Radiative $\alpha^7 m$ QED contribution to the helium Lamb shift

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We present a derivation of the last unknown part of the $\alpha^7 m$ contribution to the Lamb shift of a two-electron atom, induced by the radiative QED effects beyond the Bethe logarithm. This derivation is performed in the framework of nonrelativistic quantum electrodynamics and is valid for the triplet (spin $S = 1$) atomic states. The obtained formulas are free from any divergences and are suitable for a numerical evaluation. This opens a way for a complete numerical calculation of the $\alpha^7 m$ QED effects in helium, which will allow an accurate determination of the nuclear charge radius from measurements of helium transition frequencies.

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I. INTRODUCTION

The helium atom has been extensively studied since the very advent of quantum mechanics as the prototypical three-body problem and an ideal testing ground for various theoretical approaches describing many-electron atoms. Modern theoretical calculations of helium spectra [1] approach the level of accuracy previously achievable only for the simplest case of the hydrogen atom, with a potential for discovery of new effects beyond the standard model. Among the major topics of current interest in the helium atom are possibilities to obtain an "atomic physics" value for the fine structure constant $\alpha = e^2/(4\pi\epsilon_0\hbar c)$ [2,3] and to provide another method for the determination of the nuclear charge radius [4,5].

Up to now, theoretical calculations of the helium Lamb shift allowed accurate determinations only for the *differences* of the nuclear charge radii of two isotopes [6]. In order to determine the *absolute* value of the nuclear radius with a precision comparable to what is expected from muonic helium [7], one needs to perform a complete calculation of the $\alpha^7 m$ QED effects, which is a very challenging task.

The $\alpha^7 m$ QED effects were first calculated for hydrogen in Refs. [8–10] and recently generalized for the two-center hydrogenic problem [11]. For helium, the $\alpha^7 m$ QED effects were investigated in the context of the fine-structure splitting [2,12,13], which offered extensive simplifications to the underlying theory.

Several years ago, we started a project of calculating the $\alpha^7 m$ QED effects in the Lamb shift of helium. The first aim of the project is the triplet (spin $S = 1$) states, whose theory is simplified by the absence of the so-called contact operators $\propto \delta(\vec{r}_1 - \vec{r}_2)$. Intermediate results were published in Refs. [14,15]. In the present work, we complete the derivation of the $\alpha^7 m$ contribution, presenting formulas for the last missing part. More specifically, the $\alpha^7 m$ contribution to the Lamb shift are represented as a sum of three parts,

$$E^{(7)} = E^{(7)}_L + E^{(7)}_{\rm exch} + E^{(7)}_{\rm rad}\,, \tag{1}$$

where $E^{(7)}_L$ is the relativistic correction to the so-called Bethe logarithm, $E^{(7)}_{\rm exch}$ is the part induced by the electron-electron and electron-nucleus photon exchange, and $E^{(7)}_{\rm rad}$ is induced by the radiative QED effects beyond the Bethe logarithm. The relativistic correction to the Bethe logarithm was calculated in Ref. [14], whereas the photon-exchange contribution was derived by us in Ref. [15]. The goal of the present investigation is to perform a derivation of the last missing part in Eq. (1), thus obtaining the total set of formulas for the $\alpha^7 m$ contribution for the triplet states of a two-electron atom. The numerical evaluation of the obtained formulas is left for the forthcoming investigation.

II. BASIC APPROACH

The radiative $\alpha^7\, m$ contribution to the Lamb shift is represented by a sum of the first-order and the second-order perturbation corrections,

$$E^{(7)}_{\rm rad} = \big\langle H^{(7)}_{\rm rad}\big\rangle + 2\left\langle H^{(4)}\,\frac{1}{(E_0 - H_0)'}\,H^{(5)}_{\rm rad}\right\rangle. \tag{2}$$

Here, $H^{(7)}_{\rm rad}$ and $H^{(5)}_{\rm rad}$ are the effective Hamiltonians induced by the radiative effects of order $\alpha^7 m$ and $\alpha^5 m$, respectively, $H^{(4)}$ is the Breit Hamiltonian (of order $\alpha^4 m$), and H_0 and E_0 are the nonrelativistic Hamiltonian and the corresponding eigenvalue, respectively.

$E^{(7)}_{\rm rad}$ consists of contributions coming from the one-loop self-energy (SE), the one-loop vacuum polarization (VP), and the two-loop (rad2) and three-loop QED effects (rad3),

$$E^{(7)}_{\rm rad} = E^{(7)}_{\rm SE} + E^{(7)}_{\rm VP} + E^{(7)}_{\rm rad2} + E^{(7)}_{\rm rad3}. \tag{3}$$

The main part of the present investigation will be devoted to the evaluation of the one-loop self-energy correction, which is by far the most difficult part. The corresponding derivation is presented in Secs. III–VII. The one-loop vacuum polarization is calculated in Sec. VIII, whereas the two- and three-loop radiative effects are obtained in Sec. IX.

One of the major problems encountered in deriving formulas for higher order QED effects is connected with numerous divergences appearing on intermediate stages of the calculation. In order to systematically handle these divergences, we use dimensionally regularized nonrelativistic quantum electrodynamics (NRQED), with the dimension of the space-time $D = 4 - 2\epsilon$ and the dimension of space $d = 3 - 2\epsilon$. The parameter ϵ is considered as small, but only on the level of matrix elements, where the analytic continuation to a noninteger spatial dimension is allowed. The final results will be expanded in small ϵ, and singular contributions $\propto 1/\epsilon$ will be canceled algebraically in momentum space. Subsequently, the results will be transformed into the coordinate representation, where they can be calculated numerically. The foundation of the dimensionally regularized NRQED in the context of the hydrogen Lamb shift was laid in Ref. [16], but our approach differs in many details.

In our derivation of the radiative $\alpha^7 m$ correction for helium, we will rely on the fact that the corresponding correction is known for hydrogen-like atoms (see, e.g., a review [17]). With this in mind, in our derivation we will repeatedly drop the first-order terms containing purely the electron-nucleus Dirac δ function. (We still have to keep terms in which the electron-nucleus δ function is combined with the potential, energy, or momenta, however.) This procedure will simplify the derivation enormously and the omitted δ-like terms will be later restored by matching the known hydrogenic results. Our calculation will be performed in the Coulomb gauge, unless explicitly specified otherwise.

When working in the dimensionally regularized NRQED, we need generalizations of basic operators into the extended number of dimensions, shortly summarized below. The momentum-space representation of the photon propagator preserves its form in d dimensions, namely, $g_{\mu\nu}/k^2$. The surface area of a d-dimensional unit sphere is

$$\Omega_d = \frac{2\,\pi^{d/2}}{\Gamma(d/2)}\,. \tag{4}$$

The electron-nucleus Coulomb interaction becomes

$$\begin{aligned} V_C(r) &= -Z\,e^2 \int \frac{d^d k}{(2\,\pi)^d}\,\frac{e^{i\,\vec{k}\cdot\vec{r}}}{k^2} \\ &= -\frac{Z\,e^2}{4\,\pi\,r^{1-2\,\epsilon}}\left[(4\,\pi)^\epsilon\,\frac{\Gamma(1-2\,\epsilon)}{\Gamma(1-\epsilon)}\right] \equiv -\left[\frac{Z\alpha}{r}\right]_\epsilon. \end{aligned} \tag{5}$$

Here and in what follows, $[X]_\epsilon$ will denote the d-dimensional generalization of the $d = 3$ operator X. The d-dimensional nonrelativistic Hamiltonian of a two-electron atom is given by

$$H_0 = \sum_{a=1,2} \frac{\vec{p}_a^{\,2}}{2\,m} + V\,, \tag{6}$$

where

$$V = -\left[\frac{Z\,\alpha}{r_1}\right]_\epsilon - \left[\frac{Z\,\alpha}{r_2}\right]_\epsilon + \left[\frac{\alpha}{r}\right]_\epsilon \tag{7}$$

and $\vec{r} = \vec{r}_1 - \vec{r}_2$. The d-dimensional generalization of the Breit Hamiltonian for a two-electron atom is

$$H^{(4)} = H'^{(4)} + H''^{(4)}\,, \tag{8}$$

$$\begin{aligned} H'^{(4)} = &-\frac{\pi\,\alpha}{m^2}\,\delta^d(r) + \sum_{a=1,2}\left\{-\frac{p_a^4}{8\,m^3} + \frac{\pi\,Z\alpha}{2\,m^2}\,\delta^d(r_a)\right\} \\ &- \frac{\alpha}{2\,m^2}\,p_1^i\left[\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right]_\epsilon p_2^j - \frac{\pi\,\alpha}{d\,m^2}\,\sigma_1^{ij}\,\sigma_2^{ij}\,\delta^d(r)\,, \end{aligned} \tag{9}$$

$$\begin{aligned} H''^{(4)} = &\sum_{a=1,2} \frac{1}{4\,m^2}\,\sigma_a^{ij}\,(\nabla_a^i V)p_a^j \\ &+ \frac{1}{4\,m^2}\,\sigma_1^{ik}\,\sigma_2^{jk}\left(\nabla^i\,\nabla^j - \frac{\delta^{ij}}{d}\,\nabla^2\right)\left[\frac{\alpha}{r}\right]_\epsilon \\ &- \frac{1}{2\,m^2}\left(\sigma_1^{ij}\,\nabla^i\left[\frac{\alpha}{r}\right]_\epsilon p_2^j - \sigma_2^{ij}\,\nabla^i\left[\frac{\alpha}{r}\right]_\epsilon p_1^j\right), \end{aligned} \tag{10}$$

where $\delta^d(r)$ is the Dirac δ function in d dimensions, $\sigma^{ij} = 1/(2i)[\sigma^i, \sigma^j]$, and σ^i are the Pauli matrices. In $d = 3$ spatial dimensions, the matrices σ^{ij} reduce to $\sigma^{ij} = \epsilon^{ijk}\,\sigma^k$. The d-dimensional generalization of the algebra of the Pauli matrices is summarized in Appendix B of Ref. [15].

III. NRQED Hamiltonian

We now turn to the derivation of the NRQED Hamiltonian incorporating relativistic corrections and a class of radiative corrections that comes from the high photon momentum, in d dimensions. This Hamiltonian can be obtained from the Dirac Hamiltonian by means of the Foldy-Wouthuysen transformation. In order to incorporate a high-energy part of the radiative corrections, we start with the Dirac Hamiltonian modified by the electromagnetic form factors F_1 and F_2,

$$\begin{aligned} H_D = &\,\vec{\alpha}\cdot[\vec{p} - e\,F_1(\vec{\nabla}^2)\vec{A}] + \beta\,m + e\,F_1(\vec{\nabla}^2)\,A_0 \\ &+ F_2(\vec{\nabla}^2)\,\frac{e}{2\,m}\left(i\,\vec{\gamma}\cdot\vec{E} - \frac{\beta}{2}\,\Sigma^{ij}\,B^{ij}\right), \end{aligned} \tag{11}$$

where $B^{ij} = \nabla^i A^j - \nabla^j A^i$, $\nabla^i \equiv \nabla_i = \partial/\partial x^i$, and $\Sigma^{ij} = \frac{i}{2}\,[\gamma^i, \gamma^j]$. Formulas for the electromagnetic form factors F_1 and F_2 are summarized in Appendix A. Introducing the Foldy-Wouthuysen transformation defined by the operator S,

$$\begin{aligned} S = &-\frac{i}{2\,m}\left\{\beta\,\vec{\alpha}\cdot\vec{\pi} - \frac{1}{3\,m^2}\,\beta\,(\vec{\alpha}\cdot\vec{\pi})^3\right. \\ &\left.+\frac{e(1+\kappa)}{2\,m}\,i\,\vec{\alpha}\cdot\vec{E} - \frac{e\,\kappa}{8\,m^2}\,[\vec{\alpha}\cdot\vec{\pi}, \beta\,\Sigma^{ij}\,B^{ij}]\right\}, \end{aligned} \tag{12}$$

where $\kappa \equiv F_2(0) \approx \alpha/(2\,\pi)$ is the electron anomalous magnetic moment, the transformed Hamiltonian is obtained as

$$H_{FW} = e^{i\,S}\,(H_D - i\,\partial_t)\,e^{-i\,S}\,. \tag{13}$$

We will split the transformed Hamiltonian into two parts, δH_1 and δH_2, $H_{FW} = \delta H_1 + \delta H_2$, where δH_1 contains the form factors only in the form of the anomalous magnetic moment κ, and δH_2 is the remainder. The result is

$$\delta H_1 = \frac{\vec{\pi}^2}{2m} + eA^0 - \frac{e}{4m}(1+\kappa)\sigma^{ij}B^{ij} - \frac{\vec{\pi}^4}{8m^3} - \frac{e}{8m^2}(1+2\kappa)[\vec{\nabla}\cdot\vec{E} + \sigma^{ij}\{E^i,\pi^j\}]$$
$$+ \frac{e}{16m^3}\Big[\Big(1+\frac{\kappa}{2}\Big)\{p^2, \sigma^{ij}B^{ij}\} + 4\kappa\, p^k\sigma^{ki}B^{ij}p^j + \kappa\,\vec{p}\,\sigma\cdot B\,\vec{p}\Big] + \frac{\vec{p}^6}{16m^5} + \frac{(\kappa^2+\kappa+1)}{8m^3}e^2\vec{E}^2$$
$$+ \frac{3+4\kappa}{64m^4}e\{\vec{p}^2, \vec{\nabla}\cdot\vec{E} + \sigma^{ij}\{E^i,p^j\}\} + \frac{5ie}{128m^4}[p^2,\{\vec{p},\vec{E}\}] - \frac{e\kappa}{16m^3}\{\pi^k, \partial_t E^k + \nabla^i B^{ik}\} + \ldots, \quad (14)$$

$$\delta H_2 = e\Big[F_1'(0)\Delta + \frac{1}{2}F_1''(0)\Delta^2\Big]A^0 - \frac{e}{m}\Big(F_1'(0)\vec{p}\cdot\Delta\vec{A} + \frac{1}{4}[F_1'(0)+F_2'(0)]\sigma^{ij}\Delta B^{ij}\Big)$$
$$- \frac{e}{8m^4}[F_1'(0) + 2F_2'(0)]\Delta\vec{\nabla}\cdot\vec{E} + \cdots, \quad (15)$$

where $\Delta = \vec{\nabla}^2$, $\{X, Y\} \equiv XY + YX$, and $\vec{\pi} = \vec{p} - e\vec{A}$. The ellipsis denotes higher order terms and spin-dependent terms that do not contribute to the centroid energies.

It should be noted that the neglect of $\partial/\partial x^0$ within the F_1 and F_2 form factors is not valid for the electron-electron interactions. In this case, we will calculate effective operators from the one-photon exchange scattering amplitude in the Feynman gauge. Moreover, there is an additional radiative correction to the NRQED Hamiltonian that is not accounted for by the F_1 and F_2 form factors. It is represented by an effective local operator quadratic in the field strengths. This operator is derived separately by evaluating a low-energy limit of the electron scattering amplitude off the Coulomb field. It was calculated in Ref. [18] to be

$$\delta H_3 = \frac{e^2}{m^3}\vec{E}^2\chi, \quad (16)$$

where E is an electric field, and the function χ is given by

$$\chi = \frac{\alpha}{\pi}\Big(\frac{1}{6} - \frac{1}{3\epsilon}\Big), \quad (17)$$

where we included only the one-loop part. We follow throughout this work the convention of Ref. [18], that a common factor of $[(4\pi)^\epsilon\,\Gamma(1+\epsilon)]$ for each loop integration is pulled out from all matrix elements.

We thus obtain the effective NRQED Hamiltonian as

$$H_{\rm nrqed} = \delta H_1 + \delta H_2 + \delta H_3. \quad (18)$$

Individual operators from $H_{\rm nrqed}$ induce numerous contributions to the one-loop electron self-energy, evaluated term by term in Sec. VI C.

IV. EFFECTIVE $\alpha^5 m$ HAMILTONIAN

We now derive the self-energy part of the effective $\alpha^5 m$ operator $H^{(5)}_{\rm rad}$, which is required for evaluation of the second-order contribution in Eq. (2). Despite the fact that the $\alpha^5 m$ correction is well-known in principle [19,20], we here need a d-dimensional generalization of the corresponding effective operator. From now on, we will make the simplification of setting the electron mass equal to one, $m = 1$.

