Scalar vertex operator for bound-state QED in the Coulomb gauge

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Adkins's result [Phys. Rev. D **34**, 2489 (1986)] for the time component of the renormalized vertex operator in Coulomb-gauge QED is separated according to its tensor structure and some of the Feynman parameter integrals are carried out analytically, yielding a form suited for numerical bound-state QED calculations. This modified form is applied to the evaluation of the self-energy shift to the binding energy in hydrogenic ions of high nuclear charge.

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I. INTRODUCTION

In 1986, Adkins [1] obtained an expression for the renormalized vertex operator $\Lambda^{\mu}_{\rm ren}$ in Coulomb-gauge QED. This operator gives the first-order (one-loop) radiative correction to the interaction vertex $ie\gamma^{\mu}$. In this paper I demonstrate how the time component $\Lambda^{0}_{\rm ren}$ of the renormalized vertex operator can be put into a form suited for numerical calculations involving bound states where the scalar Coulomb interaction constitutes the binding potential. In Sec. III this modified form of $\Lambda^{0}_{\rm ren}$ is applied to the numerical evaluation of the self-energy shift of an electron in a hydrogenic, highly charged ion, where one of the contributions to the total shift can be expressed in terms of this operator.

Adkins's result has been verified for the $\mu = 0$ case using the method of dimensional regularization; a detailed derivation can be found in Ref. [2]. In the present paper I use units such that $\hbar = c = 1$ throughout.

II. SEPARATION OF $\Lambda^{0}_{\rm ren}$

The time component of the renormalized vertex operator can be written as

$$\Lambda^{0}_{\rm ren}(p,q) = \frac{\alpha}{4\pi}[\gamma^0 h_1 + (\boldsymbol{\gamma}\cdot\mathbf{p}\gamma^0\boldsymbol{\gamma}\cdot\mathbf{q})h_2 + (m\boldsymbol{\gamma}\cdot\mathbf{p}\gamma^0)h_3 + (m\gamma^0\boldsymbol{\gamma}\cdot\mathbf{q})h_4 + (\boldsymbol{\gamma}\cdot\mathbf{p})h_5 + (\boldsymbol{\gamma}\cdot\mathbf{q})h_6 + mh_7]. \tag{1}$$

The h_i factors, which can be identified from Ref. [1], are functions of $|\mathbf{p}|$, $|\mathbf{q}|$, p^0, q^0, and $\cos\vartheta$, where ϑ is the angle between $\mathbf{p}$ and $\mathbf{q}$. Moreover, they contain integrals over up to three Feynman parameters x, u, and s.

It is rather straightforward to perform some of these Feynman parameter integrations analytically; in order to do this we arrange terms in the h_i functions according to the polynomial structure of their numerators. We then obtain 22 different types of integral, for which we define the following abbreviations:

$$\{F_1,F_2,F_3,F_4,F_5,F_6\} = \int_0^1 dx\int_0^1 du\frac{\{1,x,xu,x^2,x^2u,x^2u^2\}}{\Delta_Y}, \tag{2}$$

$$\{F_7,F_8,F_9\} = \int_0^1 dx\int_0^1 du\sqrt{x}\frac{\{1,u,u^2\}}{\Delta_X}, \tag{3}$$

$$\{F_{10},F_{11}\} = \int_0^1 dx\int_0^1 du\frac{\{1,u\}}{\sqrt{x}\Delta_X}, \tag{4}$$

$$\{F_{12},F_{13},F_{14}\} = \int_0^1 dx\int_0^1 du\int_0^1 ds\, x\sqrt{xs}\frac{\{1,u,u^2\}}{(\Delta_Z)^2}, \tag{5}$$

$$\{F_{15},F_{16},F_{17},F_{18}\} = \int_0^1 dx\int_0^1 du\int_0^1 ds\, x\sqrt{x}s^2\frac{\{1,u,u^2,u^3\}}{(\Delta_Z)^2}, \tag{6}$$

$$\{F_{19},F_{20},F_{21}\} = \int_0^1 dx\int_0^1 du\int_0^1 ds\sqrt{x}\frac{\{1,s,su\}}{\Delta_Z}, \tag{7}$$

where the Δ functions are those introduced by Adkins. They can be simplified to read

$$\Delta_X = m^2 - up^2 - (1-u)q^2 + t_0^2 - x\mathbf{t}^2, \tag{8}$$

$$\Delta_Y = m^2 - up^2 - (1-u)q^2 + xt^2, \tag{9}$$

$$\Delta_Z = m^2 - up^2 - (1-u)q^2 + st_0^2 - sx\mathbf{t}^2, \tag{10}$$

with $t^{\mu} \equiv up^{\mu} + (1-u)q^{\mu}$. Finally, the following integral occurs in the h_1 function:

$$F_{22} = \int_0^1 du\,\ln\frac{\Delta}{m^2}, \tag{11}$$

where $\Delta = m^2 - u(1-u)k^2$ and $k^{\mu} \equiv q^{\mu} - p^{\mu}$.

