

Coordinate-space approach to vacuum polarization

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The vacuum-polarization correction for bound electrons or muons is examined. The objective is to formulate a framework for calculating the correction from bound-state quantum electrodynamics entirely in coordinate space, including the Uehling potential, which is usually isolated and treated separately. Pauli-Villars regularization is applied to the coordinate-space calculation and the most singular terms are shown to be eliminated, leaving the physical correction after charge renormalization. The conventional derivation of the Uehling potential in momentum space is reviewed and compared to the coordinate-space derivation.

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I. INTRODUCTION

In atomic hydrogen, an electron bound to a proton, the largest radiative correction to the energy levels of S states is the self-energy correction, which results from the electron emitting and reabsorbing a photon. This is in contrast to muonic hydrogen, a muon bound to a proton, in which the vacuum-polarization correction dominates. The reason for the difference is that for the muon, the lighter electron-positron pair that can occur in a vacuum-polarization loop produces a large effect, while for the electron, there is no lighter particle to produce a correspondingly large correction.

There has been a renewed interest in the effects of vacuum polarization due to the recent measurement of the Lamb shift in muonic hydrogen [1–3]. As mentioned above, in this atom, the Lamb shift is predominantly the effect of electron vacuum polarization. However, the radius of the proton, which is deduced by comparison of the measured transition frequencies to the theoretical predictions, differs from the value obtained from spectroscopy of hydrogen and deuterium and electron scattering experiments by 7σ [4]. In view of this discrepancy, a thorough review of the theory is warranted, and a number of such investigations have been carried out, with recent reviews given in Refs. [5–12].

In this paper, we reexamine the theory of vacuum polarization. The objective is to provide a formulation for the calculation of the vacuum-polarization effect entirely in coordinate space for any spherically symmetric binding field, in parallel with an earlier analysis of the self-energy correction in coordinate space [13]. This provides a framework for a direct numerical evaluation of the correction for strong Coulomb fields and for non-Coulombic binding fields for which a perturbation expansion is not feasible. Vacuum polarization is particularly problematic, because it contains the most severe divergences of all the bound-state corrections.

The calculation of vacuum polarization done by Wichmann and Kroll [14] is also based on a coordinate-space formulation, but it requires the explicit analytic expression

for the Green function for a point-charge nucleus. The present calculation is not based on explicit solutions, so it provides a framework for more general potentials. Here, the vacuum polarization is examined in coordinate space using Pauli-Villars regularization for an arbitrary spherically symmetric charge distribution in the nucleus. An alternative method of differential regularization has also been used to treat divergences in coordinate space [15]. We reprise the conventional derivation of the Uehling potential in momentum space in order to compare it to the coordinate-space version.

II. VACUUM POLARIZATION

In bound-state quantum electrodynamics (QED), the second-order electron vacuum-polarization correction for an electron or muon in an external potential $V(\mathbf{x})$ in the Feynman gauge is given, in units where $\{c\} = \{\hbar\} = \{m_e\} = 1$ [16], by (see, for example, [17,18])

$$E_{\text{VP}}^{(2)} = 4\pi i\alpha \int d(t_2 - t_1) \int d\mathbf{x}_2 \int d\mathbf{x}_1 D_F(x_2 - x_1) \times \text{Tr}[\gamma_\mu S_F(x_2, x_2)] \bar{\phi}_n(x_1) \gamma^\mu \phi_n(x_1). \quad (1)$$

In Eq. (1), $\phi_n(x)$ is a four-component wave function given by $\phi_n(x) = \phi_n(\mathbf{x}) e^{-iE_n t}$, where $\phi_n(\mathbf{x})$ is an eigenfunction of the Dirac equation

$$[-i\boldsymbol{\alpha} \cdot \nabla + V(\mathbf{x}) + \beta m - E_n] \phi_n(\mathbf{x}) = 0. \quad (2)$$

Here m is the bound lepton mass, the Dirac matrices are

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad (3)$$

with Pauli matrices $\boldsymbol{\sigma}$, and the γ matrices are $\gamma^0 = \beta$ and $\gamma^i = \beta\alpha^i$, $i = 1, 2, 3$. The photon propagation function is given by

$$D_F(x_2 - x_1) = -\frac{i}{(2\pi)^4} \int d^4q \frac{e^{-iq(x_2 - x_1)}}{q^2 + i\delta} = \frac{i}{8\pi^2} \int_{-\infty}^{\infty} dq^0 \frac{e^{-iq^0(t_2 - t_1)} e^{-b|x_2 - x_1|}}{|x_2 - x_1|}, \quad (4)$$

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with $b = -i(q^0{}^2 + i\delta)^{1/2}$, $\text{Re}(b) > 0$. Integration over the time difference yields

$$E_{\text{VP}}^{(2)} = -\alpha \int d\mathbf{x}_2 \int d\mathbf{x}_1 \frac{1}{|\mathbf{x}_2 - \mathbf{x}_1|} \times \text{Tr}[\gamma_\mu S_{\text{F}}(\mathbf{x}_2, \mathbf{x}_2)] \bar{\phi}_n(\mathbf{x}_1) \gamma^\mu \phi_n(\mathbf{x}_1). \quad (5)$$

Evidently, the quantity

$$e \text{Tr}[\gamma_0 S_{\text{F}}(\mathbf{x}_2, \mathbf{x}_2)] \quad (6)$$

takes the role of the vacuum-polarization charge density. The electron propagation function can be written as

$$S_{\text{F}}(\mathbf{x}_2, \mathbf{x}_1) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dz G(\mathbf{x}_2, \mathbf{x}_1, z(1 + i\delta)) \gamma^0 e^{-iz(t_2 - t_1)}, \quad (7)$$

where the Green function is the solution of the equation

$$[-i\boldsymbol{\alpha} \cdot \nabla_2 + V(\mathbf{x}_2) + \beta m - z] G(\mathbf{x}_2, \mathbf{x}_1, z) = \delta(\mathbf{x}_2 - \mathbf{x}_1), \quad (8)$$

so that

$$E_{\text{VP}}^{(2)} = \frac{i\alpha}{2\pi} \int_{-\infty}^{\infty} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1 \frac{1}{|\mathbf{x}_2 - \mathbf{x}_1|} \times \{ \text{Tr}[G(\mathbf{x}_2, \mathbf{x}_2, z(1 + i\delta))] \phi_n^\dagger(\mathbf{x}_1) \phi_n(\mathbf{x}_1) - \text{Tr}[\boldsymbol{\alpha} G(\mathbf{x}_2, \mathbf{x}_2, z(1 + i\delta))] \cdot \phi_n^\dagger(\mathbf{x}_1) \boldsymbol{\alpha} \phi_n(\mathbf{x}_1) \}. \quad (9)$$

For a spherically symmetric potential $V(\mathbf{x})$, the second term vanishes [14], but only after a formal cancellation of infinite terms (see Appendix A).

III. REGULARIZATION

The expression in Eq. (9) must be modified by regularization in order to produce a valid function for either analytical or numerical evaluation. In particular, $\text{Tr}[G(\mathbf{x}_2, \mathbf{x}_2, z)]$ is meaningless, because for $\mathbf{x}_2 \approx \mathbf{x}_1$ the trace of the Green function has a limiting form given by

$$\text{Tr}[G(\mathbf{x}_2, \mathbf{x}_1, z)] = \frac{z}{\pi |\mathbf{x}_2 - \mathbf{x}_1|} + \dots \quad (10)$$

and is undefined for equal coordinates. In addition, the integration over z is divergent.