The leading-order self-energy correction $E^{(5)}_{\rm SE}$ can be written as a sum of low-energy and high-energy contributions,

$$E^{(5)}_{\rm SE} = E_{L0} + E_{H0}. \quad (19)$$

The low-energy part comes from the radiative photon momenta of the order $k \propto \alpha^2 m$. It is represented by the one-loop self-energy contribution in the leading nonrelativistic-dipole approximation,

$$E_{L0} = e^2\int\frac{d^dk}{(2\pi)^d 2k}\,\delta^{ij}_\perp(k)$$
$$\times\langle\phi|p_1^i\,\frac{1}{E_0 - H_0 - k}\,p_1^j|\phi\rangle + (1\leftrightarrow 2), \quad (20)$$

where $\delta^{ij}_\perp(k) = \delta^{ij} - k^ik^j/k^2$. The integration over $|k|$ is split into two parts, $\int_0^\infty = \int_0^\Lambda + \int_\Lambda^\infty$, leading to the separation

$$E_{L0} = E_L^{(5)} + E^\Lambda_{L0}, \quad (21)$$

where the first term $E_L^{(5)}$ is the electron self-energy part of the Bethe logarithm in three dimensions,

$$E_L^{(5)} = \frac{2e^2}{3}\int_0^\Lambda\frac{d^3k}{(2\pi)^3 2k}\,\langle\phi|p_1^i\,\frac{1}{E_0 - H_0 - k}\,p_1^i|\phi\rangle$$
$$+(1\leftrightarrow 2), \quad (22)$$

while the second term is the remainder to be calculated in d dimensions. It is assumed that

$$\Lambda = \alpha^2\lambda, \quad (23)$$

with arbitrary large λ. Namely, it is assumed that the limit $\epsilon \to 0$ is performed as the first and $\lambda \to \infty$ as the second one. So, we obtain

$$E_L^{(5)} = -\frac{2\alpha}{3\pi}\langle\phi|p_1^i\,(H_0 - E_0)\ln\Big[\frac{(H_0 - E_0)}{\alpha^2}\Big]p_1^i|\phi\rangle$$
$$+\frac{\alpha\ln\lambda}{3\pi}\nabla_1^2 V + (1\leftrightarrow 2). \quad (24)$$

Here, the second term depends on λ, but it will cancel out in the sum in Eq. (21). The remainder E^Λ_{L0} is evaluated as

$$E^\Lambda_{L0} = e^2\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d 2k}\,\delta^{ij}_\perp(k)$$
$$\times\langle\phi|p_1^i\,\frac{1}{E_0 - H_0 - k}\,p_1^j|\phi\rangle + (1\leftrightarrow 2)$$
$$= \frac{e^2}{4}\frac{d-1}{d}\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d k^3}$$
$$\times\langle\phi|\big[p_1^i, \big[H_0 - E_0, p_1^i\big]\big]|\phi\rangle + (1\leftrightarrow 2). \quad (25)$$

Performing the integration with respect to k we obtain

$$E_{L0}^{\Lambda} = \frac{\alpha}{\pi}\mathcal{I}_\epsilon\left(\nabla_1^2 V + \nabla_2^2 V\right), \tag{26}$$

where

$$\mathcal{I}_\epsilon = \pi^2\frac{d-1}{d}\int_\Lambda^\infty \frac{d^d k}{(2\pi)^d k^3} = -\frac{2^{-d}(d-1)\pi^{2-\frac{d}{2}}[\alpha^2\lambda]^{d-3}}{(d-3)\Gamma\left(\frac{d}{2}+1\right)} = \frac{5}{18} + \frac{1}{6}\ln\Lambda_\epsilon + O(\epsilon) \tag{27}$$

and

$$\ln\Lambda_\epsilon = \frac{1}{\epsilon} + 2\ln(\alpha^{-2}) - 2\ln(2\lambda). \tag{28}$$

The high-energy contribution, E_{H0} in Eq. (19), is induced by the region where the momentum of the radiative photon is of the order of the electron mass $k \propto m$. E_{H0} is conveniently split into two parts,

$$E_{H0} = E_{H0}^A + E_{H0}^B. \tag{29}$$

The first part comes from the exchange of a transverse photon with one vertex $-\frac{e}{4}\kappa\,\sigma\cdot B$. It is calculated in the nonretardation approximation, with the result

$$\begin{aligned} E_{H0}^A = &-e^2\kappa\int\frac{d^d k}{(2\pi)^d\,2k^2}\delta_\perp^{ij}(k)\langle\phi|\left(p_1^i + \frac{1}{2}\sigma_1^{ki}\nabla_1^k\right)e^{i\vec{k}\cdot\vec{r}_1}\left(\frac{1}{2}\sigma_2^{lj}\nabla_2^l\right)e^{-i\vec{k}\cdot\vec{r}_2}|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2) \\ = &\,\alpha\kappa\left\langle\frac{1}{4}\sigma_1^{ik}\sigma_2^{jk}\left(\nabla^i\nabla^j - \frac{\delta^{ij}}{d}\nabla^2\right)\left[\frac{1}{r}\right]_\epsilon - \frac{\pi}{d}\sigma_1\cdot\sigma_2\,\delta^d(r) + \frac{1}{2}\sigma_2^{ij}\nabla_1^i\left[\frac{1}{r}\right]_\epsilon p_1^j\right\rangle + (1\leftrightarrow 2). \end{aligned} \tag{30}$$

The remaining high-energy contribution comes from the exchange of a Coulomb photon with the vertices eA^0 and $-\frac{e}{4}\kappa\vec{\nabla}\cdot\vec{E} - \frac{e}{4}\kappa\,\sigma^{ij}\{E^i, p^j\} + F_1'(0)\,\vec{\nabla}^2 eA^0$. The result is

$$E_{H0}^B = \left\langle\left[F_1'(0) + \frac{1}{4}\kappa\right]\nabla_1^2 V + \frac{1}{4}\kappa\,\sigma_1^{ij}\left\{\nabla_1^i V, p_1^j\right\}\right\rangle + (1\leftrightarrow 2). \tag{31}$$

Here $F_1'(0)$ contains the singular part $\propto 1/\epsilon$; see Appendix A. This singularity will cancel exactly with that in $\ln\Lambda_\epsilon$, so that the final result for $E_{\rm SE}^{(5)}$ is finite. We thus obtain

$$E_{\rm SE}^{(5)} = E_L^{(5)} + \left\langle H_{\rm SE}^{(5)}\right\rangle, \tag{32}$$

where the self-energy Hamiltonian $H_{\rm SE}^{(5)} = H_{\rm SE}^{\prime(5)} + H_{\rm SE}^{\prime\prime(5)}$ is given by

$$\begin{aligned} H_{\rm SE}^{\prime(5)} &= \frac{\alpha}{\pi}\left(\mathcal{I}_\epsilon - \frac{1}{6\epsilon}\right)\left(\nabla_1^2 V + \nabla_2^2 V\right) - \alpha\frac{2\pi\kappa}{d}\sigma_1\cdot\sigma_2\,\delta^d(r) \\ &\approx \frac{\alpha}{\pi}\left[\frac{5}{18} + \frac{1}{3}\ln(\alpha^{-2}) - \frac{1}{3}\ln(2\lambda)\right]\left(\nabla_1^2 V + \nabla_2^2 V\right) - \alpha\frac{2\pi\kappa}{3}\sigma_1\cdot\sigma_2\,\delta^d(r), \end{aligned} \tag{33}$$

$$H_{\rm SE}^{\prime\prime(5)} = \alpha\frac{\kappa}{2}\left\{\left[\vec{\sigma}_2\cdot\left(\vec{\nabla}_1\frac{1}{r}\right)\times\vec{p}_1 + \vec{\sigma}_1\cdot\vec{\nabla}_1 V\times\vec{p}_1 + (1\leftrightarrow 2)\right] - \sigma_1^i\sigma_2^j\left(\nabla^i\nabla^j - \frac{\delta^{ij}}{3}\nabla^2\right)\frac{1}{r}\right\}. \tag{34}$$

Here we used $d = 3$ for $H_{\rm SE}^{\prime\prime(5)}$ because the corresponding $\alpha^7 m$ second-order contribution will not contain any singularities. Note that the second line in Eq. (33) holds only for the $\alpha^5 m$ correction. For the $\alpha^7 m$ contribution coming from the second-order perturbation correction with $H_{\rm SE}^{(5)}$, we will have to keep $\mathcal{I}_\epsilon$ in the closed form because of a contribution from the linear in ϵ terms. We also note that both $E_L^{(5)}$ and $H_{\rm SE}^{(5)}$ are free of any divergencies but they depend on the cutoff parameter λ, which cancels out in their sum.

V. SECOND-ORDER $\alpha^7 m$ SELF-ENERGY CORRECTION

We now turn to the derivation of the second-order $\alpha^7 m$ self-energy contribution represented by the second term in Eq. (2),

$$E_{\rm sec,SE}^{(7)} = 2\left\langle H^{(4)}\frac{1}{(E_0 - H_0)'}H_{\rm SE}^{(5)}\right\rangle, \tag{35}$$

where $H^{(4)}$ is the Breit Hamiltonian and $H_{\rm SE}^{(5)}$ was derived in the previous section. It is convenient to split $E_{\rm sec,SE}^{(7)}$ into the spin-dependent and spin-independent parts,

$$\begin{aligned} E_{\rm sec,SE}^{(7)} = &\,2\left\langle H^{\prime(4)}\frac{1}{(E_0 - H_0)'}H_{\rm SE}^{\prime(5)}\right\rangle \\ &+ 2\left\langle H^{\prime\prime(4)}\frac{1}{(E_0 - H_0)'}H_{\rm SE}^{\prime\prime(5)}\right\rangle, \end{aligned} \tag{36}$$

where $H^{\prime(4)}$ and $H^{\prime\prime(4)}$ are given by Eqs. (9) and (10), respectively, and $H_{\rm SE}^{\prime(5)}$ and $H_{\rm SE}^{\prime\prime(5)}$ by Eqs. (33) and (34), respectively. The spin-dependent second-order contribution with $H_{\rm SE}^{\prime\prime(5)}$ is finite and can be calculated numerically as it stands. The contribution induced by $H_{\rm SE}^{\prime(5)}$, however, is divergent and needs to be regularized and transformed in order to move all $1/\epsilon$ singularities into the first-order terms where they can be canceled.

Omitting terms $\propto \delta^d(r)$ vanishing for triplet states, we rewrite the first part of the α^5 Hamiltonian as

$$H'^{(5)}_{\rm SE} = \frac{\alpha}{\pi}\left(\mathcal{I}_\epsilon - \frac{1}{6\epsilon}\right)[\vec{P},[V,\vec{P}]]\,, \tag{37}$$

where $\vec{P} = \vec{p}_1 + \vec{p}_2$ is the total momentum. The corresponding second-order contribution is thus of the form

$$\frac{2\alpha}{\pi}\left(\mathcal{I}_\epsilon - \frac{1}{6\epsilon}\right)\left\langle H'^{(4)}\,\frac{1}{(E_0-H_0)'}\,[\vec{P},[V,\vec{P}]]\right\rangle. \tag{38}$$

In order to identify divergencies in this second-order matrix element, we introduce the following identities

$$H'^{(4)} = \{H_0 - E_0, Q\} + H_R\,, \tag{39}$$

$$[P^i,[V,P^i]] = \{H_0 - E_0, Q'\} + H'_R\,, \tag{40}$$

where the operators H_R and H'_R are chosen in such a way that the second-order corrections with these operators are finite. We have

$$Q = -\frac{1}{4}\left[\frac{Z\alpha}{r_1} + \frac{Z\alpha}{r_2}\right]_\epsilon + \frac{\alpha}{2r}\,, \tag{41}$$

$$Q' = 2\left[\frac{Z\alpha}{r_1} + \frac{Z\alpha}{r_2}\right]_\epsilon\,, \tag{42}$$

and the regularized operators H_R and H'_R are defined by their action on ket states as

$$H_R|\phi\rangle = \bigg[-\frac{1}{2}(E_0-V)^2 - \frac{Z\alpha}{4}\frac{\vec{r}_1\cdot\vec{\nabla}_1}{r_1^3} - \frac{Z\alpha}{4}\frac{\vec{r}_2\cdot\vec{\nabla}_2}{r_2^3} + \frac{1}{4}\nabla_1^2\nabla_2^2 - p_1^i\frac{\alpha}{2r}\left(\delta^{ij} + \frac{r^ir^j}{r^2}\right)p_2^j\bigg]|\phi\rangle\,, \tag{43}$$

$$H'_R|\phi\rangle = -2Z\alpha\left(\frac{\vec{r}_1\cdot\vec{\nabla}_1}{r_1^3} + \frac{\vec{r}_2\cdot\vec{\nabla}_2}{r_2^3}\right)|\phi\rangle\,. \tag{44}$$

We now rewrite the second-order correction as

$$\left\langle[P^i,[V,P^i]]\frac{1}{(E_0-H_0)'}H'^{(4)}\right\rangle = \left\langle[P^i,[V,P^i]]\frac{1}{(E_0-H_0)'}H_R\right\rangle + \langle(\langle Q\rangle - Q)[P^i,[V,P^i]]\rangle \tag{45}$$

$$= \left\langle H'_R\frac{1}{(E_0-H_0)'}H_R\right\rangle + \langle H_R\,(\langle Q'\rangle - Q')\rangle + \langle(\langle Q\rangle - Q)\,[P^i,[V,P^i]]\rangle\,. \tag{46}$$

The first term in the last equation is finite. The third term is evaluated as

$$\langle(\langle Q\rangle - Q)\,[P^i,[V,P^i]]\rangle = \left\langle\left(\frac{E_0}{2} + \left\langle\frac{\alpha}{4r}\right\rangle + \frac{(Z-2)\alpha}{4r_2}\right)4\pi Z\alpha\,\delta^3(r_1) + (1\leftrightarrow 2)\right\rangle. \tag{47}$$

Here we used the identity $\delta^d(r)\,[1/r]_\epsilon = 0$, which is valid in dimensional regularization. The evaluation of the second term in Eq. (46) is more complicated. We rewrite it as

$$\langle H_R\,(\langle Q'\rangle - Q')\rangle = E^{(4)}\langle Q'\rangle - \left\langle\left(H'^{(4)} - \{H_0 - E_0, Q\}\right)Q'\right\rangle$$
$$= \left\langle E^{(4)}\left(\frac{2\alpha}{r} - 4E_0\right) + \frac{1}{2}[(\vec{\nabla}_1 Q)\cdot(\vec{\nabla}_1 Q') + (\vec{\nabla}_2 Q)\cdot(\vec{\nabla}_2 Q')] - H'^{(4)}\,Q'\right\rangle = X_1 + X_2 + X_3\,, \tag{48}$$

where $E^{(4)} = \langle H^{(4)}\rangle = \langle H_R\rangle$ since $\langle H''^{(4)}\rangle = 0$. Term X_1 needs no further simplification,

$$X_1 = \left\langle E^{(4)}\left(\frac{2\alpha}{r} - 4E_0\right)\right\rangle. \tag{49}$$

Term X_2 reduces to

$$X_2 = \frac{1}{2}[(\vec{\nabla}_1 Q)\cdot(\vec{\nabla}_1 Q') + (\vec{\nabla}_2 Q)\cdot(\vec{\nabla}_2 Q')] = -\frac{1}{4}\left[\frac{(Z\alpha)^2}{r_1^4} + \frac{(Z\alpha)^2}{r_2^4}\right]_\epsilon + \frac{1}{2}\left(\frac{Z\alpha\,\vec{r}_1}{r_1^3} - \frac{Z\alpha\,\vec{r}_2}{r_2^3}\right)\cdot\frac{\alpha\,\vec{r}}{r^3}\,, \tag{50}$$

where $[(Z\alpha)^2/r_1^4]_\epsilon = [\nabla(Z\alpha/r_1)]^2_\epsilon$. Term X_3 for triplet states is

$$X_3 = \langle -H'^{(4)}\,Q'\rangle = \left\langle\left[\frac{1}{8}(p_1^4 + p_2^4) - \frac{Z\pi\alpha}{2}[\delta^3(r_1) + \delta^3(r_2)] + \frac{\alpha}{2}p_1^i\left(\frac{\delta^{ij}}{r} + \frac{r^ir^j}{r^3}\right)p_2^j\right]Q'\right\rangle$$
$$= \left\langle\frac{1}{8}(p_1^4 + p_2^4)\,Q' - (Z\alpha)^2\pi\left[\frac{\delta^3(r_1)}{r_2} + \frac{\delta^3(r_2)}{r_1}\right] + p_1^i\left(\frac{Z\alpha}{r_1} + \frac{Z\alpha}{r_2}\right)\frac{\alpha}{r}\left(\delta^{ij} + \frac{r^ir^j}{q^2}\right)p_2^j\right\rangle. \tag{51}$$

The first term in the last equation contains singularities. We transform it as

$$\frac{1}{8}(p_1^4 + p_2^4)\,Q' = \frac{1}{8}[(p_1^2 + p_2^2)^2 - 2\,p_1^2\,p_2^2]\,Q' = \frac{1}{8}\left[(p_1^2 + p_2^2)\,Q'\,(p_1^2 + p_2^2) + \frac{1}{2}[p_1^2 + p_2^2,[p_1^2 + p_2^2, Q']] - 2\,p_1^2\,Q'\,p_2^2\right]$$
$$= \frac{1}{2}\left[2(E_0 - V)^2\left[\frac{Z\alpha}{r_1} + \frac{Z\alpha}{r_2}\right]_\epsilon + \left\{\left[\frac{(Z\alpha)^2}{r_1^4}\right]_\epsilon - \frac{Z\alpha\,\vec{r}_1}{r_1^3}\cdot\frac{\alpha\,\vec{r}}{r^3} + (1\leftrightarrow 2)\right\} - p_1^2\left(\frac{Z\alpha}{r_1} + \frac{Z\alpha}{r_2}\right)p_2^2\right]. \tag{52}$$

It is convenient to convert $[Z^3/r_a^3]_\epsilon$ into $[Z^2/r_a^4]_\epsilon$, which is achieved by the following identity,

$$\left\langle\left[\frac{(Z\alpha)^2}{r_1^4}\right]_\epsilon\right\rangle = \left\langle -2\left[\frac{Z\alpha}{r_1}\right]_\epsilon^3 - 2\,Y_1\right\rangle, \tag{53}$$

where

$$Y_1 = \left(E_0 + \frac{Z\alpha}{r_2} - \frac{\alpha}{r} - \frac{p_2^2}{2}\right)\frac{(Z\alpha)^2}{r_1^2} - \frac{1}{2}\,\vec{p}_1\,\frac{(Z\alpha)^2}{r_1^2}\,\vec{p}_1\,. \tag{54}$$

The final result for the second-order contribution is a sum $X_1 + X_2 + X_3$ and takes the form

$$\begin{aligned} E^{(7)}_{\rm sec,SE} = {}& 2\left\langle H''^{(4)}\,\frac{1}{(E_0-H_0)'}\,H''^{(5)}_{\rm SE}\right\rangle + \frac{\alpha}{\pi}\left[\frac{5}{9} + \frac{2}{3}\ln(\alpha^{-2}) - \frac{2}{3}\ln(2\lambda)\right]\Bigg(\left\langle H'_R\frac{1}{(E_0-H_0)'}H_R\right\rangle \\ & + \Bigg\langle E^{(4)}\left(\left\langle\frac{2\alpha}{r}\right\rangle - 4E_0\right) + \Bigg\{\left(2E_0 + \left\langle\frac{\alpha}{r}\right\rangle\right)\pi Z\alpha\,\delta^3(r_1) + \left(E_0 + \frac{Z\alpha}{r_2} - \frac{\alpha}{r}\right)^2\frac{Z\alpha}{r_1} + 2\left(E_0 + \frac{Z\alpha}{r_2} - \frac{\alpha}{r}\right)\frac{(Z\alpha)^2}{r_1^2} \\ & - Y_1 - \frac{1}{2}p_1^2\,\frac{Z\alpha}{r_1}\,p_2^2 - \frac{1}{4}\left[\frac{(Z\alpha)^2}{r_1^4}\right]_\epsilon - 2\pi Z\alpha^2\frac{\delta^3(r_1)}{r_2} + p_1^i\,\frac{Z\alpha}{r_1}\frac{\alpha}{r}\left(\delta^{ij} + \frac{r^i r^j}{r^2}\right)p_2^j + (1\leftrightarrow 2)\Bigg\}\Bigg\rangle\Bigg)\,. \end{aligned} \tag{55}$$

Note that the above expression is written completely in the coordinate representation. In the following derivation of other contributions, we will often find it convenient to keep the two-body electron-electron terms in the momentum representation. This is advantageous because in the momentum representation the evaluation of the electron-electron terms is simpler.