Using that Δ_X, Δ_Y, and Δ_Z are all of the form $ax + b$, the x integrations can readily be carried out, yielding

$$F_1 = \int_0^1 du\frac{1}{t^2}\ln\left(\frac{t^2+A}{A}\right), \tag{12}$$

$$\{F_2,F_3\} = \int_0^1 du\left[\frac{1}{t^2} - \frac{A}{(t^2)^2}\ln\left(\frac{t^2+A}{A}\right)\right]\times\{1,u\}, \tag{13}$$

$$\{F_4,F_5,F_6\} = \int_0^1 du\left[\frac{A^2}{(t^2)^3}\ln\left(\frac{t^2+A}{A}\right) + \frac{t^2-2A}{2(t^2)^2}\right]\times\{1,u,u^2\}, \tag{14}$$

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$$\{F_7,F_8,F_9\} = \int_0^1 du \left\{ \frac{2\sqrt{C}}{\mathbf{t}^2\sqrt{\mathbf{t}^2}} \tanh^{-1}\left[\left(\frac{\mathbf{t}^2}{C}\right)^{1/2}\right] - \frac{2}{\mathbf{t}^2}\right\} \times \{1,u,u^2\}, \tag{15}$$

$$\{F_{10},F_{11}\} = \int_0^1 du \left\{ \frac{2}{\sqrt{\mathbf{t}^2 C}} \tanh^{-1}\left[\left(\frac{\mathbf{t}^2}{C}\right)^{1/2}\right]\right\} \times \{1,u\}, \tag{16}$$

$$\{F_{12},F_{13},F_{14},F_{15},F_{16},F_{17},F_{18}\} = \int_0^1 ds \int_0^1 du \frac{s}{(s\mathbf{t}^2)^2}\left\{3 - \frac{1}{1-B/s\mathbf{t}^2} - 3\left(\frac{B}{s\mathbf{t}^2}\right)^{1/2} \tanh^{-1}\left[\left(\frac{s\mathbf{t}^2}{B}\right)^{1/2}\right]\right\} \times \{1,u,u^2,s,su,su^2,su^3\}, \tag{17}$$

$$\{F_{19},F_{20},F_{21}\} = \int_0^1 ds \int_0^1 du \frac{2}{s\mathbf{t}^2}\left\{\left(\frac{B}{s\mathbf{t}^2}\right)^{1/2} \times \tanh^{-1}\left[\left(\frac{s\mathbf{t}^2}{B}\right)^{1/2}\right] - 1\right\} \times \{1,s,su\}, \tag{18}$$

with

$$A = m^2 - up^2 - (1-u)q^2, \tag{19}$$

$$B = m^2 - up^2 - (1-u)q^2 + st_0^2, \tag{20}$$

$$C = m^2 - up^2 - (1-u)q^2 + t_0^2. \tag{21}$$

The resulting expressions [Eqs. (12)–(18)] are real and finite when q^0 and p^0 lie in the open interval $(-m,m)$, a condition that is fulfilled for bound electrons. Using the above definitions, the h_i functions of Eq. (1) take the following form:

$$h_1 = -F_{22} + F_8(2\mathbf{k}^2 - \mathbf{p}^2 + \mathbf{q}^2) - 2F_9\mathbf{k}^2 - F_7\mathbf{q}^2 + F_{10}\mathbf{q}^2 + F_{11}(\mathbf{p}^2 - \mathbf{q}^2) + 2F_1(m^2 + p_0q_0 + 2\mathbf{p}\cdot\mathbf{q}) + F_2\left(-3m^2 + q_0^2 - 5\mathbf{q}^2 - 2q_0p_0 - 2\mathbf{p}\cdot\mathbf{q}\right) + F_3\left(p_0^2 - q_0^2 - 5\mathbf{p}^2 + 5\mathbf{q}^2\right) + 4F_4\mathbf{q}^2 + 4F_5(\mathbf{p}^2 - \mathbf{q}^2 - \mathbf{k}^2) + 4F_6\mathbf{k}^2 - 2F_{19}\mathbf{p}\cdot\mathbf{q} - 2F_{12}\mathbf{q}^2\mathbf{p}\cdot\mathbf{q} - 4F_{13}(\mathbf{p}\cdot\mathbf{q} - \mathbf{q}^2)\mathbf{p}\cdot\mathbf{q} - 2F_{14}\mathbf{k}^2\mathbf{p}\cdot\mathbf{q}, \tag{22}$$