To obtain a physical prediction from Eq. (9), we carry out Pauli-Villars regularization by replacing the Green function with the regulated Green function given by [19]

$$G_{\text{R}}(\mathbf{x}_2, \mathbf{x}_1, z) = \sum_i C_i G_i(\mathbf{x}_2, \mathbf{x}_1, z), \quad (11)$$

where G_i is the Green function for a Dirac particle with mass m_i , the solution of

$$[-i\boldsymbol{\alpha} \cdot \nabla_2 + V(\mathbf{x}_2) + \beta m_i - z] G_i(\mathbf{x}_2, \mathbf{x}_1, z) = \delta(\mathbf{x}_2 - \mathbf{x}_1), \quad (12)$$

and the C_i are functions of the masses. The leading term has

$$C_0 = 1; \quad m_0 = m. \quad (13)$$

The coefficients C_i for $i > 0$ are chosen to eliminate the divergent terms from the level shift and will be seen to be quotients of polynomials in the m_i . Then for $\mathbf{x}_2 \neq \mathbf{x}_1$ we have the limit

$$\lim_{\substack{m_i \rightarrow \infty \\ i > 0}} G_{\text{R}}(\mathbf{x}_2, \mathbf{x}_1, z) = G(\mathbf{x}_2, \mathbf{x}_1, z), \quad (14)$$

where G is the unregulated bound-electron Green function. The level shift is calculated by replacing G by G_{R} in Eq. (9) and eventually taking the limit $m_i \rightarrow \infty$ for $i > 0$ after renormalization.

IV. EXPANSION IN V

To separate the singularities from the finite physical contribution, it is useful to employ the power series in V for the Green function, an approach that has been extensively discussed in connection with the evaluation of QED corrections for bound states (see, for example, [14,20,21]). The expansion is

$$G(\mathbf{x}_2, \mathbf{x}_1, z) = F(\mathbf{x}_2, \mathbf{x}_1, z) - \int d\mathbf{w} F(\mathbf{x}_2, \mathbf{w}, z) \times V(\mathbf{w}) F(\mathbf{w}, \mathbf{x}_1, z) + \dots, \quad (15)$$

where F is the free Green function, given by

$$F(\mathbf{x}_2, \mathbf{x}_1, z) = [-i\boldsymbol{\alpha} \cdot \nabla_2 + \beta m + z] \frac{e^{-c|\mathbf{x}_2 - \mathbf{x}_1|}}{4\pi |\mathbf{x}_2 - \mathbf{x}_1|}, \quad (16)$$

with $c = \sqrt{m^2 - z^2}$, $\text{Re}(c) > 0$. It satisfies the equation

$$[-i\boldsymbol{\alpha} \cdot \nabla_2 + \beta m - z] F(\mathbf{x}_2, \mathbf{x}_1, z) = \delta(\mathbf{x}_2 - \mathbf{x}_1). \quad (17)$$

The expansion is illustrated in Fig. 1.

In this context, Furry's theorem is seen by the following consideration. In the expansion of the electron Green function in powers of V , for the term with n powers of V , there will be altogether $n + 1$ vertices and free Green functions F . Thus the expression will consist of the trace of the sum of products of i α matrices, j β matrices, and k powers of z , where $i + j + k = n + 1$. The trace will vanish unless both i and j are even, and the integration over z will vanish unless k is even. Hence only terms with $n + 1$ even may be nonzero, which is just Furry's theorem.

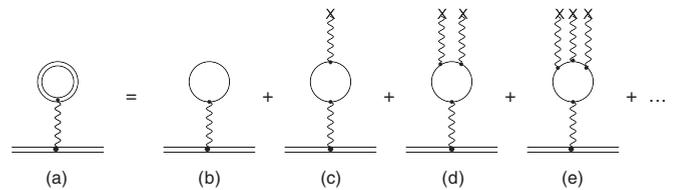


FIG. 1. Expansion of the vacuum-polarization correction in powers of the binding potential V . Diagram (a) represents the complete vacuum polarization of order α . Diagrams (b) through (e) depict the zero-, one-, two-, and three-potential contributions. Only diagrams (c) and (e) and higher-order diagrams with an even number of vertices in the loop are nonzero according to Furry's theorem.

A. Zero potential

The leading term in the expansion is the free Green function, with the zero-component trace given by

$$\text{Tr}[F(\mathbf{x}_2, \mathbf{x}_1, z)] = \frac{z e^{-c|\mathbf{x}_2 - \mathbf{x}_1|}}{\pi |\mathbf{x}_2 - \mathbf{x}_1|}. \quad (18)$$

The contribution of this term to the vacuum-polarization correction formally vanishes because of Furry's theorem. However, the term is problematic when $\mathbf{x}_2 = \mathbf{x}_1$, which is remedied by Pauli-Villars regularization. In view of the analyticity of $F(\mathbf{x}_2, \mathbf{x}_1, z)$ as a function of z and the fact that its branch points are located at $z = \pm m(1 - i\delta)$, we can modify the contour of integration to be a straight line along the imaginary axis plus contributions from two quarter circles in the first and third quadrants of the complex z plane. The contribution from the two quarter circles will vanish as their radii increase, provided the integrand of the regulated expression falls off for large $|z|$ faster than $1/|z|$ if $\mathbf{x}_2 = \mathbf{x}_1$. Letting $z = iu$, we have

$$c_i = \sqrt{m_i^2 - z^2} = \sqrt{u^2} + \frac{m_i^2}{2\sqrt{u^2}} - \frac{m_i^4}{8u^2\sqrt{u^2}} + \dots, \quad (19)$$

and the leading terms in the expansion in $1/u$ are

$$\frac{e^{-c_i|\mathbf{x}_2 - \mathbf{x}_1|}}{|\mathbf{x}_2 - \mathbf{x}_1|} = \frac{e^{-\sqrt{u^2}|\mathbf{x}_2 - \mathbf{x}_1|}}{|\mathbf{x}_2 - \mathbf{x}_1|} - \frac{m_i^2 e^{-\sqrt{u^2}|\mathbf{x}_2 - \mathbf{x}_1|}}{2\sqrt{u^2}} + \dots. \quad (20)$$

The two terms on the right-hand side of Eq. (20) lead to divergent contributions, so we eliminate them with two auxiliary mass propagators that fulfill the conditions

$$1 + C_1 + C_2 = 0, \quad (21)$$

$$m_0^2 + C_1 m_1^2 + C_2 m_2^2 = 0, \quad (22)$$

satisfied by

$$C_1 = \frac{m_0^2 - m_2^2}{m_2^2 - m_1^2}, \quad (23)$$

$$C_2 = \frac{m_1^2 - m_0^2}{m_2^2 - m_1^2}. \quad (24)$$

The regularization is implemented by writing

$$F_R(\mathbf{x}_2, \mathbf{x}_1, z) = \sum_{i=0}^2 C_i F_i(\mathbf{x}_2, \mathbf{x}_1, z), \quad (25)$$

where F_i is given by Eq. (16) with m replaced by m_i . We thus have

$$\text{Tr}[F_R(\mathbf{x}_2, \mathbf{x}_1, z)] = \sum_{i=0}^2 C_i \frac{i u e^{-c_i|\mathbf{x}_2 - \mathbf{x}_1|}}{\pi |\mathbf{x}_2 - \mathbf{x}_1|}, \quad (26)$$

and

$$\begin{aligned} \text{Tr}[F_R(\mathbf{x}_2, \mathbf{x}_2, z)] &= \lim_{|\mathbf{x}_2 - \mathbf{x}_1| \rightarrow 0} \text{Tr}[F_R(\mathbf{x}_2, \mathbf{x}_1, z)] \\ &= -\frac{i u}{\pi} \sum_{i=0}^2 C_i c_i \\ &= \frac{i}{8\pi u \sqrt{u^2}} \left[\sum_{i=0}^2 C_i m_i^4 + O\left(\frac{1}{u^2}\right) \right]. \end{aligned} \quad (27)$$

Evidently, the contribution from the quarter circles vanishes, and since the branches of the square root are specified to give $\sqrt{u^2} = |u|$ for real values of u , the integrand is an odd function of u , and we have

$$\int_{-\infty}^{\infty} du \text{Tr}[F_R(\mathbf{x}_2, \mathbf{x}_2, i u)] = 0. \quad (28)$$

B. One potential

The next term of the expansion in V is

$$G^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z) = - \int d\mathbf{w} F(\mathbf{x}_2, \mathbf{w}, z) V(\mathbf{w}) F(\mathbf{w}, \mathbf{x}_1, z). \quad (29)$$