VI. EFFECTIVE $\alpha^7 m$ HAMILTONIAN

We now turn to the derivation of the first-order self-energy $\alpha^7 m$ contribution represented by the first term in Eq. (2). This correction can be conveniently split into three parts, according to the region of the contributing photon momenta,

$$\left\langle H^{(7)}_{\rm SE}\right\rangle = E_L^\Lambda + E_M + E_H\,. \tag{56}$$

Here, the three contributions E_L^Λ, E_M, and E_H are induced by momenta k of the radiative photon of the order $m\alpha^2$, $m\alpha$, and m, respectively. These three terms will be referred to as the low-energy, middle-energy, and high-energy parts, correspondingly.

A. Low-energy part

We now turn to the evaluation of relativistic corrections of order $\alpha^7 m$ to the leading-order one-loop nonrelativistic dipole self-energy contribution, E_{L0}, given by Eq. (20). Contributions arising from the small-k region, $k < \Lambda$, give rise to the relativistic corrections to the Bethe logarithm, already computed in Ref. [14]. So, in the present work we are only concerned with the large-k region, $k > \Lambda$.

The $\alpha^7 m$ corrections to E_{L0}^Λ arise as (i) perturbations of the reference-state wave function ϕ, the zeroth-order energy E_0, and the zeroth-order Hamiltonian H_0 by the Breit Hamiltonian $H^{(4)}$, (ii) a perturbation of the current $\vec{p} \to \delta\vec{j}$, and (iii) a retardation (quadrupole) correction. The corresponding $\alpha^7 m$ corrections will be denoted as E_{L1}, E_{L2}, and E_{L3}, respectively,

$$E_L^\Lambda = E_{L1}^\Lambda + E_{L2}^\Lambda + E_{L3}^\Lambda\,. \tag{57}$$

Our calculation of these terms will be similar to that of the low-energy photon-exchange contributions, described in Sec. III of Ref. [15].

1. E_{L1}^Λ

The first term E_{L1}^Λ is due to a perturbation by the Breit Hamiltonian and is written as

$$\begin{aligned} E_{L1}^\Lambda = {}& e^2\int_\Lambda^\infty \frac{d^dk}{(2\pi)^d 2k}\,\delta_\perp^{ij}(k)\,\delta\langle\phi|p_1^i\frac{1}{E_0-H_0-k}p_1^j|\phi\rangle \\ & + (1\leftrightarrow 2)\,. \end{aligned} \tag{58}$$

Here the symbol $\delta\langle\cdots\rangle$ denotes the first-order perturbation of the matrix element $\langle\cdots\rangle$ by the Breit Hamiltonian $H^{(4)}$, which implies perturbations of the reference-state wave function ϕ, the energy E_0, and the zeroth-order Hamiltonian H_0. Since k is much bigger than $H_0 - E_0$, we can expand the integrand of Eq. (58) in large k, keeping only the $1/k^2$ term, while $1/k$ contributes at the lower order of $\alpha^6 m$. The result is

$$\begin{aligned} & \delta\langle\phi|p_1^i\frac{1}{E_0-H_0-k}p_1^j|\phi\rangle + (1\leftrightarrow 2) \\ & = \frac{1}{2\,k^2}\,\delta\langle\phi|\big[p_1^i,\big[H_0-E_0,p_1^j\big]\big]|\phi\rangle + (1\leftrightarrow 2) \\ & = \frac{1}{k^2}\,\langle\phi|\big[p_1^i,\big[V,p_1^j\big]\big]\frac{1}{(E_0-H_0)'}H^{(4)}|\phi\rangle \\ & \quad + \frac{1}{2\,k^2}\,\langle\phi|\big[p_1^i,\big[H^{(4)},p_1^j\big]\big]|\phi\rangle + (1\leftrightarrow 2)\,. \end{aligned} \tag{59}$$

The first term in the last equation is the second-order contribution already accounted for in the previous section, and thus it will be omitted here. Note that the above expansion is valid up to the electron-nucleus Dirac δ-function terms, which we are omitting for the present. They will be restored later by matching our calculation against the hydrogenic result. The same will apply also for E_{L2}^Λ and E_{L3}^Λ.

After expanding in $\epsilon = (3-d)/2$ and then in α, we obtain the result for the corresponding effective Hamiltonian H_{L1}, $E^{\Lambda}_{L1} = \langle H_{L1}\rangle$,

$$H_{L1} = \alpha^2\bigg(\frac{5}{36}+\frac{1}{12}\ln\Lambda_\epsilon\bigg)Z\left[\nabla_1^2\delta^d(r_1)+\nabla_2^2\delta^d(r_2)\right] - \alpha^2\bigg\{\sigma_1\cdot\sigma_2\bigg(-\frac{7}{27}-\frac{1}{9}\ln\Lambda_\epsilon\bigg)q^2 + \bigg(-\frac{5}{9}-\frac{1}{3}\ln\Lambda_\epsilon\bigg)\bigg[q^2+4\vec{P}_1\cdot\vec{P}_2-4\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}\bigg]\bigg\}, \tag{60}$$

where $\vec{P}_1 = \frac{1}{2}(\vec{p}_1+\vec{p}_1{}')$ and $\vec{P}_2 = \frac{1}{2}(\vec{p}_2+\vec{p}_2{}')$ are sums of the *in* and *out* momenta of the corresponding electron, and $\vec{q} = \vec{p}_1' - \vec{p}_1$. Using the identity valid for the expectation values of the operators,

$$\nabla_1^2\delta^d(r_1) = -2\,p_1^2\,\delta^d(r_1) + 2\,\vec{p}_1\,\delta^d(r_1)\,\vec{p}_1 = -4\left(E_0 - V - p_2^2/2\right)\delta^d(r_1) + 2\,\vec{p}_1\,\delta^d(r_1)\,\vec{p}_1\,, \tag{61}$$

we simplify the expression further, obtaining the final result

$$H_{L1} = \alpha^2\bigg\{Z\delta^d(r_1)\bigg(-\frac{5}{9}-\frac{1}{3}\ln\Lambda_\epsilon\bigg)\bigg(E_0-V-\frac{p_2^2}{2}\bigg)+\bigg(\frac{5}{18}+\frac{1}{6}\ln\Lambda_\epsilon\bigg)\vec{p}_1\,Z\delta^d(r_1)\,\vec{p}_1+(1\leftrightarrow 2)\bigg\} +\alpha^2\bigg\{\sigma_1\cdot\sigma_2\bigg(\frac{7}{27}+\frac{1}{9}\ln\Lambda_\epsilon\bigg)q^2+\bigg(\frac{5}{9}+\frac{1}{3}\ln\Lambda_\epsilon\bigg)\bigg[q^2+4\vec{P}_1\cdot\vec{P}_2-4\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}\bigg]\bigg\}. \tag{62}$$

Note that in the above expression we keep the electron-nucleus terms in the coordinate representation but the electron-electron terms in the momentum representation.

2. E^{Λ}_{L2}

The second term in Eq. (57), E^{Λ}_{L2}, comes from a correction to the current. Specifically, $\vec{p}_1$ gets a correction $\delta\vec{j}_1$, which is

$$\delta j_1^i = i\big[H^{(4)}, r_1^i\big] = -\frac{1}{2}p_1^i p_1^2 - \frac{\alpha}{2}\bigg[\frac{\delta^{ij}}{r}+\frac{r^i r^j}{r^3}\bigg]_\epsilon p_2^j\,, \tag{63}$$

and the same for $\vec{p}_2$. The contribution E^{Λ}_{L2} is then

$$E^{\Lambda}_{L2} = 2e^2\int_\Lambda^\infty \frac{d^dk}{(2\pi)^d 2k}\,\delta_\perp^{ij}(k)\,\langle\phi|\delta j_1^i\frac{1}{E_0-H_0-k}p_1^j|\phi\rangle + (1\leftrightarrow 2)\,. \tag{64}$$

Expanding this expression in large k and performing the angular average, we arrive at

$$E^{\Lambda}_{L2} = e^2\frac{d-1}{d}\int_\Lambda^\infty \frac{d^dk}{(2\pi)^d 2k^3}\langle\phi|\left[\delta j_1^i,\left[V,p_1^i\right]\right]|\phi\rangle + (1\leftrightarrow 2) = E^A_{L2}+E^B_{L2}+E^C_{L2}\,. \tag{65}$$

This expression consists of three-body and two-body terms. The three-body contribution E^A_{L2} is due to the first term in $\delta\vec{j}_1$; it is transformed as

$$E^A_{L2} = -e^2\frac{d-1}{2d}\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d 2k^3}\langle\phi|\bigg[p_1^i\,p_1^2,\bigg[-\bigg[\frac{Z\alpha}{r_1}\bigg]_\epsilon,p_1^i\bigg]\bigg]|\phi\rangle + (1\leftrightarrow 2) = \frac{\alpha}{\pi}\bigg(-\frac{5}{18}-\frac{1}{6}\ln\Lambda_\epsilon\bigg)\langle\phi|-\bigg[V,\bigg[p_1^2,\bigg[\frac{Z\alpha}{r_1}\bigg]_\epsilon\bigg]\bigg]+8\pi Z\alpha\,\delta^d(r_1)\,(E_0-V)-\vec{p}_2\,4\pi Z\alpha\,\delta^d(r_1)\,\vec{p}_2|\phi\rangle+(1\leftrightarrow 2)\,. \tag{66}$$

There are two two-body contributions, the first one coming from the term $[-\frac{1}{2}p_1^i\,p_1^2,[\alpha/r,p_1^i]]$. We evaluate it by switching into the momentum representation,

$$E^B_{L2} = e^2\frac{d-1}{d}\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d 2k^3}\langle\phi|\bigg[-\frac{1}{2}p_1^i\,p_1^2,\bigg[\bigg[\frac{\alpha}{r}\bigg]_\epsilon,p_1^i\bigg]\bigg]|\phi\rangle+(1\leftrightarrow 2) = \alpha^2\bigg(\frac{20}{9}+\frac{4}{3}\ln\Lambda_\epsilon\bigg)\langle\phi|\frac{1}{2}(\vec{P}_1-\vec{P}_2)^2+\vec{P}_1\cdot\vec{P}_2+\frac{1}{4}q^2+\frac{[(\vec{P}_1-\vec{P}_2)\cdot\vec{q}]^2}{q^2}+2\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}|\phi\rangle\,. \tag{67}$$

The two-body contribution induced by the second term in $\delta\vec{j}_1$ is evaluated with help of integration formulas from Appendix C of Ref. [15] as

$$E^C_{L2} = e^2\frac{d-1}{d}\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d 2k^3}\langle\phi|\bigg(-\frac{\alpha}{2}\bigg[\frac{\delta^{ij}}{r}+\frac{r^ir^j}{r^3}\bigg]_\epsilon\bigg)\bigg[p_2^j,\bigg[\bigg[\frac{\alpha}{r}\bigg]_\epsilon,p_1^i\bigg]\bigg]|\phi\rangle+(1\leftrightarrow 2) = \pi\alpha^3\langle\phi|\bigg(-\frac{4}{9}-\frac{2}{3}\ln\Lambda_\epsilon-\frac{4}{3}\ln 2+\frac{4}{3}\ln q\bigg)q|\phi\rangle\,. \tag{68}$$

Adding together the individual contributions to E_{L2}^{Λ} and using the expectation value identity

$$\alpha\frac{[(\vec{P}_1-\vec{P}_2)\cdot\vec{q}]^2}{q^2}=\left\{\frac{1}{4\pi}\left[\frac{Z\alpha\,\vec{r}_1}{r_1^3}\right]_\epsilon\cdot\left[\frac{\alpha\,\vec{r}}{r^3}\right]_\epsilon+(1\leftrightarrow 2)\right\}+\frac{\pi\alpha^2}{2}\{1+\epsilon\,(2\ln 2-2\ln q)\}q\,, \tag{69}$$

we write the result in terms of the effective Hamiltonian H_{L2}, $E_{L2}^{\Lambda}=\langle H_{L2}\rangle$, which is

$$\begin{aligned}H_{L2}=\frac{\alpha}{\pi}\bigg(\bigg(-\frac{5}{9}-\frac{1}{3}\ln\Lambda_\epsilon\bigg)\bigg\{\bigg[\frac{(Z\alpha)^2}{r_1^4}\bigg]_\epsilon-2\bigg[\frac{Z\alpha\,\vec{r}_1}{r_1^3}\bigg]_\epsilon\cdot\bigg[\frac{\alpha\,\vec{r}}{r^3}\bigg]_\epsilon+4\pi Z\alpha\,\delta^d(r_1)\bigg(E_0-V-\frac{p_2^2}{2m}\bigg)\bigg\}+(1\leftrightarrow 2)\bigg)\\+\alpha^2\bigg(\frac{20}{9}+\frac{4}{3}\ln\Lambda_\epsilon\bigg)\bigg[\frac{1}{2}(\vec{P}_1-\vec{P}_2)^2+\vec{P}_1\cdot\vec{P}_2+\frac{1}{4}q^2+2\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}\bigg]+\frac{2\pi}{3}\alpha^3\,q\,.\end{aligned} \tag{70}$$

3. E_{L3}^{Λ}

The third term in Eq. (57), E_{L3}^{Λ}, is a retardation correction. It can be expressed as

$$E_{L3}^{\Lambda}=e^2\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d2k}\,\delta_\perp^{ij}(k)\,\delta_{k^2}\langle\phi|p_1^i\,e^{i\vec{k}\cdot\vec{r}_1}\frac{1}{E_0-H_0-k}p_1^j\,e^{-i\vec{k}\cdot\vec{r}_1}|\phi\rangle+(1\leftrightarrow 2)\,, \tag{71}$$

where the symbol $\delta_{k^2}\langle\dots\rangle$ means that the exponential factors $e^{i\vec{k}\cdot\vec{r}_1}$ and $e^{-i\vec{k}\cdot\vec{r}_1}$ in the matrix element $\langle\dots\rangle$ are expanded in small k up to order k^2. Because Λ is arbitrarily large, we perform the large-k expansion of the resolvent,

$$\frac{1}{E_0-H_0-k}=-\frac{1}{k}+\frac{H_0-E_0}{k^2}-\frac{(H_0-E_0)^2}{k^3}+\frac{(H_0-E_0)^3}{k^4}+\cdots\,. \tag{72}$$

The k expansion needs to be extended up to order k^{-4} because of the additional k^2 from the expansion of the exponential factors. The resulting correction of order $\alpha^7\,m$ is

$$E_{L3}^{\Lambda}=e^2\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d2k^5}\,\delta_\perp^{ij}(k)\,\delta_{k^2}\langle\phi|p_1^i\,e^{i\vec{k}\cdot\vec{r}_1}(H_0-E_0)^3\,p_1^j\,e^{-i\vec{k}\cdot\vec{r}_1}|\phi\rangle+(1\leftrightarrow 2)\,. \tag{73}$$

The radial integration k can be performed in the same way as in the previous low-energy contributions. For the angular integration, we will use the formulas from Appendix C of Ref. [15]. The matrix element in Eq. (73) can be simplified by using identity $\exp(i\vec{k}\cdot\vec{r})\,f(\vec{p})\,\exp(-i\vec{k}\cdot\vec{r})=f(\vec{p}-\vec{k})$. We, therefore, have

$$\begin{aligned}\delta_{k^2}\big[p_1^i\,e^{i\vec{k}\cdot\vec{r}_1}(H_0-E_0)^3\,p_1^j\,e^{-i\vec{k}\cdot\vec{r}_1}\big]&=\delta_{k^2}\bigg[p_1^i\bigg(H_0-E_0-\vec{p}_1\cdot\vec{k}+\frac{k^2}{2}\bigg)^3\,p_1^j\bigg]\\&=p_1^i\bigg[\frac{3}{2}(H_0-E_0)^2\,k^2+\vec{p}_1\cdot\vec{k}\,(H_0-E_0)\,\vec{p}_1\cdot\vec{k}+2\,(\vec{p}_1\cdot\vec{k})^2\,(H_0-E_0)\bigg]p_1^j\,.\end{aligned} \tag{74}$$

We will refer to the contributions induced by the three terms in the brackets of the above expression as E_{L3}^A, E_{L3}^B, and E_{L3}^C, respectively,

$$E_{L3}^{\Lambda}=E_{L3}^A+E_{L3}^B+E_{L3}^C\,. \tag{75}$$

Starting with the three-photon contribution E_{L3}^A, we obtain

$$E_{L3}^A=\frac{3e^2}{2}\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d2k^3}\,\delta_\perp^{ij}(k)\,\langle\phi|p_1^i\,(H_0-E_0)^2\,p_1^j|\phi\rangle+(1\leftrightarrow 2)\,. \tag{76}$$

Averaging this expression over the angular variables, commuting H_0-E_0 to the left and to the right, and performing the integration, we obtain

$$\begin{aligned}E_{L3}^A=\langle\phi|\frac{\alpha}{\pi}\bigg\{\bigg(\frac{5}{6}+\frac{1}{2}\ln\Lambda_\epsilon\bigg)\bigg[\frac{(Z\alpha)^2}{r_1^4}\bigg]_\epsilon-\bigg(\frac{5}{3}+\ln\Lambda_\epsilon\bigg)\bigg[\frac{Z\alpha\,\vec{r}_1}{r_1^3}\bigg]_\epsilon\cdot\bigg[\frac{\alpha\,\vec{r}}{r^3}\bigg]_\epsilon+(1\leftrightarrow 2)\bigg\}\\+\pi\alpha^3\bigg(-\frac{5}{3}-\ln\Lambda_\epsilon-2\ln 2+2\ln q\bigg)q|\phi\rangle\,.\end{aligned} \tag{77}$$

The contribution of the second term is evaluated as

$$\begin{aligned}E_{L3}^B&=e^2\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d2k^5}\,\delta_\perp^{ij}(k)k^mk^n\,\langle\phi|p_1^ip_1^m\,(H_0-E_0)\,p_1^np_1^j|\phi\rangle+(1\leftrightarrow 2)\\&=\frac{e^2}{d(d+2)}\int_\Lambda^\infty\frac{d^dk}{(2\pi)^d2k^3}\,\langle\phi|d\,p_1^ip_1^j\,(H_0-E_0)\,p_1^ip_1^j-p_1^2\,(H_0-E_0)\,p_1^2|\phi\rangle+(1\leftrightarrow 2)\,.\end{aligned} \tag{78}$$