$$h_2 = F_7 - F_{10} + 2[-F_1 + F_{19} + F_{12}\mathbf{q}^2 + 2F_{13}(\mathbf{p}\cdot\mathbf{q} - \mathbf{q}^2) + F_{14}\mathbf{k}^2], \tag{23}$$

$$h_3 = -F_{10} + F_{19} - 2F_{13}(\mathbf{q}^2 - \mathbf{p}\cdot\mathbf{q}) + 2F_{14}\mathbf{k}^2, \tag{24}$$

$$h_4 = h_3 + 2F_{12}(\mathbf{q}^2 - \mathbf{p}\cdot\mathbf{q}) - 2F_{13}\mathbf{k}^2, \tag{25}$$

$$h_5 = 2p_0[F_3 + \mathbf{q}^2(F_{14} - F_{13})] + 2q_0\left[F_3 - 2F_5 + \tfrac{1}{2}(F_{20} - F_{19}) + F_{17}(\mathbf{p}^2 - \mathbf{q}^2) - F_{14}\mathbf{p}^2 - F_{13}\mathbf{p}\cdot\mathbf{q} + F_{16}(\mathbf{p}\cdot\mathbf{q} + \mathbf{q}^2)\right] + (q_0 - p_0)[2F_9 - F_{11} - F_8 + 4F_6 - F_{21} + 2F_{18}(\mathbf{q}^2 - \mathbf{p}^2) - 2F_{17}(\mathbf{p}\cdot\mathbf{q} + \mathbf{q}^2) + 2F_{14}\mathbf{p}\cdot\mathbf{q}], \tag{26}$$

$$h_6 = 2p_0\left[F_2 - F_3 - \tfrac{1}{2}F_{19} + 2F_{13}\mathbf{q}^2 - F_{12}\mathbf{q}^2 - F_{14}\mathbf{q}^2\right] + 2q_0\left[F_2 - F_3 + 2F_5 - 2F_4 + \tfrac{1}{2}F_{20} + F_{16}(\mathbf{p}^2 - 2\mathbf{q}^2) + F_{17}(\mathbf{q}^2 - \mathbf{p}^2) - F_{13}\mathbf{p}^2 + F_{14}\mathbf{p}^2 + F_{15}\mathbf{q}^2 + \mathbf{p}\cdot\mathbf{q}(F_{13} - F_{16} - F_{12} + F_{15})\right] + (q_0 - p_0)[F_{10} - F_7 + 3F_8 - F_{11} - 2F_9 + 4F_5 - 4F_6 - F_{21} + 2F_{17}(2\mathbf{q}^2 + \mathbf{p}\cdot\mathbf{q} - \mathbf{p}^2) - 2F_{16}(\mathbf{p}\cdot\mathbf{q} + \mathbf{q}^2) + 2F_{13}\mathbf{p}\cdot\mathbf{q} + 2F_{18}(\mathbf{p}^2 - \mathbf{q}^2) - 2F_{14}\mathbf{p}\cdot\mathbf{q}], \tag{27}$$

$$h_7 = (q_0 - p_0)(F_{10} - 2F_{11} - 4F_3) + 2[2F_2q_0 - F_1(q_0 + p_0)]. \tag{28}$$

III. NUMERICAL SELF-ENERGY CALCULATION

In the attempts at a unification of relativistic many-body perturbation theory and QED it is convenient, if not neccesary, to describe the electromagnetic field in the Coulomb gauge [3]. It is therefore of interest to be able to perform bound-state QED calculations in this gauge; this section describes how to apply Eq. (1) to calculate the self-energy shift of an electron in a hydrogenic ion of high nuclear charge Z.

In a method developed by Brown, Langer, and Schaefer [4] and improved by Blundell and Snyderman [5], large parts of the self-energy shift can be treated semianalytically by using analytical expressions for the free self-energy and vertex operators. Work to perform such calculations using Adkins's expressions for the relevant Coulomb-gauge operators is described in Ref. [6].

From Sucher's [7] level shift formula, the self-energy shift in the state $|a\rangle$ is simply given by

$$\Delta E_a^{\mathrm{SE}} = \langle a|\Sigma_{\mathrm{bou}}^{\mathrm{ren}}|a\rangle, \tag{29}$$

where $\Sigma_{\mathrm{bou}}^{\mathrm{ren}}$ is the renormalized, bound self-energy operator. Utilizing a potential expansion for the bound electron propagator, the total energy shift can be written as the sum of three terms

$$\Delta E^{\mathrm{SE}} = \Delta E^{\mathrm{ZP}} + \Delta E^{\mathrm{OP}} + \Delta E^{\mathrm{MP}}, \tag{30}$$

known as the zero-potential, one-potential, and many-potential terms, respectively. They correspond to the scattering order in the nuclear potential and are all gauge dependent.