In Appendix B we recast $\text{Tr}[G^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z)]$ into a form in which the singularity at $\mathbf{x}_2 = \mathbf{x}_1$ is isolated in a relatively simple term,

$$\begin{aligned} \text{Tr}[G^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z)] &= -\frac{Z\alpha}{2\pi} \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} \rho(\mathbf{w}) \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|} \\ &\quad - \frac{z^2}{2\pi^2} \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} V(\mathbf{w}) \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|} \\ &\quad - \frac{1}{2\pi} [V(\mathbf{x}_2) + V(\mathbf{x}_1)] \frac{e^{-c|\mathbf{x}_2 - \mathbf{x}_1|}}{|\mathbf{x}_2 - \mathbf{x}_1|}, \end{aligned} \quad (30)$$

where Z is the charge of the nucleus and ρ is the nuclear charge density normalized to 1. The limit as $\mathbf{x}_2 \rightarrow \mathbf{x}_1$ of $\text{Tr}[G^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z)]$ is undefined due to the third term, so we introduce a counterterm that cancels the singularity pointwise and vanishes when integrated over z . The counterterm is

$$\begin{aligned} G_A^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z) &= - \int d\mathbf{w} F(\mathbf{x}_2, \mathbf{w}, z) \frac{V(\mathbf{x}_2) + V(\mathbf{x}_1)}{2} F(\mathbf{w}, \mathbf{x}_1, z), \end{aligned} \quad (31)$$

and (see Appendix B)

$$\begin{aligned} \text{Tr}[G_A^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z)] &= -\frac{z^2}{2\pi^2} \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} \frac{V(\mathbf{x}_2) + V(\mathbf{x}_1)}{2} \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|} \\ &\quad - \frac{1}{2\pi} [V(\mathbf{x}_2) + V(\mathbf{x}_1)] \frac{e^{-c|\mathbf{x}_2 - \mathbf{x}_1|}}{|\mathbf{x}_2 - \mathbf{x}_1|}. \end{aligned} \quad (32)$$

The difference

$$G_B^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z) = G^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z) - G_A^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z) \quad (33)$$

has the trace

$$\begin{aligned} \text{Tr}[G_B^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z)] &= -\frac{Z\alpha}{2\pi} \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} \rho(\mathbf{w}) \\ &\quad \times \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|} - \frac{z^2}{2\pi^2} \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} \\ &\quad \times \left[V(\mathbf{w}) - \frac{V(\mathbf{x}_2) + V(\mathbf{x}_1)}{2} \right] \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|}, \end{aligned} \quad (34)$$

with the limit

$$\begin{aligned} & \text{Tr}[G_B^{(1)}(\mathbf{x}_2, \mathbf{x}_2, z)] \\ &= -\frac{Z\alpha}{2\pi} \int d\mathbf{w} \rho(\mathbf{w}) \frac{e^{-2c|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|^2} \\ & \quad - \frac{z^2}{2\pi^2} \int d\mathbf{w} [V(\mathbf{w}) - V(\mathbf{x}_2)] \frac{e^{-2c|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|^2} \end{aligned} \quad (35)$$

for $\mathbf{x}_1 \rightarrow \mathbf{x}_2$.

To show that the integral over the counterterm vanishes, we consider the expansion

$$\begin{aligned} & F(\mathbf{x}_2, \mathbf{x}_1, z + \delta z) \\ &= F(\mathbf{x}_2, \mathbf{x}_1, z) + \int d\mathbf{w} F(\mathbf{x}_2, \mathbf{w}, z) \delta z F(\mathbf{w}, \mathbf{x}_1, z) \\ & \quad + \int d\mathbf{v} \int d\mathbf{w} F(\mathbf{x}_2, \mathbf{v}, z) \delta z F(\mathbf{v}, \mathbf{w}, z) \delta z \\ & \quad \times F(\mathbf{w}, \mathbf{x}_1, z) + \dots \end{aligned} \quad (36)$$

This yields

$$\frac{\partial}{\partial \delta z} F(\mathbf{x}_2, \mathbf{x}_1, z + \delta z) \Big|_{\delta z=0} = \int d\mathbf{w} F(\mathbf{x}_2, \mathbf{w}, z) F(\mathbf{w}, \mathbf{x}_1, z), \quad (37)$$

so we can write

$$G_A^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z) = -\frac{V(\mathbf{x}_2) + V(\mathbf{x}_1)}{2} \frac{\partial}{\partial z} F(\mathbf{x}_2, \mathbf{x}_1, z). \quad (38)$$

With the contour modified as in the zero-potential case, the leading surviving term in the regulated trace is

$$\begin{aligned} & \frac{\partial}{\partial z} \text{Tr}[F_R(\mathbf{x}_2, \mathbf{x}_2, z)] \\ &= \frac{\partial}{\partial u} \frac{1}{8\pi u \sqrt{u^2}} \left[\sum_{i=0}^2 C_i m_i^4 + O\left(\frac{1}{u^2}\right) \right], \end{aligned} \quad (39)$$

so that integration gives

$$\int_{-\infty}^{\infty} dz \frac{\partial}{\partial z} \text{Tr}[F_R(\mathbf{x}_2, \mathbf{x}_1, z)] = \text{Tr}[F_R(\mathbf{x}_2, \mathbf{x}_1, iu)] \Big|_{u=-\infty}^{u=\infty} = 0 \quad (40)$$

and the counterterm vanishes.

The subtracted one-potential contribution to the Green function is regulated to be

$$\begin{aligned} G_{BR}^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z) &= -\int d\mathbf{w} \left[V(\mathbf{w}) - \frac{V(\mathbf{x}_2) + V(\mathbf{x}_1)}{2} \right] \\ & \quad \times \sum_{i=0}^2 C_i F_i(\mathbf{x}_2, \mathbf{w}, z) F_i(\mathbf{w}, \mathbf{x}_1, z), \end{aligned} \quad (41)$$

and the trace of the corresponding equal coordinate propagation function is

$$\begin{aligned} & \text{Tr}[\gamma^0 S_{FBR}^{(1)}(\mathbf{x}_2, \mathbf{x}_2)] \\ &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} dz \text{Tr}[G_{BR}^{(1)}(\mathbf{x}_2, \mathbf{x}_2, z(1+i\delta))] \end{aligned}$$

$$\begin{aligned} &= \int_0^{\infty} du \sum_{i=0}^2 C_i \left\{ -\frac{Z\alpha}{2\pi^2} \int d\mathbf{w} \rho(\mathbf{w}) \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|^2} \right. \\ & \quad \left. + \frac{u^2}{2\pi^3} \int d\mathbf{w} [V(\mathbf{w}) - V(\mathbf{x}_2)] \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|^2} \right\}. \end{aligned} \quad (42)$$

In this equation the second line follows from a contour rotation to the imaginary z axis and a variable change $z = iu$. The contribution from the quarter circles as $|z| \rightarrow \infty$ vanishes due to the exponential falloff of the integrand. For the possibly singular case of $|\mathbf{x}_2 - \mathbf{w}| \approx 0$, we note that

$$\begin{aligned} & \sum_{i=0}^2 C_i \int d\mathbf{w} \rho(\mathbf{w}) \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|^2} \\ & \rightarrow \rho(\mathbf{x}_2) \sum_{i=0}^2 C_i \int d\mathbf{w} \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|^2} \\ &= \frac{3\pi}{4} \rho(\mathbf{x}_2) \sum_{i=0}^2 C_i \frac{m_i^4}{u^5} + O\left(\frac{1}{u^7}\right) \end{aligned} \quad (43)$$

and

$$\begin{aligned} & \sum_{i=0}^2 C_i u^2 \int d\mathbf{w} [V(\mathbf{w}) - V(\mathbf{x}_2)] \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|^2} \\ & \rightarrow \sum_{i=0}^2 C_i \frac{u^2}{6} [\nabla_2^2 V(\mathbf{x}_2)] \int d\mathbf{w} e^{-2c_i|\mathbf{x}_2-\mathbf{w}|} \\ &= \frac{5\pi^2 Z\alpha}{4} \rho(\mathbf{x}_2) \sum_{i=0}^2 C_i \frac{m_i^4}{u^5} + O\left(\frac{1}{u^7}\right), \end{aligned} \quad (44)$$

which provides sufficient convergence in the integration over u for the contour rotation to be valid.