We transform this expression further with the help of the following identities,

$$p_1^2\,(H_0-E_0)\,p_1^2 = \frac{1}{2}\,[p_1^2,[H_0-E_0,p_1^2]] = \frac{1}{2}\,[p_1^2,[V,p_1^2]]\,, \tag{79}$$

$$p_1^i\,[p_1^i,[V,p_1^j]]\,p_1^j = \frac{1}{4}\,[p_1^2,[V,p_1^2]] - \frac{1}{2}\,p_1^2\,[\,p_1^i,[V,p_1^i]] + \frac{1}{2}\,p_1^i\,[p_1^j,[V,p_1^j]]\,p_1^i\,, \tag{80}$$

and

$$p_1^i p_1^j\,(H_0-E_0)\,p_1^i p_1^j = \frac{1}{2}\,p_1^2\,[\,p_1^i,[V,p_1^i]] + \frac{1}{4}\,[p_1^2,[V,p_1^2]] + \frac{1}{2}\,p_1^i\,[p_1^j,[V,p_1^j]]\,p_1^i\,. \tag{81}$$

The result for the second term is

$$\begin{aligned}
E_{L3}^B &= \frac{\alpha}{\pi}\,\langle\phi|\bigg(\frac{2}{225}+\frac{1}{120}\ln\Lambda_\epsilon\bigg)[p_1^2,[V,p_1^2]] + \bigg(\frac{3}{25}+\frac{1}{20}\ln\Lambda_\epsilon\bigg)\\
&\quad\times\big(p_1^i\,[p_1^j,[V,p_1^j]]\,p_1^i + p_1^2\,[\,p_1^i,[V,p_1^i]]\big)|\phi\rangle + (1\leftrightarrow 2)\\
&= \langle\phi|\frac{\alpha}{\pi}\bigg\{\bigg(\frac{8}{225}+\frac{1}{30}\ln\Lambda_\epsilon\bigg)\bigg(\bigg[\frac{(Z\alpha)^2}{r_1^4}\bigg]_\epsilon - \bigg[\frac{Z\alpha\,\vec r_1}{r_1^3}\bigg]_\epsilon\cdot\bigg[\frac{\alpha\,\vec r}{r^3}\bigg]_\epsilon\bigg) + \bigg(\frac{3}{25}+\frac{1}{20}\ln\Lambda_\epsilon\bigg)\\
&\quad\times\bigg[p_1^i\,4\pi Z\alpha\,\delta^d(r_1)\,p_1^i + \bigg(E_0 - V - \frac{p_2^2}{2}\bigg)\,8\pi Z\alpha\,\delta^d(r_1)\bigg] + (1\leftrightarrow 2)\bigg\}\\
&\quad+\alpha^2\bigg(-\frac{32}{225}\frac{[(\vec P_1-\vec P_2)\cdot\vec q]^2}{q^2} - \frac{24}{25}(\vec P_1-\vec P_2)^2 - \frac{48}{25}\vec P_1\cdot\vec P_2 - \frac{64}{225}\frac{(\vec P_1\cdot\vec q)(\vec P_2\cdot\vec q)}{q^2}\\
&\quad+\ln\Lambda_\epsilon\bigg\{-\frac{2}{5}(\vec P_1-\vec P_2)^2 - \frac{2}{15}\frac{[(\vec P_1-\vec P_2)\cdot\vec q]^2}{q^2} - \frac{4}{5}\vec P_1\cdot\vec P_2 - \frac{4}{15}\frac{(\vec P_1\cdot\vec q)(\vec P_2\cdot\vec q)}{q^2}\bigg\}\bigg)|\phi\rangle\,.
\end{aligned} \tag{82}$$

Finally, the term E_{L3}^C is calculated as

$$\begin{aligned}
E_{L3}^C &= 2e^2\int_\Lambda^\infty \frac{d^dk}{(2\pi)^d 2k^5}\,\delta_\perp^{ij}(k)k^m k^n\,\langle\phi|p_1^i p_1^m p_1^n\,(H_0-E_0)\,p_1^j|\phi\rangle + (1\leftrightarrow 2)\\
&= e^2\int_\Lambda^\infty \frac{d^dk}{(2\pi)^d 2k^3}\,\langle\phi|\frac{(d-1)}{d(d+2)}\,[p_1^i p_1^2,[V,p_1^i]]|\phi\rangle + (1\leftrightarrow 2)\\
&= \langle\phi|\frac{\alpha}{\pi}\bigg\{\bigg(\frac{62}{225}+\frac{2}{15}\ln\Lambda_\epsilon\bigg)\bigg(4\pi Z\alpha\,\delta^d(r_1)\bigg(E_0-V-\frac{p_2^2}{2}\bigg) + \bigg[\frac{(Z\alpha)^2}{r_1^4}\bigg]_\epsilon - \bigg[\frac{Z\alpha\,\vec r_1}{r_1^3}\bigg]_\epsilon\cdot\bigg[\frac{\alpha\,\vec r}{r^3}\bigg]_\epsilon\bigg) + (1\leftrightarrow 2)\bigg\}\\
&\quad+\alpha^2\bigg(\frac{124}{225}+\frac{4}{15}\ln\Lambda_\epsilon\bigg)\bigg(-(\vec P_1-\vec P_2)^2 - \frac{1}{2}q^2 - 2\vec P_1\cdot\vec P_1 - 2\frac{[(\vec P_1-\vec P_2)\cdot\vec q]^2}{q^2} - 4\frac{(\vec P_1\cdot\vec q)(\vec P_2\cdot\vec q)}{q^2}\bigg)|\phi\rangle\,.
\end{aligned} \tag{83}$$

Adding together E_{L3}^A, E_{L3}^B, and E_{L3}^C and transforming the sum with help of Eq. (69), we obtain the retardation correction E_{L3}^Λ as

$$\begin{aligned}
E_{L3}^\Lambda &= \langle\phi|\frac{\alpha}{\pi}\bigg\{\frac{464}{225}\pi Z\alpha\,\delta^d(r_1)\bigg(E_0-V-\frac{p_2^2}{2}\bigg) + \frac{103}{90}\bigg[\frac{(Z\alpha)^2}{r_1^4}\bigg]_\epsilon - \frac{103}{45}\bigg[\frac{Z\alpha\,\vec r_1}{r_1^3}\bigg]_\epsilon\cdot\bigg[\frac{\alpha\,\vec r}{r^3}\bigg]_\epsilon\\
&\quad+\frac{3}{25}p_1^i\,4\pi Z\alpha\,\delta^d(r_1)\,p_1^i + \ln\Lambda_\epsilon\bigg(\frac{14}{15}\pi Z\alpha\,\delta^d(r_1)\bigg(E_0-V-\frac{p_2^2}{2}\bigg)\\
&\quad+\frac{2}{3}\bigg[\frac{(Z\alpha)^2}{r_1^4}\bigg]_\epsilon - \frac{4}{3}\bigg[\frac{Z\alpha\,\vec r_1}{r_1^3}\bigg]_\epsilon\cdot\bigg[\frac{\alpha\,\vec r}{r^3}\bigg]_\epsilon + \frac{1}{20}p_1^i\,4\pi Z\alpha\,\delta^d(r_1)\,p_1^i\bigg) + (1\leftrightarrow 2)\bigg\}\\
&\quad+\alpha^2\bigg\{-\frac{68}{45}(\vec P_1-\vec P_2)^2 - \frac{62}{225}q^2 - \frac{136}{45}\vec P_1\cdot\vec P_2 - \frac{112}{45}\frac{(\vec P_1\cdot\vec q)(\vec P_2\cdot\vec q)}{q^2}\\
&\quad+\ln\Lambda_\epsilon\bigg(-\frac{2}{3}(\vec P_1-\vec P_2)^2 - \frac{2}{15}q^2 - \frac{4}{3}\vec P_1\cdot\vec P_2 - \frac{4}{3}\frac{(\vec P_1\cdot\vec q)(\vec P_2\cdot\vec q)}{q^2}\bigg)\bigg\}\\
&\quad+\pi\alpha^3\bigg(-\frac{103}{45} - \frac{4}{3}\ln\Lambda_\epsilon - \frac{8}{3}\ln 2 + \frac{8}{3}\ln q\bigg)\,q\,|\phi\rangle\,.
\end{aligned} \tag{84}$$

4. Total low-energy result

Adding together E_{L1}^{Λ}, E_{L2}^{Λ}, and E_{L3}^{Λ}, we arrive at the final result for the low-energy contribution, which is

$$
\begin{aligned}
H_L^{\Lambda} = \frac{\alpha}{\pi}\bigg\{&\pi Z\alpha\,\delta^d(r_1)\bigg[-\frac{161}{225}\bigg(E_0 - V - \frac{p_2^2}{2}\bigg) - \frac{11}{15}\ln\Lambda_\epsilon\bigg(E_0 - V - \frac{p_2^2}{2}\bigg)\bigg] + \frac{53}{90}\bigg[\frac{(Z\alpha)^2}{r_1^4}\bigg]_\epsilon - \frac{53}{45}\bigg[\frac{Z\alpha\,\vec{r}_1}{r_1^3}\bigg]_\epsilon\cdot\bigg[\frac{\alpha\,\vec{r}}{r^3}\bigg]_\epsilon \\
&+ \frac{341}{450}p_1^i\pi Z\alpha\,\delta^d(r_1)\,p_1^i + \ln\Lambda_\epsilon\bigg(\frac{1}{3}\bigg[\frac{(Z\alpha)^2}{r_1^4}\bigg]_\epsilon - \frac{2}{3}\bigg[\frac{Z\alpha\,\vec{r}_1}{r_1^3}\bigg]_\epsilon\cdot\bigg[\frac{\alpha\,\vec{r}}{r^3}\bigg]_\epsilon + \frac{11}{30}p_1^i\,\pi Z\alpha\,\delta^d(r_1)\,p_1^i\bigg) + (1\leftrightarrow 2)\bigg\} \\
&+ \pi\alpha^3\bigg\{-\frac{73}{45} - \frac{4}{3}\ln\Lambda_\epsilon - \frac{8}{3}\ln 2 + \frac{8}{3}\ln q\bigg\}q + \alpha^2\bigg\{-\frac{2}{5}(\vec{P}_1 - \vec{P}_2)^2 + \frac{188}{225}q^2 + \frac{64}{45}\vec{P}_1\cdot\vec{P}_2 \\
&- \frac{4}{15}\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2} + \ln\Lambda_\epsilon\bigg(\frac{4}{3}\vec{P}_1\cdot\vec{P}_2 + \frac{8}{15}q^2\bigg) + \sigma_1\cdot\sigma_2\bigg(\frac{7}{27} + \frac{1}{9}\ln\Lambda_\epsilon\bigg)q^2\bigg\}. \qquad (85)
\end{aligned}
$$

B. Middle-energy part

We now turn to the second term in Eq. (56), the middle-energy contribution E_M. This part originated from the region where both the radiative and the exchanged photons are of the order $k \propto m\alpha$. We separate E_M into two parts, $E_M = E_{M1} + E_{M2}$, which are examined as follows.

1. Triple seagull contribution

The first middle-energy part is the triple seagull contribution, which is expressed (with k_3 being the radiative photon) as

$$
\begin{aligned}
E_{M1} = e^6 &\int\frac{d^dk_1}{(2\pi)^d\,2k_1}\int\frac{d^dk_2}{(2\pi)^d\,2k_2}\int\frac{d^dk_3}{(2\pi)^d\,2k_3}\,\delta_\perp^{ik}(k_1)\delta_\perp^{jk}(k_2)\delta_\perp^{ij}(k_3) \\
&\times\langle\phi|e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_1}\frac{1}{E_0 - H_0 - k_1 - k_2}e^{i(\vec{k}_3-\vec{k}_1)\cdot\vec{r}_2}\frac{1}{E_0 - H_0 - k_2 - k_3}e^{-i(\vec{k}_2+\vec{k}_3)\cdot\vec{r}_2} \\
&+ e^{-i(\vec{k}_1+\vec{k}_3)\cdot\vec{r}_2}\frac{1}{E_0 - H_0 - k_1 - k_3}e^{-i(\vec{k}_2-\vec{k}_3)\cdot\vec{r}_2}\frac{1}{E_0 - H_0 - k_1 - k_2}e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_1} \\
&+ e^{-i(\vec{k}_1+\vec{k}_3)\cdot\vec{r}_2}\frac{1}{E_0 - H_0 - k_1 - k_3}e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_1}\frac{1}{E_0 - H_0 - k_2 - k_3}e^{-i(\vec{k}_2+\vec{k}_3)\cdot\vec{r}_2}|\phi\rangle + (1\leftrightarrow 2). \qquad (86)
\end{aligned}
$$

We now have to expand the resolvents for large k. To get the contribution of the order $\alpha^7 m$, it is sufficient to take the nonretardation approximation, thus omitting $H_0 - E_0$. We arrive at

$$
\begin{aligned}
E_{M1} = e^6 &\int\frac{d^dk_1}{(2\pi)^d\,2k_1}\int\frac{d^dk_2}{(2\pi)^d\,2k_2}\int\frac{d^dk_3}{(2\pi)^d\,2k_3}\,\delta_\perp^{ik}(k_1)\delta_\perp^{ik}(k_2)\frac{(d-1)}{d} \\
&\times\langle\phi|e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}}\bigg[\frac{1}{(k_1+k_2)(k_2+k_3)} + \frac{1}{(k_1+k_3)(k_1+k_2)} + \frac{1}{(k_1+k_3)(k_2+k_3)}\bigg]|\phi\rangle + (1\leftrightarrow 2). \qquad (87)
\end{aligned}
$$

Similarly to the case of the low-energy contribution, we will express E_{M1} as an expectation value of some effective operator H_{M1}. Because it contains purely two-body electron-electron terms, we express it in momentum representation. We obtain

$$
\begin{aligned}
H_{M1} = (4\pi\alpha)^3\frac{(d-1)}{8d}&\int\frac{d^dk}{(2\pi)^d}\int\frac{d^dk_3}{(2\pi)^d}\frac{\delta_\perp^{ik}(k_1)\delta_\perp^{ik}(k_2)}{k_1\,k_2\,k_3} \\
&\times\bigg[\frac{1}{(k_1+k_2)(k_2+k_3)} + \frac{1}{(k_1+k_3)(k_1+k_2)} + \frac{1}{(k_1+k_3)(k_2+k_3)}\bigg] + (1\leftrightarrow 2), \qquad (88)
\end{aligned}
$$

with $k_1 = |\vec{k} - \vec{q}/2|$ and $k_2 = |\vec{k} + \vec{q}/2|$. The integration over radiative photon k_3 is trivial. The remaining integration is performed in spheroidal coordinates as explained in Appendix B. The result for the triple seagull contribution is

$$
H_{M1} = \alpha^3\pi\bigg(-\frac{1}{3} + \frac{4}{3}\ln 2\bigg)q. \qquad (89)
$$

2. Single seagull with retardation

The second middle-energy contribution comes from the diagram with a single seagull and retardation. The diagram contains two photons, one of which is a transverse photon exchanged between the electrons and another one is a radiative photon. The corresponding contribution is expressed as

$$
\begin{aligned}
E_{M2} = e^4 \int \frac{d^d k_1}{(2\pi)^d\, 2k_1} \int \frac{d^d k_2}{(2\pi)^d\, 2k_2} \delta_\perp^{in}(k_1)\delta_\perp^{im}(k_2) \\
\times \langle\phi| j_1^n(k_1)\, e^{i\vec{k}_1\cdot\vec{r}_1} \frac{1}{E_0-H_0-k_1} e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2} \frac{1}{E_0-H_0-k_2} j_2^m(k_2)\, e^{i\vec{k}_2\cdot\vec{r}_2} \\
+ j_2^n(k_1)\, e^{i\vec{k}_1\cdot\vec{r}_2} \frac{1}{E_0-H_0-k_1} e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2} \frac{1}{E_0-H_0-k_2} j_1^m(k_2)\, e^{i\vec{k}_2\cdot\vec{r}_1} \\
+ j_1^n(k_1)\, e^{i\vec{k}_1\cdot\vec{r}_1} \frac{1}{E_0-H_0-k_1} j_2^m(k_2)\, e^{i\vec{k}_2\cdot\vec{r}_2} \frac{1}{E_0-H_0-k_1-k_2} e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2} \\
+ j_2^n(k_1)\, e^{i\vec{k}_1\cdot\vec{r}_2} \frac{1}{E_0-H_0-k_1} j_1^m(k_2)\, e^{i\vec{k}_2\cdot\vec{r}_1} \frac{1}{E_0-H_0-k_1-k_2} e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2} \\
+ e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2} \frac{1}{E_0-H_0-k_1-k_2} j_1^n(k_1)\, e^{i\vec{k}_1\cdot\vec{r}_1} \frac{1}{E_0-H_0-k_2} j_2^m(k_2)\, e^{i\vec{k}_2\cdot\vec{r}_2} \\
+ e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2} \frac{1}{E_0-H_0-k_1-k_2} j_2^n(k_1)\, e^{i\vec{k}_1\cdot\vec{r}_2} \frac{1}{E_0-H_0-k_2} j_1^m(k_2)\, e^{i\vec{k}_2\cdot\vec{r}_1} |\phi\rangle + (1 \leftrightarrow 2),
\end{aligned}
\tag{90}
$$

where $j_i^l(k)$ is defined as

$$
j_i^l(k) = p_i^l + \frac{i}{2}\sigma_i^{kl} k^k. \tag{91}
$$

The first two terms in the matrix element vanish after performing the retardation expansion and carrying out the integration over the momentum of the radiative photon as $\int d^d k\, k^\alpha = 0$, which is true by definition in the dimensional regularization. The remainder of the expression can be cast in the form

$$
\begin{aligned}
E_{M2} = -2e^4 \int \frac{d^d k_1}{(2\pi)^d\, 2k_1} \int \frac{d^d k_2}{(2\pi)^d\, 2k_2} \frac{1}{k_1^2(k_1+k_2)} \\
\times \delta_\perp^{in}(k_1)\delta_\perp^{im}(k_2) \\
\times \langle\phi| \big[\big[j_1^n(k_1)\, e^{i\vec{k}_1\cdot\vec{r}_1}, H_0 - E_0\big], j_2(k_2)\, e^{i\vec{k}_2\cdot\vec{r}_2}\big] \\
\times e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2} |\phi\rangle + (1 \leftrightarrow 2).
\end{aligned}
\tag{92}
$$

The above expression was rearranged so that only photon k_2 is radiative (thus the additional factor of 2 in the front). Taking into account that only spin-independent terms survive the double commutator and performing the angular average for the radiative photon, we arrive at

$$
\begin{aligned}
E_{M2} = -\frac{(4\pi\alpha)^2}{2} \frac{(d-1)}{d} \int \frac{d^d k_1}{(2\pi)^d} \int \frac{d^d k_2}{(2\pi)^d} \frac{1}{k_1^3 k_2(k_1+k_2)} \\
\times \delta_\perp^{mn}(k_1) \langle\phi| e^{i\vec{k}_1\cdot\vec{r}}\, \partial_1^m \partial_2^n V |\phi\rangle + (1 \leftrightarrow 2).
\end{aligned}
\tag{93}
$$

This can be again expressed as an expectation value of an effective operator H_{M2}, which is in momentum space

$$
\begin{aligned}
H_{M2} = -(4\pi\alpha)^3 \frac{(d-1)}{d} \int \frac{d^d k_1}{(2\pi)^d} \int \frac{d^d k_2}{(2\pi)^d} \\
\times \frac{\delta_\perp^{mn}(k_1) q^m q^n}{k_1^3\, |\vec{k}_1 - \vec{q}|^2\, k_2(k_1+k_2)}.
\end{aligned}
\tag{94}
$$

Performing the remaining integrations, we obtain the result

$$
H_{M2} = \alpha^3 \pi \left(\frac{4}{9} + \frac{2}{3\epsilon} - \frac{8}{3} \ln q \right) q. \tag{95}
$$

3. Total result for the middle-energy contribution

Adding together H_{M1} and H_{M2}, we obtain the total result for the effective operator responsible for the middle-energy contribution,

$$
H_M = \pi\alpha^3 \left(\frac{1}{9} + \frac{2}{3\epsilon} + \frac{4}{3}\ln 2 - \frac{8}{3}\ln q \right) q. \tag{96}
$$

It is not obvious that $E_M = \langle H_M \rangle$ is the complete middle-energy contribution, so we have verified this by calculating the corresponding scattering amplitude and obtaining agreement with the above result.