The relevant term for the present paper is the one-potential term, which for the binding potential $A^\mu = (V_{\rm nuc},0,0,0)$ is given by the expression

$$\Delta E^{\rm OP} = -e\langle a|\Lambda^\mu_{\rm ren} A_\mu|a\rangle = -e\langle a|\Lambda^0_{\rm ren} V_{\rm nuc}|a\rangle. \quad (31)$$

We use our modified form of $\Lambda^0_{\rm ren}$ to evaluate this contribution.

For high Z it is not feasible to treat the electron-nucleus interaction perturbatively. An alternative approach is to take the bound Dirac solutions as a basis for second quantization in what is known as the Furry picture, a method that treats the electron-nucleus interaction to all orders in $Z\alpha$.

To represent our states we use the Fourier-transformed bound solutions to the Dirac equation in a spherically symmetric potential, which are of the form

$$\langle \mathbf{p}|a\rangle = \Phi_a(\mathbf{p}) = \begin{pmatrix} P(|\mathbf{p}|)\chi^m_\kappa(\hat{p}) \\ Q(|\mathbf{p}|)\chi^m_{-\kappa}(\hat{p}) \end{pmatrix}, \quad (32)$$

where χ is a two-component ls-coupled spherical spinor with $\kappa = (-1)^{j+l+1/2}(j+\frac{1}{2})$ and P and Q are the radial components in momentum space. In this case the scalar components p^0 and q^0 of the incoming and outgoing momenta are both equal to the energy E_a of the bound state $|a\rangle$. Substituting Eqs. (32) and (1) into Eq. (31), we obtain

$$\Delta E^{\rm OP} = -e\int d^3\mathbf{p}\int d^3\mathbf{q}\,\Phi^\dagger_a(\mathbf{p})\gamma^0\Lambda^0_{\rm ren}V_{\rm nuc}(|\mathbf{k}|)\Phi_a(\mathbf{q}). \quad (33)$$

Using that $(\boldsymbol{\sigma}\cdot\mathbf{p})\chi^m_\kappa(\hat{p}) = -|\mathbf{p}|\chi^m_{-\kappa}(\hat{p})$, we can write

$$\begin{aligned}
&\frac{4\pi}{\alpha}\Phi^\dagger_a(\mathbf{p})\gamma^0\Lambda^0_{\rm ren}\Phi_a(\mathbf{q}) \\
&\quad = \chi^{m\dagger}_\kappa(\hat{p})\chi^m_\kappa(\hat{q})[h_1P_pP_q + h_2pqQ_pQ_q - h_3mpQ_pP_q \\
&\qquad - h_4mqP_pQ_q - h_5pQ_pP_q - h_6qP_pQ_q + h_7mP_pP_q] \\
&\qquad + \chi^{m\dagger}_{-\kappa}(\hat{p})\chi^m_{-\kappa}(\hat{q})[h_1Q_pQ_q + h_2pqP_pP_q + h_3mpP_pQ_q \\
&\qquad + h_4mqQ_pP_q - h_5pP_pQ_q - h_6qQ_pP_q - h_7mQ_pQ_q],
\end{aligned} \quad (34)$$

where $p \equiv |\mathbf{p}|$, $q \equiv |\mathbf{q}|$; $P_p = P(p)$, $Q_q = Q(q)$; and so on.

For the scalar nuclear potential the vertex correction is independent of the magnetic quantum number m, so a summation over m followed by a division by $2j+1$ is an identity operation. We can then use the relation

$$\frac{1}{2j+1}\sum_{m=-j}^{j}\chi^{m\dagger}_\kappa(\hat{p})\chi^m_\kappa(\hat{q}) = \frac{1}{4\pi}\mathcal{P}_{|\kappa+1/2|-1/2}(\cos\vartheta), \quad (35)$$

where $\mathcal{P}_l(\cos\vartheta)$ is the lth Legendre polynomial in $\cos\vartheta$. We finally obtain, setting $z = \cos\vartheta$,

$$\begin{aligned}
\Delta E^{\rm op} = -e\frac{\alpha}{2}\int_0^\infty dp\,p^2\int_0^\infty dq\,q^2\int_{-1}^1 dz\,V_{\rm nuc}(p,q,z) \\
\times\{\mathcal{P}_{|\kappa+1/2|-1/2}(z)[h_1P_pP_q + h_2pqQ_pQ_q - h_3mpQ_pP_q - h_4mqP_pQ_q - h_5pQ_pP_q - h_6qP_pQ_q + h_7mP_pP_q] \\
+ \mathcal{P}_{|-\kappa+1/2|-1/2}(z)[h_1Q_pQ_q + h_2pqP_pP_q + h_3mpP_pQ_q + h_4mqQ_pP_q - h_5pP_pQ_q - h_6qQ_pP_q - h_7mQ_pQ_q]\}.
\end{aligned} \quad (36)$$

