) - \mathrm{sgn}(E_u)]\frac{1}{E_t - E_u}, \tag{19}$$

$$G = 1 + [\mathrm{sgn}(E_t) - \mathrm{sgn}(E_u)]\frac{k}{E_t - E_u}. \tag{20}$$

The summation over the intermediate states $|t\rangle$ and $|u\rangle$ is performed over the spectrum of free single-electron states.

IV. RESULTS AND DISCUSSION

For comparison we have also performed corresponding calculations in the Feynman gauge, and our results in the two gauges for the $1s$ states with various nuclei are given in Table I, where we also compare our results to those obtained by Mohr and Soff [13–15]. We also note that the results of Yerokhin *et al.* [16] are in complete agreement with Mohr's point-nucleus calculations.

In Table I the self-energy is expressed in terms of the function $F(Z\alpha)$ defined through

$$\Delta E^{\mathrm{SE}} = \frac{\alpha}{\pi}\frac{(Z\alpha)^4 mc^2}{n^3}F(Z\alpha). \tag{21}$$

Our calculations use $\alpha = 137.035\,999\,679^{-1}$ for the fine-structure constant and $E_{\mathrm{H}} = 27.211\,383\,86$ eV for the Hartree energy. The nucleus is treated as a uniform, spherical charge distribution of radius R_{nuc}.

Table II shows a comparison of the contributions to the total self-energy shift in the two gauges. An important feature of the Coulomb gauge is that the contribution from the many-potential term is significantly smaller than in the Feynman gauge. It is the many-potential term which limits the overall accuracy of this scheme, and by reducing its importance, the final uncertainty is reduced in the Coulomb gauge. This feature is clearly seen in Figure 2, where we plot the contributions to the total self-energy from the analytical free-QED operators (the zero- and one-potential terms) as a function of Z.

TABLE I. Inferred values for the function $F(Z\alpha)$ from the results obtained in this work are compared to previously reported results. The nuclear radii are given in fm.

Z	R_{nuc}	Coulomb gauge	Feynman gauge	Other
18	3.423	3.444 043(9)	3.444 04(3)	3.4438(12)[a]
26	3.730	2.783 762(3)	2.783 77(1)	2.783 766(1)[a,b]
36	4.230	2.279 314(2)	2.279 316(7)	2.279 314(1)[a,b]
54	4.826	1.781 866 2(6)	1.781 868(3)	1.781 866(1)[a,b]
66	5.210	1.604 461 5(4)	1.604 462(2)	1.604 52(1)[a,c]
82	5.505	1.487 258 4(4)	1.487 259(1)	1.487 258(1)[a,b]
92	5.863	1.472 424 1(4)	1.472 425(1)	1.472 424(1)[a,b]

[a]Values with point nucleus by Mohr [13,14].
[b]Nuclear-size correction from Mohr and Soff [15].
[c]Missing nuclear-size correction cubic spline interpolated.

TABLE II. Comparison between the Feynman and Coulomb gauges for the contributions to the self-energy obtained in the present work. Values are given in eV.

Z	Term	Coulomb gauge	Feynman gauge
18	ΔE^{ZP}	1.341 668 068(1)	−67.924 837 74(5)
	ΔE^{OP}	0.054 770 997(7)	49.511 443 05(6)
	ΔE^{MP}	−0.179 538(3)	19.630 296(10)
	Sum	1.216 901(3)	1.216 90(1)
54	ΔE^{ZP}	43.590 621 48(6)	−285.092 638 6(1)
	ΔE^{OP}	17.387 986 7(3)	190.356 052 0(3)
	ΔE^{MP}	−9.981 343(16)	145.733 90(8)
	Sum	50.997 27(2)	50.997 31(8)
66	ΔE^{ZP}	79.791 727 3(2)	−355.317 806 4(6)
	ΔE^{OP}	43.151 260 4(7)	248.819 551(1)
	ΔE^{MP}	−20.471 793(25)	208.969 5(1)
	Sum	102.471 19(3)	102.471 3(1)
92	ΔE^{ZP}	210.068 220 5(7)	−516.318 598(4)
	ΔE^{OP}	213.739 094(4)	472.000 597(6)
	ΔE^{MP}	−68.764 3(1)	399.361 2(2)
	Sum	355.043 0(1)	355.043 2(2)

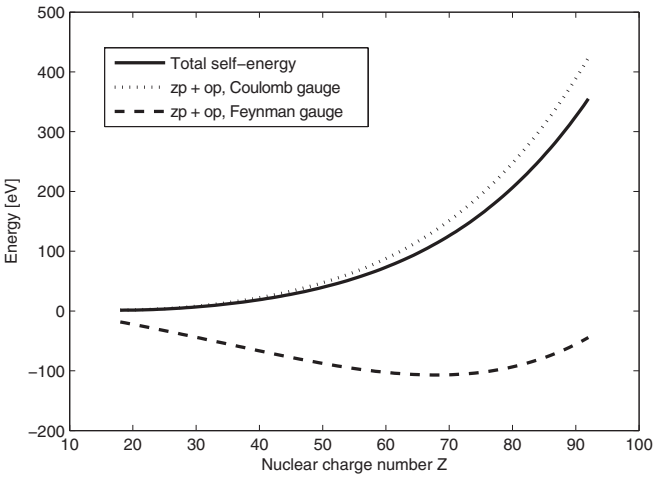

FIG. 2. Contribution to the total self-energy of the 1s state from the zero- and one-potential terms in the two gauges.

The uncertainty of the zero-potential term is solely due to the statistical variation from choosing different grid-sizes in position space. This effect is also present in the one-potential term, but here additional uncertainties come from the extrapolation to continuous space in the numerical integrations over the two Feynman parameters. The many-potential term acquires its uncertainty from two extrapolations to infinity—one in the total number of grid points in position space, and one in the sum over partial waves l.

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