Integration by parts in Eq. (42) yields

$$\begin{aligned} & \text{Tr}[\gamma^0 S_{FBR}^{(1)}(\mathbf{x}_2, \mathbf{x}_2)] \\ &= \int_0^{\infty} du \sum_{i=0}^2 C_i \left\{ -\frac{Z\alpha u^2}{\pi^2 c_i} \int d\mathbf{w} \rho(\mathbf{w}) \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|} \right. \\ & \quad \left. + \frac{u^4}{3\pi^3 c_i} \int d\mathbf{w} [V(\mathbf{w}) - V(\mathbf{x}_2)] \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|} \right\}, \end{aligned} \quad (45)$$

where estimates analogous to those in Eqs. (43) and (44) show that the integration over u converges and that the surface terms at $u = \infty$ from the partial integration vanish even for $|\mathbf{x}_2 - \mathbf{w}| \approx 0$. For the second term we have

$$\begin{aligned} & \int d\mathbf{w} [V(\mathbf{w}) - V(\mathbf{x}_2)] \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|} \\ &= -Z\alpha \int d\mathbf{w} \int d\mathbf{r} \rho(\mathbf{r}) \left(\frac{1}{|\mathbf{w}-\mathbf{r}|} - \frac{1}{|\mathbf{x}_2-\mathbf{r}|} \right) \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{w}|}}{|\mathbf{x}_2-\mathbf{w}|} \\ &= \frac{\pi Z\alpha}{c_i^2} \int d\mathbf{r} \rho(\mathbf{r}) \frac{e^{-2c_i|\mathbf{x}_2-\mathbf{r}|}}{|\mathbf{x}_2-\mathbf{r}|} \end{aligned} \quad (46)$$

so that

$$\begin{aligned} & \text{Tr}[\gamma^0 S_{\text{FBR}}^{(1)}(x_2, x_2)] \\ &= \frac{Z\alpha}{\pi^2} \int_0^\infty du \int d\mathbf{r} \rho(\mathbf{r}) \sum_{i=0}^2 C_i \left(-\frac{u^2}{c_i} + \frac{u^4}{3c_i^3} \right) \frac{e^{-2c_i|x_2-r|}}{|\mathbf{x}_2 - \mathbf{r}|}. \end{aligned} \quad (47)$$

Thus the one-potential level shift

$$\begin{aligned} E_{\text{VP}}^{(2,1)} &= -\alpha \int d\mathbf{x}_2 \int d\mathbf{x}_1 \frac{1}{|\mathbf{x}_2 - \mathbf{x}_1|} \text{Tr}[\gamma^0 S_{\text{FBR}}^{(1)}(x_2, x_2)] \\ &\quad \times \phi_n^\dagger(\mathbf{x}_1) \phi_n(\mathbf{x}_1) \end{aligned} \quad (48)$$

is the expectation value of a vacuum-polarization potential given by

$$\begin{aligned} V_{\text{VP}}^{(2,1)}(\mathbf{x}_1) &= \frac{Z\alpha^2}{\pi^2} \int d\mathbf{x}_2 \frac{1}{|\mathbf{x}_2 - \mathbf{x}_1|} \int_0^\infty du \\ &\quad \times \int d\mathbf{r} \rho(\mathbf{r}) \sum_{i=0}^2 C_i \left(\frac{u^2}{c_i} - \frac{u^4}{3c_i^3} \right) \frac{e^{-2c_i|x_2-r|}}{|\mathbf{x}_2 - \mathbf{r}|}. \end{aligned} \quad (49)$$

Integration over \mathbf{x}_2 ,

$$\int d\mathbf{x}_2 \frac{1}{|\mathbf{x}_2 - \mathbf{x}_1|} \frac{e^{-2c_i|x_2-r|}}{|\mathbf{x}_2 - \mathbf{r}|} = \frac{\pi}{c_i^2 |\mathbf{x}_1 - \mathbf{r}|} (1 - e^{-2c_i|x_1-r|}), \quad (50)$$

yields

$$\begin{aligned} V_{\text{VP}}^{(2,1)}(\mathbf{x}_1) &= \frac{Z\alpha^2}{\pi} \int_0^\infty du \int d\mathbf{r} \rho(\mathbf{r}) \sum_{i=0}^2 C_i \left(\frac{u^2}{c_i^3} - \frac{u^4}{3c_i^5} \right) \\ &\quad \times \frac{1 - e^{-2c_i|x_1-r|}}{|\mathbf{x}_1 - \mathbf{r}|}. \end{aligned} \quad (51)$$

We have

$$\int_0^\infty du \sum_{i=0}^2 C_i \left(\frac{u^2}{c_i^3} - \frac{u^4}{3c_i^5} \right) = -\frac{1}{3} \sum_{i=0}^2 C_i \ln m_i^2, \quad (52)$$

which produces a potential corresponding to a mass-dependent charge proportional to the charge distribution ρ . This is ultimately eliminated by charge renormalization. For the remaining part of Eq. (51), the contribution from each i is separately finite because of the exponential factor, and there is no contribution from the terms with $i > 0$ in the limit of large auxiliary masses. This can be seen from the nonrelativistic estimate for the level shift from each of these terms

$$\begin{aligned} & -\frac{Z\alpha^2}{\pi} |\phi_n(0)|^2 \int d\mathbf{x}_1 \int_0^\infty du \\ & \quad \times \int d\mathbf{r} \rho(\mathbf{r}) C_i \left(\frac{u^2}{c_i^3} - \frac{u^4}{3c_i^5} \right) \frac{e^{-2c_i|x_1-r|}}{|\mathbf{x}_1 - \mathbf{r}|} \\ &= -Z\alpha^2 |\phi_n(0)|^2 \int_0^\infty du C_i \left(\frac{u^2}{c_i^5} - \frac{u^4}{3c_i^7} \right) \\ &= -\frac{4Z\alpha^2}{15} |\phi_n(0)|^2 \frac{C_i}{m_i^2}. \end{aligned} \quad (53)$$

The surviving term of Eq. (51) with $i = 0$ is just the Uehling potential $V_U(\mathbf{x}_1)$ [22,23]. We thus have

$$V_{\text{VP}}^{(2,1)}(\mathbf{x}_1) = -\frac{Z\alpha^2}{3\pi} \int d\mathbf{r} \frac{\rho(\mathbf{r})}{|\mathbf{x}_1 - \mathbf{r}|} \sum_{i=0}^2 C_i \ln m_i^2 + V_U(\mathbf{x}_1), \quad (54)$$

where

$$\begin{aligned} V_U(\mathbf{x}_1) &= -\frac{Z\alpha^2}{\pi} \int d\mathbf{r} \rho(\mathbf{r}) \int_0^\infty du \left(\frac{u^2}{c_0^3} - \frac{u^4}{3c_0^5} \right) \frac{e^{-2c_0|x_1-r|}}{|\mathbf{x}_1 - \mathbf{r}|} \\ &= -\frac{Z\alpha^2}{3\pi} \int d\mathbf{r} \rho(\mathbf{r}) \int_1^\infty dt \sqrt{t^2 - 1} \left(\frac{2}{t^2} + \frac{1}{t^4} \right) \\ &\quad \times \frac{e^{-2tm_0|x_1-r|}}{|\mathbf{x}_1 - \mathbf{r}|}, \end{aligned} \quad (55)$$

and in the case of a point charge

$$V_U(\mathbf{x}_1) = -\frac{Z\alpha^2}{3\pi} \int_1^\infty dt \sqrt{t^2 - 1} \left(\frac{2}{t^2} + \frac{1}{t^4} \right) \frac{e^{-2tm_0x_1}}{x_1}, \quad (56)$$

where $x_1 = |\mathbf{x}_1|$.

To summarize, the Green function in the expression for the vacuum polarization is not defined for equal coordinates as it appears formally, so a counterterm that removes this singularity is subtracted, the Pauli-Villars regularization sum is made for unequal coordinates, and the regulated expression is taken to be the limit as the coordinates become equal. Then, integration over the energy parameter in the Green function is carried out, the charge is renormalized, after which the auxiliary masses are taken to the infinite limit. The result is just the Uehling potential.