We use a numerical representation of the nuclear potential $V_{\rm nuc}(r)$, treating the nucleus as a uniform spherical charge distribution of radius $R_{\rm nuc}$. The radial Dirac equation is solved on a grid (see Ref. [8]) and the Fourier-transformed solutions P and Q serve as a numerical representation of the states. All of the integrals in Eq. (36), including those implicit in the h_i functions, are performed with Gauss-Legendre quadrature, extrapolating to infinite grid size when necessary. The integrable Coulomb singularity at $p = q$ is removed with the variable substitutions introduced by Blundell [9].

The numerical integration of F_4, F_5, and F_6 in Eq. (14) requires some care. Setting $y \equiv t^2/A$, their integrands can be written as (dropping the factors $\{1,u,u^2\}$)

$$\frac{A^2}{(t^2)^3}\ln\left(\frac{t^2+A}{A}\right) + \frac{t^2-2A}{2(t^2)^2} \equiv \frac{f(y)}{2A}, \quad (37)$$

with

$$f(y) = 2\left(\frac{\ln(1+y)}{y^3} - \frac{1}{y^2}\right) + \frac{1}{y}, \quad (38)$$

which can be expanded as a power series for small y.

IV. RESULTS AND DISCUSSION

The calculated results for the one-potential term of the self-energy in hydrogenic $1s$ states with different nuclei are shown in Table I. The one-potential term is added to the contributions from the zero- and many-potential terms calculated in Ref. [6] in order to obtain the total self-energy shift, which is compared to results from other works. Our calculations were performed using $\alpha^{-1} = 137.035\,999\,679$ for the inverse fine-structure constant and $E_H = 27.211\,383\,86$ eV for the Hartree energy. A discussion of these results is given in Ref. [6]; here we

TABLE I. Results for the one-potential term (OP) added to the zero- and many-potential terms (ZP and MP, respectively), which are described in Ref. [6], to obtain the self-energy (SE) for hydrogenic 1*s* states with various nuclei. A comparison is made with results from other works. The values given in Refs. [10–12] have been converted to energies using $mc^2 = 510.998\,928$ keV for the rest energy of the electron. All values are given in eV.

Z	R_{nuc} (fm)	ZP	OP	MP	Total SE	Other
18	3.423	1.341668068(1)	0.054770997(7)	−0.179538(3)	1.216901(3)	1.2168(4)[a]
26	3.730	4.446768313(3)	0.540671056(7)	−0.705680(5)	4.281759(5)	4.281765(2)[b,c]
36	4.230	12.485838189(7)	2.71976160(3)	−2.319815(8)	12.885784(8)	12.885786(6)[b,c]
54	4.826	43.59062148(6)	17.3879867(3)	−9.981343(16)	50.99727(2)	50.99726(3)[b,c]
82	5.505	151.3929093(5)	119.825027(2)	−44.88978(6)	226.32816(6)	226.3281(2)[b,c] 226.33[d]
92	5.863	210.0682205(7)	213.739094(3)	−68.7643(1)	355.0430(1)	355.0430(2)[b,c] 355.05[d]

[a]Results for a point nucleus taken from Ref. [10].
[b]Results for a point nucleus taken from Ref. [11].
[c]Correction due to the finite nuclear size taken from Ref. [12].
[d]Results for a point nucleus taken from Ref. [13].

simply note that our Coulomb-gauge calculation is seen to produce values in good agreement with previously reported ones.

The numerical implementation of Eq. (36) is reasonably straightforward and by using the substitutions in Eqs. (37) and (38), the numerical scheme is stable and accurate. Extrapolation to a continuous domain of integration is needed in the numerical quadrature for evaluating the F functions. The uncertainty is estimated by performing this extrapolation while excluding one data point at a time, thus forming an ensemble of extrapolated values. The mean of this ensemble estimates the true value and the standard deviation estimates the error. Together with the statistical error from choosing different grid sizes in radial position space, this estimation accounts for the uncertainty in the one-potential term.

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