C. High-energy part

We now turn to the third term in Eq. (56), the high-energy part E_H. It consists of 16 terms originating from the anomalous magnetic moment κ and the slopes of form factors $F_1'(0)$ and $F_2'(0)$,

$$
E_H = \sum_{i=1}^{16} E_i. \tag{97}
$$

The contributions E_i are derived as corrections to the one-photon and two-photon exchange amplitudes induced by individual terms in the NRQED Hamiltonian $H_{\rm nrqed}$, see Eq. (18), as illustrated by Table I. The computational method is very similar to the one used in the derivation of the $\alpha^6 m$ correction to the helium Lamb shift [21]. Each contribution E_i will be expressed as an expectation value of the corresponding effective operator, $E_i = \langle H_i \rangle$, and we now examine the contributions E_i one by one.

1. E_1

E_1 is the retardation correction to the one-photon exchange between the electrons, where one vertex is $-\frac{e}{4}\sigma \cdot B$ and the

TABLE I. Contributions originating from δH_1, δH_2, and δH_3, given by Eqs. (14), (15), and (16).

Vertex	Vertex	Vertex	Retardation order	Diagram
$-\frac{e}{4}\sigma\cdot B$	$-\frac{e}{4}\kappa\,\sigma\cdot B$		$(H-E)^2$	E_1
$\frac{e^2}{2}\vec{A}^{\,2}$	$-\frac{e}{4}\kappa\,\sigma\cdot B$	$-\frac{e}{4}\sigma\cdot B$	$(H-E)^0$	E_2
$\frac{e}{16}\{\vec{p}^{\,2},\,\sigma\cdot B\}$	$-\frac{e}{4}\kappa\,\sigma\cdot B$		$(H-E)^0$	E_3
$-\frac{e}{4}\sigma\cdot B$	$\frac{e}{16}\kappa\,(\frac{1}{2}\{\vec{p}^{\,2},\sigma\cdot B\}+4p^k\sigma^{ki}B^{ij}\,p^j+\vec{p}\,\sigma\cdot B\,\vec{p})$		$(H-E)^0$	E_4
$\frac{e^2}{4}\sigma^{ij}E_\parallel^i A^j$	$-\frac{e}{4}\kappa\,\sigma\cdot B$	eA^0	$(H-E)^0$	E_5
$-\frac{e}{4}\sigma\cdot B$	$\frac{e^2}{2}\kappa\,\sigma^{ij}E_\parallel^i A^j$	eA^0	$(H-E)^0$	E_6
$-\frac{e}{4}\sigma\cdot B$	$-\frac{e}{4m^2}\kappa\,\sigma^{ij}\{E_\perp^i,\,p^j\}$		$(H-E)$	E_7
$-\frac{e}{8}\,\sigma^{ij}\{E_\perp^i,\,p^j\}$	$-\frac{e}{4}\kappa\,\sigma\cdot B$		$(H-E)$	E_8
eA^0	$-\frac{e}{8}[F_1'(0)+2F_2'(0)+4F_1''(0)]\vec{\nabla}^2\vec{\nabla}\cdot\vec{E}$		$(H-E)^0$	E_{10}
eA^0	$\frac{1}{16}\kappa\,\{\vec{p}^2,\,\vec{\nabla}\cdot\vec{E}\}$		$(H-E)^0$	E_{11}
eA^0	$\frac{e^2}{8}\kappa\,\vec{E}_\parallel^2$	eA^0	$(H-E)^0$	E_{12}
eA^0	$e^2\,\vec{E}_\parallel^2\,\chi$	eA^0	$(H-E)^0$	E_{13}
$-\frac{e}{8}\,(\vec{\nabla}\cdot\vec{E}+\sigma^{ij}\,\{E_\parallel^i,\,p^j\})$	$-\frac{e}{4}\,\kappa\,(\vec{\nabla}\cdot\vec{E}+\sigma^{ij}\,\{E_\parallel^i,\,p^j\})$		$(H-E)^0$	E_{14}
$-e\,\vec{p}\cdot\vec{A}$	$-\frac{e\kappa}{16}\,\{p^k,\,\partial_t E_\perp^k+\nabla^i B^{ik}\}$		$(H-E)^0$	E_{15}
eA^0	$-\frac{e\kappa}{16}\,\{p^k,\,\partial_t E_\parallel^k\}$		$(H-E)^0$	E_{16}

second vertex is $-\frac{e}{4}\kappa\,\sigma\cdot B$. We have

$$E_1 = -\,e^2\kappa\int\frac{d^dk}{(2\pi)^d\,2k^4}\delta_\perp^{ij}(k)\langle\phi|\left(\frac{1}{2}\sigma_1^{ki}\nabla_1^k\right)e^{i\vec{k}\cdot\vec{r}_1}\times(H_0-E_0)^2\left(\frac{1}{2}\sigma_2^{lj}\nabla_2^l\right)e^{-i\vec{k}\cdot\vec{r}_2}|\phi\rangle+\text{H.c.}+(1\leftrightarrow 2)\,. \tag{98}$$

Commuting H_0-E_0 to the left and to the right and performing the spin averaging, we obtain

$$E_1 = -\,\frac{e^2}{4}\kappa\,\frac{\sigma_1\cdot\sigma_2}{d}\int\frac{d^dk}{(2\pi)^dk^2}\times\langle\phi|\left[\frac{p_2^2}{2}\left[e^{i\vec{k}\cdot\vec{r}},\,\frac{p_1^2}{2}\right]\right]|\phi\rangle+(1\leftrightarrow 2)\,. \tag{99}$$

We now use the result for $\kappa\equiv F_2(0)$ from Appendix A,

$$\kappa = \frac{\alpha}{\pi}\left[\frac{1}{2}+2\epsilon\right], \tag{100}$$

and transform the momenta into $\vec{P}_1$ and $\vec{P}_2$. We obtain in the momentum representation

$$H_1 = -\frac{\alpha^2}{3}\sigma_1\cdot\sigma_2\,\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}\,. \tag{101}$$

2. E_2

E_2 is induced by the single-seagull diagram with the double vertex $\frac{e^2}{2}\vec{A}^{\,2}$ and the single vertices $-\frac{e}{4}\sigma\cdot B$ and $-\frac{e}{4}\kappa\,\sigma\cdot B$. The corresponding contribution is written as

$$\begin{aligned}E_2 = e^4\kappa\int\frac{d^dk_1}{(2\pi)^d\,2k_1}\int\frac{d^dk_2}{(2\pi)^d\,2k_2}\delta_\perp^{in}(k_1)\delta_\perp^{im}(k_2)\\ \times\Bigg\{\langle\phi|\left(\frac{1}{2}\sigma_1^{rn}\nabla_1^r\right)e^{i\vec{k}_1\cdot\vec{r}_1}\,\frac{1}{E_0-H_0-k_1}\,e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2}\,\frac{1}{E_0-H_0-k_2}\left(\frac{1}{2}\sigma_1^{sm}\nabla_1^s\right)e^{i\vec{k}_2\cdot\vec{r}_1}|\phi\rangle\\ +\langle\phi|\left(\frac{1}{2}\sigma_1^{rn}\nabla_1^r\right)e^{i\vec{k}_1\cdot\vec{r}_1}\,\frac{1}{E_0-H_0-k_1}\left(\frac{1}{2}\sigma_1^{sm}\nabla_1^s\right)e^{i\vec{k}_2\cdot\vec{r}_1}\,\frac{1}{E_0-H_0-k_1-k_2}\,e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2}|\phi\rangle\\ +\langle\phi|e^{-i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}_2}\,\frac{1}{E_0-H_0-k_1-k_2}\left(\frac{1}{2}\sigma_1^{rn}\nabla_1^r\right)e^{i\vec{k}_1\cdot\vec{r}_1}\,\frac{1}{E_0-H_0-k_2}\left(\frac{1}{2}\sigma_1^{sm}\nabla_1^s\right)e^{i\vec{k}_2\cdot\vec{r}_1}|\phi\rangle\Bigg\}+(1\leftrightarrow 2)\,.\end{aligned} \tag{102}$$

Expanding denominators in large k, we get the α^7m contribution of the form

$$\begin{aligned}E_2 &= \frac{e^4}{2}\kappa\int\frac{d^dk_1}{(2\pi)^d\,k_1^2}\int\frac{d^dk_2}{(2\pi)^d\,k_2^2}\delta_\perp^{in}(k_1)\delta_\perp^{im}(k_2)\langle\phi|\left(\frac{i}{2}\sigma_1^{rn}k_1^r\right)e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}}\left(\frac{i}{2}\sigma_1^{sm}k_2^s\right)|\phi\rangle+(1\leftrightarrow 2)\\ &= -\frac{e^4}{8}\kappa\int\frac{d^dk_1}{(2\pi)^d\,k_1^2}\int\frac{d^dk_2}{(2\pi)^d\,k_2^2}\sigma_1^{rn}\sigma_1^{sm}k_1^rk_2^s\,\delta_\perp^{in}(k_1)\delta_\perp^{im}(k_2)\langle\phi|\,e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{r}}|\phi\rangle+(1\leftrightarrow 2)\,.\end{aligned} \tag{103}$$

Averaging the spin matrices and performing the integrations by using formulas from Appendix C of Ref. [15], we obtain the result for E_2 in the momentum representation,

$$H_2 = -\pi\alpha^3\,\frac{q}{4}\,. \tag{104}$$

3. E_3

E_3 is induced by the exchange of a single transverse photon, with one vertex $-\frac{e}{4}\kappa\,\sigma\cdot B$ and the other $\frac{e}{4}\{\vec p^{\,2}, \frac{1}{4}\,\sigma\cdot B\}$. We thus get

$$\begin{aligned} E_3 &= \frac{e^2}{4}\kappa\int\frac{d^dk}{(2\pi)^d\,2k^2}\delta_\perp^{ij}(k)\langle\phi|\left(\frac{1}{2}\sigma_1^{ki}\nabla_1^k\right)e^{i\vec k\cdot\vec r_1}\left\{p_2^2,\,\frac{1}{2}\sigma_2^{lj}\nabla_2^l\,e^{-i\vec k\cdot\vec r_2}\right\}|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2)\\ &= \frac{e^2}{32}\kappa\,\frac{\sigma_1\cdot\sigma_2}{d}\int\frac{d^dk}{(2\pi)^d}\langle\phi|\left\{p_2^2,\,e^{i\vec k\cdot\vec r}\right\}|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2)\,. \end{aligned}\tag{105}$$

This expression is proportional to $\{p_2^2, \delta^d(r)\}$, which vanishes for triplet states. Therefore, $E_3 = 0$.

4. E_4

E_4 comes from the exchange of a single transverse photon, with one vertex being $-\frac{e}{4}\sigma\cdot B$ and the other $\frac{e}{16}\kappa\,(\frac{1}{2}\{\vec p, \{\vec p, \sigma\cdot B\}\} + 4p^k\sigma^{ki}B^{ij}\,p^j)$. The corresponding contribution is written as

$$\begin{aligned} E_4 = \frac{e^2}{16}\kappa\int\frac{d^dk}{(2\pi)^d\,2k^2}\delta_\perp^{ij}(k)\langle\phi|\left(\frac{1}{2}\sigma_1^{ki}\nabla_1^k\right)e^{i\vec k\cdot\vec r_1}\\ \times\Big[\big\{p_2^l,\,\big\{p_2^l,\,\sigma_2^{mj}\nabla_2^m\,e^{-i\vec k\cdot\vec r_2}\big\}\big\} + 4p_2^l\big(\sigma_2^{lm}\nabla_2^m\,e^{-i\vec k\cdot\vec r_2}\,p_2^j - \sigma_2^{lj}\nabla_2^m\,e^{-i\vec k\cdot\vec r_2}\,p_2^m\big)\Big]|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2)\,. \end{aligned}\tag{106}$$

After differentiating and spin averaging, we arrive at

$$E_4 = \frac{e^2}{16}\kappa\,\frac{\sigma_1\cdot\sigma_2}{d}\int\frac{d^dk}{(2\pi)^d\,k^2}\langle\phi|\frac{1}{4}\{\vec p_2, \{\vec p_2, k^2\,e^{i\vec k\cdot\vec r}\}\} - \frac{\delta_\perp^{ij}(k)}{(d-1)}\,p_2^i\,k^2\,e^{i\vec k\cdot\vec r}\,p_2^j - p_2^k\,k^kk^m\,e^{i\vec k\cdot\vec r}\,p_2^m\,|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2)\,. \tag{107}$$

Transforming the momenta in this expression into $\vec P_1$ and $\vec P_2$, we obtain the result in the momentum space,

$$H_4 = \alpha^2\sigma_1\cdot\sigma_2\left\{\frac{1}{24}(\vec P_1 - \vec P_2)^2 + \frac{1}{12}\vec P_1\cdot\vec P_2 - \frac{1}{24}\frac{[(\vec P_1 - \vec P_2)\cdot\vec q]^2}{q^2} + \frac{1}{24}q^2 - \frac{1}{12}\frac{(\vec P_1\cdot\vec q)(\vec P_2\cdot\vec q)}{q^2}\right\}. \tag{108}$$

5. E_5 and E_6

The terms E_5 and E_6 are examined together, because they both are given by the one-photon exchange amplitude with one vertex $-\frac{1}{4}\sigma\cdot B$ and the other vertex $e^2\,\sigma^{ij}E_\parallel^iA^j$, multiplied by a factor $\kappa/2$ in the case of E_6 and $\kappa/4$ in the case of E_5. The sum of the contributions is

$$\begin{aligned} E_5 + E_6 &= -\frac{3e^2}{8}\kappa\int\frac{d^dk}{(2\pi)^d\,2k^2}\delta_\perp^{ij}(k)\langle\phi|\sigma_1^{ki}\nabla_1^k\,e^{i\vec k\cdot\vec r}\,\sigma_2^{lj}\,\nabla_2^l\,V|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2)\\ &= -\frac{3e^2}{16}\kappa\,\frac{\sigma_1\cdot\sigma_2}{d}\int\frac{d^dk}{(2\pi)^d}\,\frac{k^l}{k^2}\langle\phi|\,e^{i\vec k\cdot\vec r}\left[V,\,p_2^l\right]|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2)\,. \end{aligned}\tag{109}$$

The result in a mixed coordinate and momentum representations is

$$H_5 + H_6 = \sigma_1\cdot\sigma_2\left(\left\{-\frac{\alpha}{16\pi}\left[\frac{Z\alpha\,\vec r_1}{r_1^3}\right]_\epsilon\cdot\left[\frac{\alpha\,\vec r}{r^3}\right]_\epsilon + (1\leftrightarrow 2)\right\} - \frac{\pi\alpha^3}{8}q\right). \tag{110}$$

6. E_7 and E_8

The terms E_7 and E_8 are induced by the one-photon exchange amplitude with one vertex $-\frac{e}{4}\sigma\cdot B$ and the other vertex $-e\kappa\,\sigma^{ij}\{E_\perp^i, p^j\}$, multiplied by either $\kappa/4$ or $\kappa/8$. The sum of the corresponding contributions is

$$\begin{aligned} E_7 + E_8 &= \frac{3e^2}{8}\kappa\int\frac{d^dk}{(2\pi)^d\,2k^3}\delta_\perp^{ij}(k)\langle\phi|\sigma_1^{ik}\left\{ik\,e^{i\vec k\cdot\vec r_1},\,p_1^k\right\}(H_0 - E_0)\left(\frac{1}{2}\sigma_2^{lj}\nabla_2^l\right)e^{-i\vec k\cdot\vec r_2}\,|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2)\\ &= \frac{3e^2}{32}\kappa\,\sigma_1^{ik}\sigma_2^{lj}\int\frac{d^dk}{(2\pi)^d\,k^2}\delta_\perp^{ij}(k)\,\langle\phi|\left\{e^{i\vec k\cdot\vec r_1},\,p_1^k\right\}\left[H_0 - E_0,\,\left[e^{-i\vec k\cdot\vec r_2},\,p_2^l\right]\right]|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2)\,. \end{aligned}\tag{111}$$

Spin averaging this expression, we get

$$E_7 + E_8 = -\frac{3e^2}{32}\kappa\,\frac{\sigma_1\cdot\sigma_2}{d}\int\frac{d^dk}{(2\pi)^d\,k^2}\langle\phi|\left[\frac{p_2^2}{2},\,\left[\left\{e^{i\vec{k}\cdot\vec{r}},\,p_1^i\right\},\,p_2^i\right]\right]|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2). \tag{112}$$

The result in momentum representation is

$$H_7 + H_8 = \alpha^2\,\frac{\sigma_1\cdot\sigma_2}{2}\,\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}\,. \tag{113}$$