C. Two potential

The next term in the expansion of the Green function in powers of V is

$$\begin{aligned} G^{(2)}(\mathbf{x}_2, \mathbf{x}_1, z) &= \int d\mathbf{v} \int d\mathbf{w} F(\mathbf{x}_2, \mathbf{v}, z) V(\mathbf{v}) F(\mathbf{v}, \mathbf{w}, z) \\ &\quad \times V(\mathbf{w}) F(\mathbf{w}, \mathbf{x}_1, z). \end{aligned} \quad (57)$$

This gives a divergent contribution to the level shift, which is expected to vanish when regulated because of Furry's theorem. To confirm that the regulated contribution vanishes in our framework, we consider the approximation given by

$$\begin{aligned} G_A^{(2)}(\mathbf{x}_2, \mathbf{x}_1, z) &= \int d\mathbf{v} \int d\mathbf{w} F(\mathbf{x}_2, \mathbf{v}, z) V(\mathbf{x}_2) F(\mathbf{v}, \mathbf{w}, z) \\ &\quad \times V(\mathbf{x}_1) F(\mathbf{w}, \mathbf{x}_1, z). \end{aligned} \quad (58)$$

From Eq. (36), we have

$$\begin{aligned} & \frac{1}{2} \frac{\partial^2}{\partial \delta z^2} F(\mathbf{x}_2, \mathbf{x}_1, z + \delta z) \Big|_{\delta z=0} \\ &= \int d\mathbf{v} \int d\mathbf{w} F(\mathbf{x}_2, \mathbf{v}, z) F(\mathbf{v}, \mathbf{w}, z) F(\mathbf{w}, \mathbf{x}_1, z), \end{aligned} \quad (59)$$

so we can write

$$G_A^{(2)}(\mathbf{x}_2, \mathbf{x}_1, z) = \frac{1}{2} V(\mathbf{x}_2) V(\mathbf{x}_1) \frac{\partial^2}{\partial z^2} F(\mathbf{x}_2, \mathbf{x}_1, z). \quad (60)$$

The zero-component trace is

$$\begin{aligned} \frac{\partial^2}{\partial z^2} \text{Tr}[F_i(\mathbf{x}_2, \mathbf{x}_1, z)] &= \frac{\partial^2}{\partial z^2} \frac{z e^{-c_i |\mathbf{x}_2 - \mathbf{x}_1|}}{\pi |\mathbf{x}_2 - \mathbf{x}_1|} \\ &= -\frac{\partial^2}{\partial z^2} \frac{z c_i}{\pi} + O(|\mathbf{x}_2 - \mathbf{x}_1|), \end{aligned} \quad (61)$$

which is finite for equal coordinates. We thus have

$$\begin{aligned} \frac{\partial^2}{\partial z^2} \text{Tr}[F_i(\mathbf{x}_2, \mathbf{x}_2, z)] &= \frac{\partial^2}{\partial u^2} \frac{i u}{\pi} \sqrt{m_i^2 + u^2} \\ &= \frac{\partial}{\partial u} \frac{i \sqrt{u^2}}{\pi} \left(2 + \frac{m_i^4}{4u^4} + \dots \right) \end{aligned} \quad (62)$$

and the regulated Green function has the factor

$$\begin{aligned} \frac{\partial^2}{\partial z^2} \text{Tr}[F_R(\mathbf{x}_2, \mathbf{x}_2, z)] \\ = \frac{\partial}{\partial u} \frac{i}{4\pi u^2 \sqrt{u^2}} \left[\sum_{i=0}^2 C_i m_i^4 + O\left(\frac{1}{u^2}\right) \right], \end{aligned} \quad (63)$$

which vanishes when integrated over u . The trace of the full regulated two-potential Green function $\text{Tr}[G_R^{(2)}(\mathbf{x}_2, \mathbf{x}_1, z)]$ will have a similar analytic behavior, and it is an odd function of z , so it also vanishes.

D. Three potential

The three-potential Green function is

$$\begin{aligned} G^{(3)}(\mathbf{x}_2, \mathbf{x}_1, z) &= -\int ds \int dv \int d\mathbf{w} F(\mathbf{x}_2, s, z) V(s) F(s, \mathbf{v}, z) \\ &\quad \times V(\mathbf{v}) F(\mathbf{v}, \mathbf{w}, z) V(\mathbf{w}) F(\mathbf{w}, \mathbf{x}_1, z). \end{aligned} \quad (64)$$

This expression gives the leading term in powers of $Z\alpha$ in the all-order calculation by Wichmann and Kroll [14] for a point nucleus. For the effect of the finite size of the nucleus on this and higher-order terms, see Soff and Mohr [24] and papers cited therein. A first approximation for this function is given by

$$\begin{aligned} G_A^{(3)}(\mathbf{x}_2, \mathbf{x}_1, z) &= -\int ds \int dv \int d\mathbf{w} F(\mathbf{x}_2, s, z) V(\mathbf{x}_2) F(s, \mathbf{v}, z) \\ &\quad \times V(\mathbf{x}_2) F(\mathbf{v}, \mathbf{w}, z) V(\mathbf{x}_2) F(\mathbf{w}, \mathbf{x}_1, z) \\ &= -\frac{[V(\mathbf{x}_2)]^3}{6} \frac{\partial^3}{\partial z^3} F(\mathbf{x}_2, \mathbf{x}_1, z). \end{aligned} \quad (65)$$

The zero-component trace of the i th mass term is proportional to

$$\begin{aligned} \frac{\partial^3}{\partial z^3} \text{Tr}[F_i(\mathbf{x}_2, \mathbf{x}_1, z)] &= \frac{\partial^3}{\partial z^3} \frac{z e^{-c_i |\mathbf{x}_2 - \mathbf{x}_1|}}{\pi |\mathbf{x}_2 - \mathbf{x}_1|} \\ &= -\frac{\partial^3}{\partial z^3} \frac{z c_i}{\pi} + O(|\mathbf{x}_2 - \mathbf{x}_1|), \end{aligned} \quad (66)$$

which is finite for equal coordinates, and

$$\begin{aligned} \frac{\partial^3}{\partial z^3} \text{Tr}[F_i(\mathbf{x}_2, \mathbf{x}_2, z)] &= \frac{\partial^3}{\partial u^3} \frac{u}{\pi} \sqrt{m_i^2 + u^2} \\ &= \frac{\partial}{\partial u} \frac{\sqrt{u^2}}{\pi} \left(\frac{2}{u} - \frac{3m_i^4}{4u^5} + \dots \right). \end{aligned} \quad (67)$$

Evidently, the integral over u of this expression is finite and nonzero, because the relevant branch of the square root is positive at $u = \pm\infty$. This well-known property of the ‘‘light-by-light’’ Feynman diagram yields a spurious finite gauge-noninvariant part [25]. On the other hand, the integral of the regulated approximate expression vanishes with no ambiguity from the quarter circles. It is of interest to note that the spurious contribution is not present if the correction is calculated from an expansion of the Green function in angular momentum eigenfunctions [24].

E. All-order generalization

The higher-order terms in the potential expansion of the vacuum polarization are finite and unambiguous, and according to Furry’s theorem, only closed loops with an even number of vertices are nonzero. In the case considered here, there is one vertex from the interaction with the bound electron or muon and an odd number from the expansion of the bound Green function in powers of the external potential.

V. MOMENTUM-SPACE APPROACH

Here, the conventional momentum-space derivation of the Uehling potential for a point-charge nucleus is reprised in order to provide a comparison to the coordinate-space approach.