7. E_9

We now move to contributions originating from the δH_2 part of the FW Hamiltonian, given by Eq. (15). It is possible to evaluate them in the same way as the previous E_i contributions, with the difference that one has to use the Feynman gauge instead of the Coulomb gauge. This difference is caused by the presence of q_0^2 in the expansion of form factors F_1 and F_2. We will use a different approach, however, which is more advantageous and illustrative, namely, the so-called scattering amplitude approach. We recall that the electromagnetic form factors F_1 and F_2 modify the vertex γ^μ as

$$\gamma^\mu \to \Gamma^\mu = \gamma^\mu + \gamma^\mu\,F_1\big(q_0^2 - q^2\big) + \frac{i}{2}F_2\big(q_0^2 - q^2\big)\Big(\frac{i}{2}\Big)[\gamma^\mu,\,\not{q}]. \tag{114}$$

The amplitude of the exchange of one photon between the electrons with one of the vertices perturbed in this way is

$$M_{fi} = e^2(\bar{u}_1'\Gamma^\mu u_1)D_{\mu\nu}(q)(\bar{u}_2'\gamma^\nu u_2) + (1\leftrightarrow 2)\,, \tag{115}$$

where $q = p_1' - p_1 = p_2 - p_2'$ with p_1 and p_1' being the *in* and *out* momenta of the first electron, and the same for the second electron. To obtain contributions up to the order $\alpha^7 m$, we expand the expression of the vertex as

$$\Gamma^\mu \to \left\{\gamma^\mu\left[F_1'(0) - \frac{1}{2}F_1''(0)\,q^2\right] - \frac{1}{4}F_2'(0)\,q^j[\gamma^j,\gamma^\mu]\right\} \times\big[q_0^2 - q^2\big]\,, \tag{116}$$

where we omitted terms with q_0 which contribute to higher orders in α, and we also excluded anomalous magnetic moment contribution $\propto F_2(0)$. We now pull the factor $q_0^2 - q^2$ out of this expression to cancel it with the denominator of the photon propagator. The photon propagator thus becomes

$$(q_0^2 - q^2)D_{\mu\nu}(q) = g_{\mu\nu}. \tag{117}$$

The scattering amplitude is then

$$\begin{aligned} M_{fi} = e^2\Bigg\{&\left[F_1'(0) - \frac{1}{2}F_1''(0)\,q^2\right] \\ &\times\left[(\bar{u}_1'\gamma^0 u_1)(\bar{u}_2'\gamma^0 u_2) - (\bar{u}_1'\gamma^i u_1)(\bar{u}_2'\gamma^i u_2)\right] \\ &-\frac{1}{4}F_2'(0)\big[(\bar{u}_1' q^j[\gamma^j,\gamma^0]u_1)(\bar{u}_2'\gamma^0 u_2) \\ &-(\bar{u}_1' q^j[\gamma^j,\gamma^i]u_1)(\bar{u}_2'\gamma^i u_2)\big] + (1\leftrightarrow 2)\Bigg\}. \end{aligned} \tag{118}$$

For the bispinor u, we take

$$u = \begin{pmatrix} \big(1 - \frac{p^2}{8}\big)\,w \\ \frac{(\vec{\sigma}\cdot\vec{p})}{2}\,w \end{pmatrix}, \tag{119}$$

where w is the spinor amplitude of the plane wave that includes the relativistic correction to the kinetic energy. Then,

$$\begin{aligned} (\bar{u}_1'\gamma^0 u_1) &= (w_1')^*\Big(1 - \frac{q^2}{8} + \frac{i}{4}\sigma_1^{ij}q^i p_1^j\Big)w_1\,, \\ (\bar{u}_1'\gamma^i u_1) &= \frac{1}{2}(w_1')^*\big(i\,\sigma_1^{ji}q^j + 2p_1^i + q^i\big)\,w_1\,, \\ (\bar{u}_1' q^j[\gamma^j,\gamma^0]u_1) &= (w_1')^*\big(q^2 + 2\,i\,\sigma_1^{ij}q^j p_1^i\big)w_1\,, \\ (\bar{u}_1' q^j[\gamma^j,\gamma^i]u_1) &= (w_1')^*\,2\,i\,\sigma_1^{ij}q^j\,w_1\,. \end{aligned} \tag{120}$$

The corresponding expressions for the second electron are obtained from the above formulas by changing the index $1\to 2$ and reversing the transferred momentum $\vec{q}\to-\vec{q}$. We thus obtain for the scattering amplitude

$$M_{fi} = -(w_1')^*(w_2')^*\,U(\vec{p}_1,\vec{p}_2,\vec{q})\,w_1 w_2\,, \tag{121}$$

where (omitting higher order terms and terms contributing only to the fine structure)

$$\begin{aligned} U(\vec{p}_1,\vec{p}_2,\vec{q}) = e^2\Bigg\{&F_1'(0)\bigg[-1 + \frac{q^2}{4} + \frac{1}{4}\Big(\sigma_1^{ik}\sigma_2^{jk}\,q^i q^j \\ &+ (2\vec{p}_1 + \vec{q})(2\vec{p}_2 - \vec{q})\Big)\bigg] + \frac{1}{2}F_1''(0)\,q^2 \\ &+ F_2'(0)\left[\frac{q^2}{4} + \frac{1}{4}\sigma_1^{ik}\sigma_2^{jk}\,q^i q^j\right] + (1\leftrightarrow 2)\Bigg\}. \end{aligned} \tag{122}$$

Transforming the expression from momenta $\vec{p}_1$ and $\vec{p}_2$ to $\vec{P}_1$ and $\vec{P}_2$ and spin-averaging it using the identity

$$\sigma_1^{ik}\sigma_2^{jk}\,q^i q^j = \frac{\sigma_1\cdot\sigma_2}{d}\,q^2\,, \tag{123}$$

we finally obtain

$$\begin{aligned} U(\vec{p}_1,\vec{p}_2,\vec{q}) = e^2\Bigg\{&F_1'(0)\left[-1 + \frac{q^2}{4} + \vec{P}_1\cdot\vec{P}_2 + \frac{\sigma_1\cdot\sigma_2}{4d}\,q^2\right] \\ &+ \frac{1}{2}F_1''(0)\,q^2 + F_2'(0)\left[\frac{q^2}{4} + \frac{\sigma_1\cdot\sigma_2}{4d}\,q^2\right] \\ &+ (1\leftrightarrow 2)\Bigg\}. \end{aligned} \tag{124}$$

The first term in this equation corresponds to the leading-order contribution while the remaining ones are the $\alpha^7 m$

corrections. Using the explicit results for the form factors, we get

$$H_9 = \alpha^2\Big[-\frac{9}{20}q^2 - \vec{P}_1\cdot\vec{P}_2 + \frac{1}{\epsilon}\Big(-\frac{8}{15}q^2 - \frac{4}{3}\vec{P}_1\cdot\vec{P}_2\Big) + \sigma_1\cdot\sigma_2\Big(-\frac{11}{108} - \frac{1}{9\epsilon}\Big)q^2\Big]. \tag{125}$$

8. E_{10}

Next, we have to take into account the exchange of a Coulomb photon between an electron and the nucleus, originating from the Hamiltonian δH_2. This gives a correction in which one vertex is eA^0 while the second one is $-\frac{e}{8}[F_1'(0) + 2F_2'(0) + 4F_1''(0)]\vec{\nabla}^2\vec{\nabla}\cdot\vec{E}$. Only the electron-nucleus part needs to be taken because the complete electron-electron contribution due to derivative of the form factors was accounted for in E_9. So, the term E_{10} is

$$E_{10} = \frac{1}{8}[F_1'(0) + 2F_2'(0) + 4F_1''(0)]\langle\phi|\vec{\nabla}_1^4\Big[-\frac{Z\alpha}{r_1}\Big]_\epsilon|\phi\rangle + (1\leftrightarrow 2). \tag{126}$$

Using the relation (61) and results for the form factors from Appendix A, we evaluate it as (omitting linear in ϵ terms)

$$H_{10} = \alpha^2\Big(-\frac{13}{40} - \frac{11}{30\epsilon}\Big)\Big[-2\Big(E_0 - V - \frac{p_2^2}{2}\Big)Z\,\delta^d(r_1) + \vec{p}_1\,Z\delta^d(r_1)\,\vec{p}_1 + (1\leftrightarrow 2)\Big]. \tag{127}$$

9. E_{11}

We now continue to examine contributions originating from the exchange of the Coulomb photons. The first such contribution, E_{11}, originates from the exchange of a Coulomb photon with one vertex being $\frac{1}{16}\kappa\,\{\vec{p}^2, \vec{\nabla}\cdot\vec{E}\}$. The corresponding contribution is

$$E_{11} = -\tfrac{1}{8}\kappa\,\langle\phi|\vec{p}_1^{\,2}\,\vec{\nabla}_1^2 V|\phi\rangle + (1\leftrightarrow 2). \tag{128}$$

After some simplifications, we get

$$H_{11} = \alpha^2\Big[-\frac{1}{2}\Big(E_0 - V - \frac{p_2^2}{2}\Big)Z\,\delta^d(r_1) + (1\leftrightarrow 2)\Big], \tag{129}$$

where we omitted terms $p_1^2\,\delta^d(r)$ which vanish for triplet states.

10. E_{12} and E_{13}

We treat the terms E_{12} and E_{13} together because they have similar structure. Specifically, they both come from the exchange of a Coulomb photon where one vertex is either $\frac{e^2}{8}\kappa\,\vec{E}_\parallel^2$ or $\delta H_3 = e^2\,\vec{E}_\parallel^{\,2}\,\chi$. We thus have

$$E_{12} + E_{13} = \Big(\frac{\kappa}{8} + \chi\Big)\langle\phi|(\vec{\nabla}_1 V)^2|\phi\rangle + (1\leftrightarrow 2). \tag{130}$$

Taking into account that

$$(\vec{\nabla}_1 V)^2 = \Big[\frac{(Z\alpha)^2}{r_1^4}\Big]_\epsilon - 2\Big[\frac{Z\alpha\,\vec{r}_1}{r_1^3}\Big]_\epsilon\cdot\Big[\frac{\alpha\,\vec{r}}{r^3}\Big]_\epsilon - \pi^2\alpha^2\{1 + \epsilon\,(2\ln 2 - 2\ln q)\}q, \tag{131}$$

we obtain

$$H_{12} + H_{13} = \alpha\Big(\frac{11}{48} - \frac{1}{3\epsilon} + \frac{1}{4}\epsilon\Big)\Big\{\frac{1}{\pi}\Big[\frac{(Z\alpha)^2}{r_1^4}\Big]_\epsilon - \frac{2}{\pi}\Big[\frac{Z\alpha\,\vec{r}_1}{r_1^3}\Big]_\epsilon\cdot\Big[\frac{\alpha\,\vec{r}}{r^3}\Big]_\epsilon + (1\leftrightarrow 2)\Big\} + \pi\alpha^3\Big(-\frac{11}{24} + \frac{2}{3\epsilon} + \frac{4}{3}\ln 2 - \frac{4}{3}\ln q\Big)q. \tag{132}$$

11. E_{14}

E_{14} is induced by the exchange of a Coulomb photon with vertices $-\frac{e}{8}\,(\vec{\nabla}\cdot\vec{E} + \sigma^{ij}\,\{E_\parallel^i, p^j\})$ and $-\frac{e}{4}\,\kappa\,(\vec{\nabla}\cdot\vec{E} + \sigma^{ij}\,\{E_\parallel^i, p^j\})$. The corresponding contribution is

$$E_{14} = \frac{e^2}{32}\kappa\int\frac{d^dk}{(2\pi)^d\,k^2}\langle\phi|\big(k^2 - 2i\sigma_1^{ij}k^i p_1^j\big)\times e^{i\vec{k}\cdot\vec{r}}\,\big(k^2 + 2i\sigma_2^{kl}k^k p_2^l\big)|\phi\rangle + (1\leftrightarrow 2). \tag{133}$$

Simplifying this expression, we get

$$H_{14} = \alpha^2\Big[\frac{1}{8}q^2 + \sigma_1\cdot\sigma_2\Big(\frac{1}{12}\vec{P}_1\cdot\vec{P}_2 - \frac{1}{12}\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}\Big)\Big]. \tag{134}$$

12. E_{15}

E_{15} originates from the one-photon exchange with one vertex $-\frac{e\kappa}{16}\,\{p^k, \partial_t E_\perp^k + \nabla^i B^{ik}\}$ and the other vertex $-e\,\vec{p}\cdot\vec{A}$. We calculate this contribution starting from the corresponding Feynman diagram,

$$\begin{aligned}E_{15} &= \frac{e^2}{16}\kappa\int\frac{d^Dk}{(2\pi)^D i}\frac{(-1)}{\omega^2 - \vec{k}^2}\delta_\perp(k)^{ij}\langle\phi|\big\{p_1^i, (\omega^2 - \vec{k}^2)e^{i\vec{k}\cdot\vec{r}_1}\big\}\\&\quad\times\frac{1}{E_0 - H_0 - \omega + i\epsilon}p_2^j\,e^{-i\vec{k}\cdot\vec{r}_2}|\phi\rangle + \text{H.c} + (1\leftrightarrow 2)\\&= -\frac{e^2}{16}\kappa\int\frac{d^Dk}{(2\pi)^D \mathrm{i}}\delta_\perp(k)^{ij}\langle\phi|\big\{p_1^i, e^{i\vec{k}\cdot\vec{r}_1}\big\}\\&\quad\times\frac{1}{E_0 - H_0 - \omega + i\epsilon}p_2^j\,e^{-i\vec{k}\cdot\vec{r}_2}|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2).\end{aligned} \tag{135}$$

Performing the ω integration and expressing the result in the momentum space, we obtain

$$\begin{aligned}E_{15} &= \frac{e^2}{32}\kappa\int\frac{d^dk}{(2\pi)^d}\delta_\perp^{ij}(k)\langle\phi|\big\{p_1^i, e^{i\vec{k}\cdot\vec{r}}\big\}p_2^j\,|\phi\rangle + \text{H.c.} + (1\leftrightarrow 2)\\&= \alpha^2\Big\langle\frac{1}{2}\vec{P}_1\cdot\vec{P}_2 - \frac{1}{2}\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}\Big\rangle.\end{aligned} \tag{136}$$

13. E_{16}

E_{16} is induced by the exchange of a Coulomb photon with one vertex of the form $-\frac{e\kappa}{16}\,\{p^k, \partial_t E_\parallel^k\}$. The contribution from the corresponding Feynman diagram is

$$E_{16} = \frac{e^2}{16}\kappa \int \frac{d^D k}{(2\pi)^D i}\left(\frac{-1}{\vec{k}^2}\right)\Big\{\langle\phi|\{\vec{p}_1, \vec{k}\omega e^{i\vec{k}\cdot\vec{r}_1}\} \times \frac{1}{E_0 - H_0 - \omega + i\epsilon} e^{-i\vec{k}\cdot\vec{r}_2}|\phi\rangle - \langle\phi|e^{-i\vec{k}\cdot\vec{r}_2}\frac{1}{E_0 - H_0 - \omega + i\epsilon}\{\vec{p}_1, \vec{k}\omega e^{i\vec{k}\cdot\vec{r}_1}\}|\phi\rangle\Big\} + (1 \leftrightarrow 2)\,, \tag{137}$$

where in the second term we introduced a mirror transformation $\vec{k} \to -\vec{k}$. The denominator is now expanded for small $E_0 - H_0$ up to the linear term and the ω integration is performed as

$$\int \frac{d\omega}{2\pi i}\frac{\omega}{(\omega - i\epsilon)^2} = \frac{1}{2}. \tag{138}$$

We then obtain

$$E_{16} = -\frac{e^2}{32}\kappa \int \frac{d^d k}{(2\pi)^d k^2}\Big\{\langle\phi|\{\vec{p}_1, \vec{k}e^{i\vec{k}\cdot\vec{r}_1}\}\Big[\frac{p_2^2}{2}, e^{-i\vec{k}\cdot\vec{r}_2}\Big]|\phi\rangle - \langle\phi|\Big[e^{-i\vec{k}\cdot\vec{r}_2}, \frac{p_2^2}{2}\Big]\{\vec{p}_1, \vec{k}e^{i\vec{k}\cdot\vec{r}_1}\}|\phi\rangle\Big\} + (1 \leftrightarrow 2)$$
$$= -\frac{e^2}{32}\kappa \int \frac{d^d k}{(2\pi)^d k^2}\langle\phi|\big[p_2^2, \{p_1^i, [p_1, e^{i\vec{k}\cdot\vec{r}}]\}\big]|\phi\rangle + (1 \leftrightarrow 2)$$
$$= \frac{\alpha^2}{2}\left\langle\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}\right\rangle. \tag{139}$$

14. Total high-energy part

Adding together all E_i contributions, we arrive at the final result for the high-energy contribution,

$$E_H = \left\langle\frac{\alpha}{\pi}\left\{\frac{11}{48}\left[\frac{(Z\alpha)^2}{r_1^4}\right]_\epsilon - \left(\frac{11}{24} + \frac{\sigma_1\cdot\sigma_2}{16}\right)\left[\frac{Z\alpha\,\vec{r}_1}{r_1^3}\right]_\epsilon \cdot \left[\frac{\alpha\,\vec{r}}{r^3}\right]_\epsilon - \frac{13}{40}\vec{p}_1\,\pi Z\alpha\,\delta^d(r_1)\,\vec{p}_1 + \frac{1}{\epsilon}\left(-\frac{1}{3}\left[\frac{(Z\alpha)^2}{r_1^4}\right]_\epsilon + \frac{2}{3}\left[\frac{Z\alpha\,\vec{r}_1}{r_1^3}\right]_\epsilon\cdot\left[\frac{\alpha\,\vec{r}}{r^3}\right]_\epsilon - \frac{11}{30}\vec{p}_1\,\pi Z\alpha\,\delta^d(r_1)\,\vec{p}_1\right) + \pi Z\alpha\,\delta^d(r_1)\left[\frac{3}{20}\left(E_0 - V - \frac{p_2^2}{2}\right) + \frac{11}{15\epsilon}\left(E_0 - V - \frac{p_2^2}{2}\right)\right] + (1\leftrightarrow 2)\right\} + \pi\alpha^3\left(-\frac{17}{24} - \frac{\sigma_1\cdot\sigma_2}{8} + \frac{2}{3\epsilon} + \frac{4}{3}\ln 2 - \frac{4}{3}\ln q\right)q + \alpha^2\left\{-\frac{1}{2}\vec{P}_1\cdot\vec{P}_2 - \frac{13}{40}q^2 + \frac{1}{\epsilon}\left(-\frac{4}{3}\vec{P}_1\cdot\vec{P}_2 - \frac{8}{15}q^2\right) + \sigma_1\cdot\sigma_2\left[\frac{1}{24}(\vec{P}_1 - \vec{P}_2)^2 + \frac{1}{6}\vec{P}_1\cdot\vec{P}_2 + \left(-\frac{13}{216} - \frac{1}{9\epsilon}\right)q^2 - \frac{1}{24}\frac{[(\vec{P}_1 - \vec{P}_2)\cdot\vec{q}]^2}{q^2}\right]\right\}\right\rangle + \delta\,Z^3\,\langle\delta^d(r_1) + \delta^d(r_2)\rangle\,. \tag{140}$$

Here, δ is as yet undetermined state-independent coefficient, which will be obtained in the next section by matching the hydrogenic result.