We consider the Fourier transform of the trace of the propagation function in Eq. (5) starting from the unequal coordinate case $\text{Tr}[\gamma^0 S_F(\mathbf{x}_2, \mathbf{x}_1)]$. From the transforms

$$F(\mathbf{x}_2, \mathbf{x}_1, z) = -\frac{1}{(2\pi)^3} \int d\mathbf{p} e^{i\mathbf{p}\cdot\mathbf{x}_2} \frac{1}{\boldsymbol{\gamma}\cdot\mathbf{p} - m} \gamma^0 e^{-i\mathbf{p}\cdot\mathbf{x}_1}, \quad (68)$$

where $p^0 = z$, and

$$V(\mathbf{x}) = -\frac{Z\alpha}{2\pi^2} \int d\mathbf{p} e^{i\mathbf{p}\cdot\mathbf{x}} \frac{1}{p^2} \quad (69)$$

for the point-nucleus potential, we have from Eq. (29), after integration over \mathbf{w} ,

$$\begin{aligned} G^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z) &= \frac{Z\alpha}{16\pi^5} \int d\mathbf{k} \int d\mathbf{p} e^{i\mathbf{k}\cdot\mathbf{x}_2} e^{i\mathbf{p}\cdot(\mathbf{x}_2 - \mathbf{x}_1)} \\ &\quad \times \frac{1}{\boldsymbol{\gamma}\cdot(\mathbf{k} + \mathbf{p}) - m} \gamma^0 \frac{1}{k^2} \frac{1}{\boldsymbol{\gamma}\cdot\mathbf{p} - m} \gamma^0, \end{aligned} \quad (70)$$

where $k^0 = 0$. The singularity for $\mathbf{x}_2 \rightarrow \mathbf{x}_1$, as seen in Eq. (30), is here manifested in the divergence of the integral over \mathbf{p} for large momenta when $\mathbf{x}_2 = \mathbf{x}_1$. This singularity is removed by regulating with the Pauli-Villars summation in the integrand, which gives

$$\begin{aligned} G_R^{(1)}(\mathbf{x}_2, \mathbf{x}_2, z) \\ = \frac{Z\alpha}{16\pi^5} \int d\mathbf{k} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{k^2} \int d\mathbf{p} \sum_{i=0}^2 C_i \frac{1}{\boldsymbol{\gamma}\cdot(\mathbf{k} + \mathbf{p}) - m_i} \gamma^0 \\ \times \frac{1}{\boldsymbol{\gamma}\cdot\mathbf{p} - m_i} \gamma^0. \end{aligned} \quad (71)$$

We thus have

$$\begin{aligned} & \text{Tr}[\gamma^0 S_{\text{FR}}^{(1)}(x_2, x_2)] \\ &= \frac{Z\alpha}{32\pi^6 i} \int d\mathbf{k} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{k^2} \int d^4 p \sum_{i=0}^2 C_i \\ & \times \text{Tr} \left[\frac{1}{\gamma \cdot (k+p) - m_i} \gamma^0 \frac{1}{\gamma \cdot p - m_i} \gamma^0 \right], \end{aligned} \quad (72)$$

where it is understood that the variable p^0 in the integrand includes a factor of $(1 + i\delta)$, which is equivalent to specification of the Feynman contour. This expression can be written as

$$\text{Tr}[\gamma^0 S_{\text{FR}}^{(1)}(x_2, x_2)] = \frac{Z\alpha}{32\pi^6 i} \int d\mathbf{k} \frac{e^{i\mathbf{k}\cdot\mathbf{x}_2}}{k^2} I^{00}(k), \quad (73)$$

where

$$I^{\mu\nu}(k) = \int d^4 p \sum_{i=0}^2 C_i \text{Tr} \left[\gamma^\mu \frac{1}{\gamma \cdot (k+p) - m_i} \gamma^\nu \frac{1}{\gamma \cdot p - m_i} \right]. \quad (74)$$

Rotation of the contour of the variable p^0 to the imaginary axis and application of standard Feynman integral evaluation methods yields (see Appendix C for details)

$$\begin{aligned} I^{\mu\nu}(k) &= 16\pi^2 i \int_0^\infty dr r^3 \sum_{i=0}^2 C_i \int_0^1 dy \frac{(g^{\mu\nu} k^2 - k^\mu k^\nu) y(1-y)}{[r^2 + k^2 y(1-y) + m_i^2]^2} \\ &+ 2\pi^2 i \int_0^\infty dr \frac{d}{dr} r^4 \sum_{i=0}^2 C_i \int_0^1 dy \frac{g^{\mu\nu}}{r^2 + k^2 y(1-y) + m_i^2}. \end{aligned} \quad (75)$$

The second term is not formally gauge invariant, but the regulated integrand falls off sufficiently rapidly that the integral of the derivative vanishes. A single mass counterterm regularization would yield a nonzero result for this term. For the first term, the change of variable $y = (t - \sqrt{t^2 - 1})/2t$ and integration by parts gives

$$\begin{aligned} \int_0^1 dy \frac{y(1-y)}{[r^2 + k^2 y(1-y) + m_i^2]^2} &= \int_0^{1/2} dy \frac{2y(1-y)}{[r^2 + k^2 y(1-y) + m_i^2]^2} = \int_1^\infty dt \frac{1}{4t^4 \sqrt{t^2 - 1}} \frac{1}{(r^2 + k^2/4t^2 + m_i^2)^2} \\ &= \frac{1}{6} \frac{1}{(r^2 + m_i^2)^2} - \int_1^\infty dt \frac{\sqrt{t^2 - 1}}{12} \left(\frac{2}{t^4} + \frac{1}{t^6} \right) \frac{k^2}{(r^2 + k^2/4t^2 + m_i^2)^3}, \end{aligned} \quad (76)$$

and hence

$$\begin{aligned} \int_0^\infty dr r^3 \sum_{i=0}^2 C_i \int_0^1 dy \frac{y(1-y)}{[r^2 + k^2 y(1-y) + m_i^2]^2} &= -\frac{1}{12} \sum_{i=0}^2 C_i \left[\ln m_i^2 + \int_1^\infty dt \sqrt{t^2 - 1} \left(\frac{2}{t^2} + \frac{1}{t^4} \right) \frac{k^2}{k^2 + 4t^2 m_i^2} \right] \\ &= -\frac{1}{12} \sum_{i=0}^2 C_i \ln m_i^2 + \frac{1}{3} \int_1^\infty dt \sqrt{t^2 - 1} \left(2 + \frac{1}{t^2} \right) \sum_{i=0}^2 \frac{C_i m_i^2}{k^2 + 4t^2 m_i^2}. \end{aligned} \quad (77)$$

Integration over \mathbf{k} in Eq. (73) yields

$$\text{Tr}[\gamma^0 S_{\text{FR}}^{(1)}(x_2, x_2)] = \frac{Z\alpha}{3\pi} \sum_{i=0}^2 C_i \ln m_i^2 \delta(x_2) - \frac{Z\alpha}{3\pi^2} \int_1^\infty dt \sqrt{t^2 - 1} \left(2 + \frac{1}{t^2} \right) \sum_{i=0}^2 C_i m_i^2 \frac{e^{-2tm_i x_2}}{x_2}. \quad (78)$$

According to Eq. (48), the level shift corresponds to a potential energy given by

$$\begin{aligned} V_{\text{VP}}^{(2,1)}(\mathbf{x}_1) &= -\alpha \int d\mathbf{x}_2 \frac{1}{|\mathbf{x}_2 - \mathbf{x}_1|} \text{Tr}[\gamma^0 S_{\text{FR}}^{(1)}(x_2, x_2)] \\ &= -\frac{Z\alpha^2}{3\pi} \left\{ \sum_{i=0}^2 C_i \frac{\ln m_i^2}{x_1} - \int_1^\infty dt \sqrt{t^2 - 1} \left(\frac{2}{t^2} + \frac{1}{t^4} \right) \sum_{i=0}^2 C_i \frac{1 - e^{-2tm_i x_1}}{x_1} \right\} \\ &= -\frac{Z\alpha^2}{3\pi} \left\{ \sum_{i=0}^2 C_i \frac{\ln m_i^2}{x_1} + \int_1^\infty dt \sqrt{t^2 - 1} \left(\frac{2}{t^2} + \frac{1}{t^4} \right) \frac{e^{-2tm_0 x_1}}{x_1} \right\}. \end{aligned} \quad (79)$$

The term on the second line that is independent of mass vanishes from the condition on C_i , and the terms with the exponential factor and with $i > 0$ make no contribution in the large mass limit, as shown by an estimate analogous to that in Eq. (53). The first term on the third line is eliminated by charge renormalization, and the second term is just the Uehling potential, in agreement with Eq. (56).

The results of the coordinate-space and momentum-space calculations agree, as they must, since Pauli-Villars regularization makes the result finite, but the charge renormalization terms arise in different ways. This is seen by comparing the point-charge special case of Eq. (47),

$$\text{Tr}[\gamma^0 S_{\text{FBR}}^{(1)}(x_2, x_2)] = \frac{Z\alpha}{\pi^2} \int_0^\infty du \sum_{i=0}^2 C_i \left(-\frac{u^2}{c_i} + \frac{u^4}{3c_i^3} \right) \times \frac{e^{-2c_i x_2}}{x_2}, \quad (80)$$

to Eq. (78). For $x_2 \neq 0$, only the second term of Eq. (78) is nonzero. In Eq. (80), the exponential factor provides convergence for large u , so that the integrals in the sum over i are separately finite. Thus, the mass-dependent variable change $t = c_i/m_i$ may be made for each i and the result is the same as the second term in Eq. (78). However, if $x_2 = 0$, then the integrals over u are not separately finite and a mass-dependent variable change is not valid. The effect of including the point $x_2 = 0$ can be checked by integrating either expression over x_2 . The result of integration of Eq. (78) is

$$\int dx_2 \text{Tr}[\gamma^0 S_{\text{FR}}^{(1)}(x_2, x_2)] = \frac{Z\alpha}{3\pi} \sum_{i=0}^2 C_i \ln m_i^2, \quad (81)$$

since the integral over the second term vanishes. Integration of Eq. (80) gives

$$\begin{aligned} \int dx_2 \text{Tr}[\gamma^0 S_{\text{FBR}}^{(1)}(x_2, x_2)] &= \frac{Z\alpha}{\pi} \int_0^\infty du \sum_{i=0}^2 C_i \left(-\frac{u^2}{c_i^3} + \frac{u^4}{3c_i^5} \right) \\ &= \frac{Z\alpha}{3\pi} \sum_{i=0}^2 C_i \ln m_i^2. \end{aligned} \quad (82)$$

These results are in agreement, although the evolution of the logarithmic terms is quite different.

It is worth pointing out that if the (incorrect) variable change $u \rightarrow m_i u$ were made in each term in the sum over i in Eq. (82), the mass dependence would drop out and the sum would vanish. This illustrates the fact that the order of

summation and integration is crucial and particular care is needed in dealing with such potentially divergent expressions.

VI. CONCLUSION

Vacuum polarization for a spherically symmetric potential is examined in coordinate space in this work. For the contribution of first order in the expansion in powers of the potential, a counterterm is introduced to remove the equal coordinate singularity, which could be problematic for a purely numerical calculation. Although this singularity is removed in principle by Pauli-Villars regularization, in practice, the subtraction can be expected to improve the numerical convergence by providing a pointwise removal of the singularity before numerical integrations are carried out. Moreover, this approach can be expected to be useful for more general calculations.

The coordinate-space calculation is compared to the momentum-space calculation. With Pauli-Villars regularization, the logarithmic charge renormalization term is seen to be the same in either case, despite the fact that it arises in a completely different way in the two approaches. As with the coordinate-space calculation, the momentum-space calculation is explicitly based on the use of two Pauli-Villars auxiliary mass subtraction terms, and it can be seen that the result is not well defined unless both terms are included.

APPENDIX A: VECTOR VACUUM POLARIZATION

For a spherically symmetric binding potential, the vector contribution to the vacuum polarization, in the last line of Eq. (9), is finite and vanishes when Pauli-Villars regularization is applied. The fact that it formally vanishes follows from the spin-angular momentum expansion of the Green function for a spherically symmetric potential. In particular, in this case the wave function can be written in terms of the Dirac spin-angle functions χ as (see, for example, [26] and references therein)

$$\phi_n(\mathbf{x}) = \begin{bmatrix} f_1(x) \chi_\kappa^\mu(\hat{\mathbf{x}}) \\ f_2(x) \chi_{-\kappa}^\mu(\hat{\mathbf{x}}) \end{bmatrix} \quad (A1)$$

and the Green function is given by

$$G(\mathbf{x}_2, \mathbf{x}_1, z) = \sum_{\kappa\mu} \begin{bmatrix} G_\kappa^{11}(x_2, x_1, z) \chi_\kappa^\mu(\hat{\mathbf{x}}_2) \chi_\kappa^{\mu\dagger}(\hat{\mathbf{x}}_1) & -i G_\kappa^{12}(x_2, x_1, z) \chi_\kappa^\mu(\hat{\mathbf{x}}_2) \chi_{-\kappa}^{\mu\dagger}(\hat{\mathbf{x}}_1) \\ i G_\kappa^{21}(x_2, x_1, z) \chi_{-\kappa}^\mu(\hat{\mathbf{x}}_2) \chi_\kappa^{\mu\dagger}(\hat{\mathbf{x}}_1) & G_\kappa^{22}(x_2, x_1, z) \chi_{-\kappa}^\mu(\hat{\mathbf{x}}_2) \chi_{-\kappa}^{\mu\dagger}(\hat{\mathbf{x}}_1) \end{bmatrix}, \quad (A2)$$

where

$$G_\kappa^{ij}(x_2, x_1, z) = \sum_n \frac{f_i(x_2) f_j(x_1)}{E_n - z} \quad (A3)$$

and

$$\sum_\mu \chi_\kappa^\mu(\hat{\mathbf{x}}_2) \chi_\kappa^{\mu\dagger}(\hat{\mathbf{x}}_1) = \frac{|\kappa|}{4\pi} \left[I P_{\kappa+}(\xi) + \frac{i}{\kappa} \boldsymbol{\sigma} \cdot (\hat{\mathbf{x}}_2 \times \hat{\mathbf{x}}_1) P'_{\kappa+}(\xi) \right], \quad (A4)$$

$$\sum_\mu \chi_{-\kappa}^\mu(\hat{\mathbf{x}}_2) \chi_\kappa^{\mu\dagger}(\hat{\mathbf{x}}_1) = \frac{1}{4\pi} \frac{\kappa}{|\kappa|} \{ \boldsymbol{\sigma} \cdot \hat{\mathbf{x}}_2 P'_{\kappa-}(\xi) - \boldsymbol{\sigma} \cdot \hat{\mathbf{x}}_1 P'_{\kappa+}(\xi) \}, \quad (A5)$$

with $\xi = \hat{\mathbf{x}}_2 \cdot \hat{\mathbf{x}}_1$ and $\kappa_{\pm} = |\kappa \pm 1/2| - 1/2$. The vector trace in Eq. (9) is

$$\begin{aligned} & \text{Tr}[\alpha G(\mathbf{x}_2, \mathbf{x}_1, z)] \\ &= \frac{i}{2\pi} \sum_{\kappa} \frac{\kappa}{|\kappa|} \{G_{\kappa}^{21}(\mathbf{x}_2, \mathbf{x}_1, z)[\hat{\mathbf{x}}_2 P'_{\kappa_-}(\xi) - \hat{\mathbf{x}}_1 P'_{\kappa_+}(\xi)] \\ & \quad + G_{\kappa}^{12}(\mathbf{x}_2, \mathbf{x}_1, z)[\hat{\mathbf{x}}_2 P'_{\kappa_+}(\xi) - \hat{\mathbf{x}}_1 P'_{\kappa_-}(\xi)]\}. \end{aligned} \quad (\text{A6})$$

The equal coordinate limit is ambiguous due to the discontinuity in the radial factor at $x_2 = x_1$, but the angular factors are just

$$[\hat{\mathbf{x}}_2 P'_{\kappa_{\pm}}(\xi) - \hat{\mathbf{x}}_1 P'_{\kappa_{\mp}}(\xi)]_{\hat{\mathbf{x}}_1 = \hat{\mathbf{x}}_2} = \pm \kappa \hat{\mathbf{x}}_2, \quad (\text{A7})$$

and integration of the level-shift expression in Eq. (9) includes

$$\int d\Omega_2 \frac{\hat{\mathbf{x}}_2}{|\mathbf{x}_2 - \mathbf{x}_1|} = \frac{4\pi}{3} \hat{\mathbf{x}}_1 \frac{x_{<}}{x_{>}^2}, \quad (\text{A8})$$

so the vector term is proportional to

$$\phi_n^{\dagger}(\mathbf{x}_1) \alpha \cdot \hat{\mathbf{x}}_1 \phi_n(\mathbf{x}_1) = 0. \quad (\text{A9})$$

Although the vector term vanishes as shown above, the integrals giving the level shift from the first few terms in the expansion of the Green function in powers of the potential are not convergent. However, these terms are well defined when Pauli-Villars regularization is applied. The analysis is similar to that employed in evaluating the nonvanishing terms of the vacuum polarization and is not repeated in this case.