VII. TOTAL RESULT FOR $\alpha^7 m$ ONE-LOOP SELF-ENERGY

In this section, we will obtain the total result for the $\alpha^7 m$ one-loop self-energy correction that is beyond the relativistic correction to the Bethe logarithm already calculated in Ref. [15]. We add together the previously calculated parts, namely, the second-order contribution given by Eq. (55), the low-energy contribution given by Eq. (85), the middle-energy contribution given by Eq. (96), and the high-energy contribution given by Eq. (140),

$$E_{\rm SE}^{(7)} = E_{\rm sec,SE}^{(7)} + E_L^\Lambda + E_M + E_H = E_{\rm SE}^A + E_{\rm SE}^B\,. \tag{141}$$

We have split the total result into two parts, $E_{\rm SE}^A$ and $E_{\rm SE}^B$. $E_{\rm SE}^A$ contains those two-body and three-body terms that are already in the coordinate representation, whereas $E_{\rm SE}^B$ consists of the remaining electron-electron two-body terms that are presently written in the momentum representation. We find that all terms $\propto 1/\epsilon$ cancel each other in the sum, so we can make the transition $d \to 3$. The result is still dependent on the intermediate momentum cutoff parameter λ. The examination presented in Appendix C demonstrates that all λ-dependent terms cancel when we add together $E_{\rm SE}^{(7)}$, the photon-exchange contribution derived in Ref. [15], and the Bethe-logarithm corrections calculated in Ref. [14]. Therefore, we can just set $\lambda \to 1$ everywhere. The resulting expression, in atomic units and with the factor α^7 pulled out, is

$$E_{\rm SE}^A = 2\left\langle H_{\rm SE}^{\prime\prime(5)}\frac{1}{(E_0 - H_0)'}H^{\prime\prime(4)}\right\rangle + \frac{1}{\pi}\left(\frac{5}{9} + \frac{1}{3}\mathcal{L}\right)\left\langle H_R'\frac{1}{(E_0 - H_0)'}H_R\right\rangle + \left\langle\frac{1}{\pi}\left\{\frac{163}{240}\frac{Z^2}{r_1^4} - \left(\frac{589}{360} + \frac{7\sigma_1\cdot\sigma_2}{96}\right)\frac{Z\vec{r}_1}{r_1^3}\cdot\frac{\vec{r}}{r^3} + \frac{5}{9}\left[\left(E_0 + \frac{Z}{r_2} - \frac{1}{r}\right)^2\frac{Z}{r_1} + 2\left(E_0 + \frac{Z}{r_2} - \frac{1}{r}\right)\frac{Z^2}{r_1^2} - \frac{1}{2}\,p_1^2\frac{Z}{r_1}\,p_2^2 - \left(E_0 + \frac{Z}{r_2} - \frac{1}{r} - \frac{p_2^2}{2}\right)\frac{Z^2}{r_1^2} + \frac{1}{2}\,\vec{p}_1\,\frac{Z^2}{r_1^2}\,\vec{p}_1 + p_1^i\,\frac{Z}{r_1\,r}\left(\delta^{ij} + \frac{r^i r^j}{r^2}\right)p_2^j\right] + \frac{779}{1800}\,\vec{p}_1\,\pi Z\delta^3(r_1)\,\vec{p}_1 + \mathcal{L}\left(\frac{1}{4}\frac{Z^2}{r_1^4} + \frac{1}{3}\left[\left(E_0 + \frac{Z}{r_2} - \frac{1}{r}\right)^2\frac{Z}{r_1} + 2\left(E_0 + \frac{Z}{r_2} - \frac{1}{r}\right)\frac{Z^2}{r_1^2}\right.\right.$$

$$-\frac{1}{2}\,p_1^2\frac{Z}{r_1}\,p_2^2-\left(E_0+\frac{Z}{r_2}-\frac{1}{r}-\frac{p_2^2}{2}\right)\frac{Z^2}{r_1^2}+\frac{1}{2}\,\vec{p}_1\,\frac{Z^2}{r_1^2}\,\vec{p}_1+p_1^i\,\frac{Z}{r_1\,r}\left(\delta^{ij}+\frac{r^ir^j}{r^2}\right)p_2^j\Bigg]-\frac{2}{3}\frac{Z\vec{r}_1}{r_1^3}\cdot\frac{\vec{r}}{r^3}+\frac{11}{30}\,\vec{p}_1\,\pi Z\delta^3(r_1)\,\vec{p}_1\Bigg)$$
$$+\pi Z\delta^3(r_1)\left[\frac{491}{900}E_0-\frac{491}{900\,r_2}-\frac{509}{900}\frac{Z}{r_2}+\frac{509}{1800}p_2^2+\frac{5}{9}\left\langle\frac{1}{r}\right\rangle+\mathcal{L}\left(-\frac{E_0}{15}+\frac{1}{15\,r_2}-\frac{11}{15}\frac{Z}{r_2}+\frac{11}{30}p_2^2+\frac{1}{3}\left\langle\frac{1}{r}\right\rangle\right)\right]+(1\leftrightarrow 2)\Bigg\}$$
$$+\frac{2E^{(4)}}{\pi}\left(\frac{5}{9}+\frac{1}{3}\mathcal{L}\right)\left(\left\langle\frac{1}{r}\right\rangle-2E_0\right)\Bigg\rangle+\delta\,Z^3\,\langle\delta^3(r_1)+\delta^3(r_2)\rangle\,, \tag{142}$$
$$E_{\rm SE}^{B}=\Bigg\langle-\frac{2}{5}(\vec{P}_1-\vec{P}_2)^2+\frac{919}{1800}q^2+\frac{83}{90}\vec{P}_1\cdot\vec{P}_2-\frac{4}{15}\frac{(\vec{P}_1\cdot\vec{q})(\vec{P}_2\cdot\vec{q})}{q^2}+\mathcal{L}\left(\frac{8}{15}q^2+\frac{4}{3}\vec{P}_1\cdot\vec{P}_2\right)+\sigma_1\cdot\sigma_2\Bigg[\frac{1}{24}(\vec{P}_1-\vec{P}_2)^2$$
$$+\frac{1}{6}\vec{P}_1\cdot\vec{P}_2+\left(\frac{43}{216}+\frac{1}{9}\mathcal{L}\right)q^2\Bigg]+\pi\left(-\frac{799}{360}-\frac{7\sigma_1\cdot\sigma_2}{48}-\frac{4}{3}\mathcal{L}-\frac{4}{3}\ln q-\frac{4}{3}\ln\alpha\right)q\Bigg\rangle. \tag{143}$$

Here, we transformed term $[(\vec{P}_1-\vec{P}_2)\cdot\vec{q}]^2/q^2$ into a three-photon form using Eq. (69). The operators $1/r_1^4$ and $1/r_1^3$ are understood as distributions examined in Appendix E, so that their matrix elements are well defined. $\mathcal{L}$ is obtained from $\ln\Lambda_\epsilon$ by dropping $1/\epsilon$ and $\ln\lambda$, $\mathcal{L}=2\ln(\alpha^{-2})-2\ln 2$.

We now recall that the result (142) is not complete because it contains as yet undefined coefficient δ originating from the electron-nucleus Dirac δ-function terms omitted in our derivation. There are several sources of such terms. One of them is the forward scattering amplitude of the three-photon exchange perturbed by the Breit Hamiltonian, the correction to the current, and the retardation. Furthermore, such terms originate from the singular operator $[Z^2/r_1^4]_\epsilon$.

We now proceed to obtaining the coefficient δ. To this end, we first evaluate the hydrogenic limit of Eq. (142) and compare it with the literature hydrogenic result for the normalized difference $n^3E(nS)-E(1S)$. We should get an agreement because all terms proportional to the electron-nucleus Dirac δ function vanish in the normalized difference. Second, we match the hydrogenic limit of Eq. (142) with the known 1S hydrogenic result and thus obtain the coefficient δ in Eq. (142).

A. Restoration of the electron-nucleus Dirac δ term

Dropping the electron-electron terms, writing $r_1\equiv r$, and omitting terms that do not contribute to the S states, we obtain the hydrogenic limit of Eq. (142) as

$$E_{\rm SE}^{(7)}({\rm hydr},nS)=\frac{1}{\pi}\left(\frac{5}{9}+\frac{1}{3}\mathcal{L}\right)\left\langle H_R'\frac{1}{(E_0-H_0)'}H_R\right\rangle+\Bigg\langle\frac{1}{\pi}\Bigg\{\left(\frac{163}{240}+\frac{1}{4}\mathcal{L}\right)\frac{Z^2}{r^4}+\left(\frac{5}{9}+\frac{1}{3}\mathcal{L}\right)\left(-2E_0^3+E_0\frac{Z^2}{r^2}\right.$$
$$\left.+\frac{1}{2}\vec{p}\,\frac{Z^2}{r^2}\,\vec{p}-4\,E_0E^{(4)}\right)+\left(\frac{779}{1800}+\frac{11}{30}\mathcal{L}\right)\vec{p}\,\pi Z\delta^3(r)\,\vec{p}+E_0\,\pi Z\delta^3(r)\left(\frac{491}{900}-\frac{1}{15}\mathcal{L}\right)\Bigg\}+\delta\,Z^3\,\delta^3(r)\Bigg\rangle. \tag{144}$$

We note that the hydrogenic limit of Eq. (143) vanishes because this expression contains only the electron-electron terms. With help of the formulas from Appendix F, we obtain for the normalized difference

$$\frac{\pi}{Z^6}\left[n^3E_{\rm SE}^{(7)}({\rm hydr},nS)-E_{\rm SE}^{(7)}({\rm hydr},1S)\right]=-\frac{16087}{5400}+\frac{263}{60n}-\frac{7583}{5400n^2}+\frac{163}{30}[\gamma+\Psi(n)-\ln n]$$
$$+\ln\frac{\alpha^{-2}}{2}\left\{-\frac{103}{45}+\frac{4}{n}-\frac{77}{45n^2}+4[\gamma+\Psi(n)-\ln n]\right\}. \tag{145}$$

This result agrees with Eq. (3.43) of Ref. [18] (with the Bethe-logarithm part omitted and with Z set to 1), which indicates consistency of the derived formulas with the hydrogen theory. The reason for setting $Z=1$ in the result of Ref. [18] is that we are now using a different scaling in the low-energy part. In particular, in Eq. (24) we define the Bethe logarithm to be rescaled by a factor of α^2, whereas in Ref. [18] it was rescaled by a factor of $(Z\alpha)^2$.

We will now take into account that for the 1S hydrogenic state, our result (142) should match the one-loop self-energy part of the function F_H given by Eq. (5.116) from Ref. [8], which is

$$F_H=-\frac{121}{60}+\frac{5}{2}\zeta(3)-\frac{5}{18}\pi^2-\frac{61}{90}\ln 2-3\ln^2 2+\ln(Z\alpha)\left(\frac{163}{30}-4\ln 2-4\ln\Lambda\right)-\frac{5}{3}\ln\Lambda-\frac{22}{3}\ln 2\ln\Lambda+\ln^2\Lambda\,. \tag{146}$$

Here, Λ is the intermediate momentum cutoff used in Ref. [8], which is the same as the cutoff Λ in the present work; see Eq. (23). We now restore the cutoff dependence of our result (144) by shifting

$$\mathcal{L}\to\mathcal{L}'=2\ln[\alpha^{-2}]-2\ln(2\lambda)=-2\ln\Lambda-2\ln 2\,. \tag{147}$$

Equation (144) for the $1S$ state thus becomes

$$\frac{\pi}{Z^6} E^{(7)}_{\rm SE}({\rm hydr}, 1S) = -\frac{7271}{1800} + \frac{221}{30}\ln 2 - 4\ln^2 2 + \ln\Lambda\left(\frac{29}{15} - 4\ln 2 - 4\ln Z\right) + \ln Z\left(\frac{163}{30} - 4\ln 2\right) + \delta\,. \tag{148}$$

The matching condition

$$F_H = \frac{\pi}{Z^6} E^{(7)}_{\rm SE}({\rm hydr}, 1S) \tag{149}$$

leads to the following result for δ,

$$\delta = \frac{3641}{1800} - \frac{362}{45}\ln 2 + \ln^2 2 + \frac{5}{2}\zeta(3) - \frac{5}{18}\pi^2 + \ln\alpha\left(\frac{163}{30} - 4\ln 2\right) + \ln\Lambda\left(-\frac{18}{5} - 4\ln\alpha - \frac{10}{3}\ln 2\right) + \ln^2\Lambda\,. \tag{150}$$

Next, we check that the cutoff dependence disappears when Eq. (150) is combined together with the Bethe logarithm. This is done in Appendix D; the conclusion is that we can just replace $\ln\Lambda \to \ln\alpha^2$ in the above expression. In this way, we obtain the final result for the δ coefficient as

$$\delta = \frac{3641}{1800} - \frac{362}{45}\ln 2 + \ln^2 2 + \frac{5}{2}\zeta(3) - \frac{5}{18}\pi^2 + \ln\alpha^{-2}\left(\frac{53}{60} + \frac{16}{3}\ln 2\right) - \ln^2\alpha^{-2}\,. \tag{151}$$

Inserting Eq. (151) into Eq. (142), employing the explicit form of $\mathcal{L}$, and using the identity $\sigma_1\cdot\sigma_2 = 2\,\vec\sigma_1\cdot\vec\sigma_2 = 2$ valid for $d=3$ and triplet states, we obtain for $E^A_{\rm SE}$ the following result:

$$\begin{aligned}
E^A_{\rm SE} =& \left\langle H''^{(5)}_{\rm SE}\frac{1}{(E_0-H_0)'}H''^{(4)}\right\rangle + \frac{1}{\pi}\left(\frac{5}{9} + \frac{2}{3}\ln\frac{\alpha^{-2}}{2}\right)\left\langle H'_R\frac{1}{(E_0-H_0)'}H_R\right\rangle\\
&+\left\langle\frac{1}{\pi}\left\{\frac{163}{240}\frac{Z^2}{r_1^4} + \frac{5}{9}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}\right)^2\frac{Z}{r_1} + \frac{10}{9}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}\right)\frac{Z^2}{r_1^2} - \frac{5}{18}p_1^2\frac{Z}{r_1}p_2^2 - \frac{5}{9}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}-\frac{p_2^2}{2}\right)\frac{Z^2}{r_1^2}\right.\right.\\
&+\frac{5}{18}\vec p_1\frac{Z^2}{r_1^2}\vec p_1 + \frac{5}{9}p_1^i\frac{Z}{r_1 r}\left(\delta^{ij}+\frac{r^ir^j}{r^2}\right)p_2^j - \frac{1283}{720}\frac{Z\vec r_1\cdot\vec r}{r_1^3 r^3} + \frac{779}{1800}\vec p_1\,\pi Z\delta^3(r_1)\,\vec p_1 + \ln\frac{\alpha^{-2}}{2}\left(\frac{1}{2}\frac{Z^2}{r_1^4} - \frac{4}{3}\frac{Z\vec r_1\cdot\vec r}{r_1^3 r^3}\right.\\
&+\frac{11}{15}\vec p_1\,\pi Z\delta^3(r_1)\,\vec p_1 + \frac{2}{3}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}\right)^2\frac{Z}{r_1} + \frac{4}{3}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}\right)\frac{Z^2}{r_1^2} - \frac{1}{3}p_1^2\frac{Z}{r_1}p_2^2 - \frac{2}{3}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}-\frac{p_2^2}{2}\right)\frac{Z^2}{r_1^2}\\
&\left.+\frac{1}{3}\vec p_1\frac{Z^2}{r_1^2}\vec p_1 + \frac{2}{3}p_1^i\frac{Z}{r_1 r}\left(\delta^{ij}+\frac{r^ir^j}{r^2}\right)p_2^j\right) + \pi Z\delta^3(r_1)\left[\frac{491}{900}E_0 - \frac{491}{900\,r_2} - \frac{509}{900}\frac{Z}{r_2} + \frac{509}{1800}p_2^2 + \frac{5}{9}\left\langle\frac{1}{r}\right\rangle + \ln\frac{\alpha^{-2}}{2}\right.\\
&\times\left(-\frac{2E_0}{15} + \frac{2}{15\,r_2} - \frac{22}{15}\frac{Z}{r_2} + \frac{11}{15}p_2^2 + \frac{2}{3}\left\langle\frac{1}{r}\right\rangle\right) + Z^2\left\{\frac{3641}{1800} - \frac{1289}{180}\ln 2 + \frac{16}{3}\ln^2 2 + \frac{5}{2}\zeta(3) - \frac{5}{18}\pi^2 - \ln^2\frac{\alpha^{-2}}{2}\right.\\
&\left.\left.\left.\left.+\ln\frac{\alpha^{-2}}{2}\left(\frac{53}{60}+\frac{10}{3}\ln 2\right)\right\}\right] + (1\leftrightarrow 2)\right\} + \frac{2E^{(4)}}{\pi}\left(\frac{5}{9}+\frac{2}{3}\ln\frac{\alpha^{-2}}{2}\right)\left(\left\langle\frac{1}{r}\right\rangle - 2E_0\right)\right\rangle.
\end{aligned} \tag{152}$$

B. Transformation of $E^B_{\rm SE}$ into coordinate space

The expression for $E^B_{\rm SE}$, given by Eq. (143), is written in momentum space and needs to be transformed into the coordinate representation to make a numerical evaluation tractable. We first express the momenta $\vec P_1$ and $\vec P_2$ in terms of new variables $\vec P$, $\vec p$, and $\vec q$, defined as

$$\vec P = \vec p_1 + \vec p_2\,,\quad \vec p = \tfrac{1}{2}(\vec p_1 - \vec p_2)\,,\quad\text{and}\quad \vec q = \vec p_1{}' - \vec p_1\,. \tag{153}$$

We thus have

$$(\vec P_1 - \vec P_2)^2 = q^2 + 4\,\vec p\cdot\vec p\,'\,,\qquad \vec P_1\cdot\vec P_2 = \frac{1}{4}(P^2 - q^2 - 4\,\vec p\cdot\vec p\,')\,, \tag{154}$$

$$\frac{(\vec P_1\cdot\vec q)(\vec P_2\cdot\vec q)}{q^2} = \left(\frac{1}{4}P^iP^j - p^ip'^j\right)\frac{q^iq^j - \frac{\delta^{ij}}{3}q^2}{q^2} - \frac{1}{4}q^2 + \frac{1}{12}P^2 - \frac{1}{3}\,\vec p\cdot\vec p\,'\,. \tag{155}$$

Furthermore, we employ the relation $\sigma_1\cdot\sigma_2 = 2$ valid in $d=3$ and take into account that the operators $P^2\,\delta^3(r)$ and $p^2\,\delta^3(r)$ vanish for triplet states. Moreover, we perform the replacement $q^2 \to -2\,\vec p\cdot\vec p\,'$ because there are no $q^2\,\ln q$ terms. Performing these transformations and using formulas for the Fourier transform from Appendix G, we bring the expression for $E^B_{\rm SE}$ into the coordinate representation (with the overall factor α^7 pulled out),

$$E^B_{\rm SE} = \bigg\langle -\left(\frac{2108}{675} + \frac{196}{45}\ln\frac{\alpha^{-2}}{2}\right)\vec{p}\,\delta^3(r)\,\vec{p} - \frac{1}{60\pi}P^iP^j\frac{(\delta^{ij}r^2 - 3r^ir^j)}{r^5} + \frac{1}{15\pi}p^i\frac{(\delta^{ij}r^2 - 3r^ir^j)}{r^5}p^j + \frac{1}{3\pi\,r^4}\left(\frac{203}{15} + 6\ln\frac{\alpha^{-2}}{2} - 2\ln 2 - 4\gamma - 4\ln r\right)\bigg\rangle. \tag{156}$$

The final result for the $\alpha^7 m$ one-loop self-energy contribution beyond the Bethe-logarithmic part is given by the sum of Eqs. (152) and (156).