APPENDIX B: ONE-POTENTIAL GREEN FUNCTION

From Eqs. (16) and (29), we have

$$\begin{aligned} \text{Tr}[G^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z)] &= -\frac{1}{4\pi^2} [\nabla_2 \cdot \nabla_1 + m^2 + z^2] \\ & \quad \times \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} V(\mathbf{w}) \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|}. \end{aligned} \quad (\text{B1})$$

Since $2\nabla_2 \cdot \nabla_1 = (\nabla_2 + \nabla_1)^2 - \nabla_2^2 - \nabla_1^2$, Eq. (30) follows from

$$\begin{aligned} & (\nabla_2 + \nabla_1)^2 \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} V(\mathbf{w}) \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|} \\ &= \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} [\nabla_w^2 V(\mathbf{w})] \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|} \end{aligned} \quad (\text{B2})$$

together with

$$\nabla_w^2 V(\mathbf{w}) = 4\pi Z\alpha \rho(\mathbf{w}) \quad (\text{B3})$$

and

$$(\nabla_i^2 - c^2) \frac{e^{-c|\mathbf{x}_i - \mathbf{w}|}}{|\mathbf{x}_i - \mathbf{w}|} = -4\pi \delta(\mathbf{x}_i - \mathbf{w}). \quad (\text{B4})$$

For the counterterm in Eq. (31), we have

$$\begin{aligned} & \text{Tr}[G_A^{(1)}(\mathbf{x}_2, \mathbf{x}_1, z)] \\ &= -\frac{1}{4\pi^2} \left\{ [\nabla_2 \cdot \nabla_1 + m^2 + z^2] \right. \\ & \quad \left. \times \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|} \right\} \frac{V(\mathbf{x}_2) + V(\mathbf{x}_1)}{2} \end{aligned} \quad (\text{B5})$$

and Eq. (32) follows from

$$\begin{aligned} & \nabla_2 \cdot \nabla_1 \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|} \\ &= \frac{2\pi}{c} \nabla_2 \cdot \nabla_1 e^{-c|\mathbf{x}_2 - \mathbf{x}_1|} \\ &= \frac{2\pi}{c} \left(\frac{2c}{|\mathbf{x}_2 - \mathbf{x}_1|} - c^2 \right) e^{-c|\mathbf{x}_2 - \mathbf{x}_1|} \\ &= \frac{4\pi}{|\mathbf{x}_2 - \mathbf{x}_1|} e^{-c|\mathbf{x}_2 - \mathbf{x}_1|} + (z^2 - m^2) \\ & \quad \times \int d\mathbf{w} \frac{e^{-c|\mathbf{x}_2 - \mathbf{w}|}}{|\mathbf{x}_2 - \mathbf{w}|} \frac{e^{-c|\mathbf{w} - \mathbf{x}_1|}}{|\mathbf{w} - \mathbf{x}_1|}. \end{aligned} \quad (\text{B6})$$

APPENDIX C: MOMENTUM-SPACE INTEGRATION

Here we give some details of the evaluation of the function

$$\begin{aligned} I^{\mu\nu}(k) &= \int d^4 p \sum_{i=0}^2 C_i \\ & \quad \times \text{Tr} \left[\gamma^{\mu} \frac{1}{\gamma \cdot (k + p) - m_i} \gamma^{\nu} \frac{1}{\gamma \cdot p - m_i} \right] \end{aligned} \quad (\text{C1})$$

that appears in Sec. V. Rationalization of the propagation functions and application of the Feynman denominator formula

$$\frac{1}{AB} = \int_0^1 dy \frac{1}{[Ay + B(1-y)]^2} \quad (\text{C2})$$

yields

$$\begin{aligned} I^{\mu\nu}(k) &= \int d^4 p \sum_{i=0}^2 C_i \int_0^1 dy \\ & \quad \times \frac{\text{Tr}[\gamma^{\mu}(\gamma \cdot p + \gamma \cdot k + m_i)\gamma^{\nu}(\gamma \cdot p + m_i)]}{[(p + ky)^2 + k^2 y(1-y) - m_i^2 + i\epsilon]^2}, \end{aligned} \quad (\text{C3})$$

where $\epsilon = 2\delta p^{02}$ and $\delta^2 p^{02}$ is dropped. After the translation $p \rightarrow p - ky$, the numerator is

$$\begin{aligned} & \text{Tr}\{\gamma^{\mu}[\gamma \cdot p + \gamma \cdot k(1-y) + m_i]\gamma^{\nu}(\gamma \cdot p - \gamma \cdot ky + m_i)\} \\ & \quad \rightarrow 8(g^{\mu\nu}k^2 - k^{\mu}k^{\nu})y(1-y) - 4g^{\mu\nu} \\ & \quad \times [p^2 + k^2 y(1-y) - m_i^2] + 8p^{\mu}p^{\nu}, \end{aligned} \quad (\text{C4})$$

where terms odd in p are not included, and the denominator is

$$\begin{aligned} & p^2 + k^2 y(1-y) - m_i^2 + i\epsilon \\ &= p^{02} - \mathbf{p}^2 - \mathbf{k}^2 y(1-y) - m_i^2 + i\epsilon. \end{aligned} \quad (\text{C5})$$

Poles of the integrand are located at

$$p^0 = \pm [p^2 + \mathbf{k}^2 y(1-y) + m_i^2 - i\epsilon]^{1/2} \quad (\text{C6})$$

in the second and fourth quadrants of the complex p^0 plane, so the contour of the p^0 integration may be rotated to the imaginary axis, and p may be replaced by a Cartesian vector q , where $p^0 = iq_0$ and $p^i = q_i$ for $i = 1, 2, 3$. The integrals over the four-vector p are thus expressed as integrals over

$r = (q_0^2 + q_1^2 + q_2^2 + q_3^2)^{1/2}$, the magnitude of the Cartesian four-vector q , where

$$\int d^4 p f(p^2) = 2\pi^2 i \int_0^\infty dr r^3 f(-r^2), \quad (\text{C7})$$

$$\int d^4 p p^\mu p^\nu f(p^2) = -\frac{\pi^2 i}{2} \int_0^\infty dr r^5 g^{\mu\nu} f(-r^2). \quad (\text{C8})$$

We thus have

$$\begin{aligned} I^{\mu\nu}(k) &= 16\pi^2 i \int_0^\infty dr r^3 \sum_{i=0}^2 C_i \\ &\times \int_0^1 dy \frac{(g^{\mu\nu} k^2 - k^\mu k^\nu) y(1-y)}{[r^2 + \mathbf{k}^2 y(1-y) + m_i^2]^2} \\ &+ 2\pi^2 i \int_0^\infty dr \frac{d}{dr} r^4 \sum_{i=0}^2 C_i \\ &\times \int_0^1 dy \frac{g^{\mu\nu}}{r^2 + \mathbf{k}^2 y(1-y) + m_i^2}. \quad (\text{C9}) \end{aligned}$$

It is evident that the second term vanishes with Pauli-Villars regularization from the identity

$$\sum_{i=0}^2 \frac{C_i}{R^2 + m_i^2} = \frac{C_0 m_1^2 m_2^2 + C_1 m_0^2 m_2^2 + C_2 m_0^2 m_1^2}{(R^2 + m_0^2)(R^2 + m_1^2)(R^2 + m_2^2)}, \quad (\text{C10})$$

where $R^2 = r^2 + \mathbf{k}^2 y(1-y)$. Note that in the numerator on the right-hand side of Eq. (C10), a possible term proportional to R^4 has the vanishing coefficient $\sum_{i=0}^2 C_i$ and a possible term proportional to R^2 has the coefficient

$$\begin{aligned} &C_0(m_1^2 + m_2^2) + C_1(m_0^2 + m_2^2) + C_2(m_0^2 + m_1^2) \\ &= C_0(m_1^2 + m_2^2) + C_1(m_0^2 + m_2^2) + C_2(m_0^2 + m_1^2) \\ &+ \sum_{i=0}^2 C_i m_i^2 = \left(\sum_{i=0}^2 C_i \right) \left(\sum_{j=0}^2 m_j^2 \right), \quad (\text{C11}) \end{aligned}$$

which also vanishes.

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