VIII. ONE-LOOP VACUUM POLARIZATION

We now turn to the derivation of the $\alpha^7 m$ correction induced by the one-loop vacuum polarization. Its calculation is much simpler than that of the self-energy. It will be convenient to split the vacuum-polarization correction into the electron-nucleus (en) and the electron-electron (ee) parts,

$$E^{(7)}_{\rm VP} = E^{en}_{\rm VP} + E^{ee}_{\rm VP}\,. \tag{157}$$

The electron vacuum polarization modifies the photon propagator as

$$\frac{g_{\mu\nu}}{q_0^2 - q^2} \to \frac{g_{\mu\nu}}{q_0^2 - q^2}\left[1 - \omega\big(q_0^2 - q^2\big)\right]. \tag{158}$$

Here, the function $\omega(q^2)$ is the Uehling correction defined as

$$\omega(q^2) = \frac{\alpha}{\pi}\,q^2\int_4^\infty d(k^2)\frac{1}{k^2(k^2 - q^2)}u(k^2)\,, \tag{159}$$

where

$$u(k^2) = \frac{1}{3}\sqrt{1 - \frac{4}{k^2}}\left(1 + \frac{2}{k^2}\right). \tag{160}$$

The low-momentum expansion of Eq. (159) is

$$\omega(q^2) = \frac{\alpha}{15\pi}\,q^2 + \frac{\alpha}{140\pi}\,q^4 + \cdots\,. \tag{161}$$

In the coordinate representation and for the electron-nucleus interaction, these expansion terms give rise to the following corrections to the Coulomb potential,

$$\delta V^{(1)} = -\frac{4\,\alpha^2}{15}Z\,\delta^d(r_1) + (1 \leftrightarrow 2)\,, \tag{162}$$

$$\delta V^{(2)} = -\frac{\alpha^2}{35}\vec{\nabla}^2 Z\,\delta^d(r_1) + (1 \leftrightarrow 2)\,. \tag{163}$$

A. Electron-nucleus vacuum polarization

We start with the electron-nucleus part of the vacuum polarization. The corresponding correction is represented as a sum of four parts,

$$E^{en}_{\rm VP} = E^{en}_{\rm sec} + E^{en}_L + E^{en}_H + E^{en}_{\rm WK}\,, \tag{164}$$

where $E^{en}_{\rm sec}$ is the second-order Uehling correction, E^{en}_L and E^{en}_H are the low-energy and the high-energy Uehling contributions, respectively; and $E^{\rm WK}_{\rm VP}$ is the Wichman-Kroll part. The low- and the high-energy contributions are induced by the exchanged momentum of the order $\alpha\,m$ and m, respectively.

The low-energy part E^{en}_L is induced by an effective operator H^{en}_L, $E^{en}_L = \langle H^{en}_L\rangle$, which is evaluated as

$$\begin{aligned} H^{en}_L &= \delta V^{(2)} + \frac{1}{8}\vec{\nabla}^2\,\delta^{(1)}V \\ &= -\frac{13\,\alpha^2}{210}\vec{\nabla}^2 Z\,\delta^d(r_1) + (1 \leftrightarrow 2) \\ &= \frac{13\,\alpha^2}{105}\left[2\left(E_0 - V - \frac{p_2^2}{2}\right)Z\,\delta^d(r_1) - \vec{p}_1\,Z\,\delta^d(r_1)\,\vec{p}_1\right]. \end{aligned} \tag{165}$$

The second-order contribution is

$$E^{en}_{\rm sec} = 2\left\langle\delta V^{(1)}\,\frac{1}{(E_0 - H_0)'}\,H'^{(4)}\right\rangle. \tag{166}$$

Rewriting it as

$$E^{en}_{\rm sec} = -\frac{2\alpha}{15\pi}\left\langle[\vec{P},[V,\vec{P}]]\,\frac{1}{(E_0 - H_0)'}\,H'^{(4)}\right\rangle, \tag{167}$$

we obtain the second-order correction we encountered earlier. The result thus is

$$\begin{aligned} E^{en}_{\rm sec} = -\frac{2\alpha}{15\pi}\Bigg(\left\langle H'_R\frac{1}{(E_0 - H_0)'}H_R\right\rangle + \left\langle E^{(4)}\right\rangle\!\left(\left\langle\frac{2\alpha}{r}\right\rangle - 4E_0\right) + \Bigg\{\left[2E_0 - \frac{2\alpha}{r_2} + \left\langle\frac{\alpha}{r}\right\rangle + \frac{(Z\alpha)^2}{2\epsilon} - 2(Z\alpha)^2\right]\pi Z\alpha\,\delta^3(r_1) \\ -\frac{1}{4}\frac{(Z\alpha)^2}{r_1^4} + \left(E_0 + \frac{Z\alpha}{r_2} - \frac{\alpha}{r}\right)^2\frac{Z\alpha}{r_1} + 2\left(E_0 + \frac{Z\alpha}{r_2} - \frac{\alpha}{r}\right)\frac{(Z\alpha)^2}{r_1^2} - \left(E_0 + \frac{Z\alpha}{r_2} - \frac{\alpha}{r} - \frac{p_2^2}{2}\right)\frac{(Z\alpha)^2}{r_1^2} \\ +\frac{1}{2}\vec{p}_1\frac{(Z\alpha)^2}{r_1^2}\,\vec{p}_1 - \frac{1}{2}p_1^2\,\frac{Z\alpha}{r_1}\,p_2^2 + p_1^i\,\frac{Z\alpha^2}{r_1\,r}\left(\delta^{ij} + \frac{r^ir^j}{r^2}\right)p_2^j + (1 \leftrightarrow 2)\Bigg\}\Bigg)\,. \end{aligned} \tag{168}$$

The high-energy part is expressed as

$$E_H^{en} = (4\pi Z\alpha)^3\,\phi^2(0)\int\frac{d^dq_1}{(2\pi)^d}\int\frac{d^dq_2}{(2\pi)^d}\frac{1}{(\vec q_1)^4\,(\vec q_2)^4\,(\vec q_{12})^2}\mathrm{Tr}\Big[(\not p_1+1)\gamma_0(\not p_2+1)\frac{(\gamma_0+I)}{4}\Big]$$
$$\times\big[\omega\big(-\vec q_1^{\,2}\big)+\omega\big(-\vec q_2^{\,2}\big)+\omega\big(-\vec q_{12}^{\,2}\big)\big], \tag{169}$$

where $\vec q_{12}=\vec q_1-\vec q_2$ and $p_i=(1,\vec q_i)$. We evaluate the trace as

$$\mathrm{Tr}\Big[(\not p_1+1)\gamma_0(\not p_2+1)\frac{(\gamma_0+I)}{4}\Big]=4+\vec q_1\cdot\vec q_2\,. \tag{170}$$

Denoting the part of E_H induced by the first term in the right-hand side of Eq. (170) as E_{H1}, we obtain

$$E_{H1}=-\frac{\alpha(4\pi Z\alpha)^3}{\pi}\,4\phi^2(0)\int_4^\infty d(k^2)\int\frac{d^dq_1}{(2\pi)^d}\int\frac{d^dq_2}{(2\pi)^d}\frac{u(k^2)}{k^2}\frac{1}{q_1^4\,q_2^4\,\vec q_{12}^{\,2}}\left(\frac{q_1^2}{k^2+q_1^2}+\frac{q_2^2}{k^2+q_2^2}+\frac{\vec q_{12}^{\,2}}{k^2+\vec q_{12}^{\,2}}\right). \tag{171}$$

We evaluate this integral with help of the following formula:

$$\int\frac{d^dk}{(2\,\pi)^d}\int\frac{d^dq}{(2\,\pi)^d}\,\frac{1}{[k^2]^{n_1}}\,\frac{1}{[(k-q)^2]^{n_2}}\,\frac{1}{[q^2+m^2]^{n_3}}$$
$$=\frac{m^{2\,(d-n_1-n_2-n_3)}}{(4\,\pi)^d}\,\frac{\Gamma(d/2-n_1)\,\Gamma(d/2-n_2)\,\Gamma(n_1+n_2-d/2)\,\Gamma(n_1+n_2+n_3-d)}{\Gamma(n_1)\,\Gamma(n_2)\,\Gamma(n_3)\,\Gamma(d/2)}\,. \tag{172}$$

In the special case of $m=0$, the integral vanishes because of the dimensional regularization. We obtain

$$E_{H1}=-\frac{2}{7}\alpha^4\,\langle Z^3\delta^3(r_1)+Z^3\delta^3(r_2)\rangle\,. \tag{173}$$

Similarly, we evaluate the contribution due to the second term in the right-hand side of Eq. (170),

$$E_{H2}=\alpha^4\left(-\frac{32}{225}+\frac{1}{15\epsilon}\right)\langle Z^3\delta^3(r_1)+Z^3\delta^3(r_2)\rangle\,. \tag{174}$$

The final result for the one-loop Uehling electron-nucleus vacuum polarization (in atomic units) is

$$E_{\rm Ue}^{en}=E_{\rm sec}^{en}+\langle H_L^{en}\rangle+E_H^{en}=-\frac{2}{15\pi}\,\bigg\{\Big\langle H_R'\frac{1}{(E_0-H_0)'}H_R\Big\rangle+\Big\langle E^{(4)}\Big(\Big\langle\frac{2}{r}\Big\rangle-4E_0\Big)$$
$$+\bigg\{\bigg(\frac{1}{7}E_0-\frac{1}{7\,r_2}-\frac{13Z}{7\,r_2}+\frac{13p_2^2}{14}+\Big\langle\frac{1}{r}\Big\rangle+\frac{127}{105}Z^2-2Z^2\ln\alpha\bigg)\pi Z\delta^3(r_1)-\frac{1}{4}\frac{Z^2}{r_1^4}+\Big(E_0+\frac{Z}{r_2}-\frac{1}{r}\Big)^2\frac{Z}{r_1}$$
$$+2\Big(E_0+\frac{Z}{r_2}-\frac{1}{r}\Big)\frac{Z^2}{r_1^2}+\frac{13}{14}\vec p_1\,\pi Z\delta^3(r_1)\,\vec p_1-\Big(E_0+\frac{Z}{r_2}-\frac{1}{r}-\frac{p_2^2}{2}\Big)\frac{Z^2}{r_1^2}+\frac{1}{2}\vec p_1\,\frac{Z^2}{r_1^2}\,\vec p_1$$
$$-\frac{1}{2}p_1^2\,\frac{Z}{r_1}\,p_2^2+p_1^i\,\frac{Z}{r_1\,r}\Big(\delta^{ij}+\frac{r^ir^j}{r^2}\Big)\,p_2^j+(1\leftrightarrow 2)\bigg\}\Big\rangle\bigg\}\,. \tag{175}$$

The term with $\ln\alpha$ comes from rescaling of the operator $(Z\alpha)^2/r_1^4$ into atomic units. The hydrogenic limit of this expression for nS states is (with $r_1\equiv r$)

$$E_{\rm Ue}^{en}(\mathrm{hydr},nS)=-\frac{2}{15\pi}\,\bigg\{\Big\langle H_R'\frac{1}{(E_0-H_0)'}H_R\Big\rangle+\Big\langle-4E_0E^{(4)}-2E_0^3+\Big(\frac{1}{7}E_0+\frac{127}{105}Z^2+Z^2\ln\alpha^{-2}\Big)\pi Z\delta^3(r)$$
$$-\frac{1}{4}\frac{Z^2}{r^4}+E_0\frac{Z^2}{r^2}+\frac{1}{2}\vec p\,\frac{Z^2}{r^2}\,\vec p\Big\rangle\bigg\}. \tag{176}$$

Using the expectation values of operators from Appendix F, we get

$$E_{\rm Ue}^{en}(\mathrm{hydr},nS)=Z^6\left[\frac{19}{35\,n^5}-\frac{4}{15\,n^4}-\frac{1724}{1575\,n^3}+\frac{4}{15\,n^3}\Big(\gamma+\Psi(n)-\ln\frac{n}{2}\Big)-\frac{2}{15n^3}\ln[(Z\alpha)^{-2}]\right], \tag{177}$$

in agreement with the known result [22].

To complete our treatment of the electron-nucleus vacuum polarization, we have to include the Wichman-Kroll correction, which is purely a Dirac-δ-like type of contribution. It is given by

$$E_{\rm WK}^{en}=\left(\frac{19}{45}-\frac{\pi^2}{27}\right)\langle Z^3\,\delta^3(r_1)+Z^3\,\delta^3(r_2)\rangle. \tag{178}$$

B. Electron-electron vacuum polarization

The electron-electron part of the vacuum polarization is simpler to evaluate because the corresponding high-energy and second-order contributions vanish for triplet states. The low-energy part consists of two parts. The first one is due to the q^4 term of the expansion (161). Denoting the corresponding operator as H^{ee}_{L1}, we obtain

$$\begin{aligned} H^{ee}_{L1} &= \delta V^{(2)} = \frac{\alpha^2}{35}\vec{\nabla}_1^2 \delta^d(r) + (1 \leftrightarrow 2) \\ &= \frac{4\alpha^2}{35}\vec{p}\,\delta^d(r)\,\vec{p}\,. \end{aligned} \tag{179}$$

The remaining part of the electron-electron contribution is induced by the $q_0^2 - q^2$ term of the expansion (161). For its calculation, we again use the scattering amplitude approach in the Feynman gauge, like in the derivation of E_9 in the one-loop self-energy calculation. In this case, the perturbed vertex is

$$\Gamma^\mu = -\frac{\alpha}{15\,\pi}\big(q_0^2 - q^2\big)\,\gamma^\mu \equiv \alpha_{\rm VP}\big(q_0^2 - q^2\big)\,\gamma^\mu. \tag{180}$$

Again, we pull out the factor $q_0^2 - q^2$ and cancel it with the same factor in the denominator of the photon propagator. The derivation then proceeds in the same way as in the self-energy calculation, leading to the result

$$\begin{aligned} U(\vec{p}_1, \vec{p}_2, \vec{q}) = \alpha_{\rm VP} e^2\bigg[-1 + \frac{q^2}{4} + \vec{P}_1\cdot\vec{P}_2 + \frac{\sigma_1\cdot\sigma_2}{4\,d}\,q^2\bigg] \\ + (1 \leftrightarrow 2)\,. \end{aligned} \tag{181}$$

The first term here corresponds to the leading vacuum polarization correction, whereas the remaining terms are the $\alpha^7 m$ corrections. We now transform them into the coordinate representation with help of the following transformations,

$$\vec{P}_1\cdot\vec{P}_2 = \frac{1}{4}(\vec{P}^2 - \vec{q}^{\,2} - 4\,\vec{p}\cdot\vec{p}^{\,\prime})\,, \tag{182}$$

$$\vec{q}^{\,2} \to -2\,\vec{p}\cdot\vec{p}^{\,\prime}\,, \tag{183}$$

$$\sigma_1\cdot\sigma_2 \to 2\,, \tag{184}$$

where the second and third equations are valid for triplet states. We then get

$$H^{ee}_{L2} = -\alpha_{\rm VP} e^2\,\frac{8}{3}\vec{p}\,\delta^3(r)\,\vec{p} = \left(\frac{4\alpha^2}{15}\right)\frac{8}{3}\vec{p}\,\delta^3(r)\,\vec{p}\,. \tag{185}$$

The total electron-electron part of the $\alpha^7 m$ vacuum polarization is the sum of H^{ee}_{L1} and H^{ee}_{L2}, with the result in atomic units

$$H^{ee}_{\rm VP} = \frac{52}{63}\,\vec{p}\,\delta^3(r)\,\vec{p}\,. \tag{186}$$

C. Total vacuum polarization

Adding together the electron-nucleus and the electron-electron parts, we get the final result for the one-loop vacuum polarization to the order $\alpha^7 m$ in atomic units,

$$\begin{aligned} E^{(7)}_{\rm VP} = -\frac{2}{15\pi}\bigg\{\bigg\langle H'_R\frac{1}{(E_0 - H_0)'}H_R\bigg\rangle + \bigg\langle E^{(4)}\bigg(\bigg\langle\frac{2}{r}\bigg\rangle - 4E_0\bigg) \\ + \bigg[\bigg(\frac{1}{7}E_0 - \frac{1}{7\,r_2} - \frac{13Z}{7\,r_2} + \frac{13p_2^2}{14} + \bigg\langle\frac{1}{r}\bigg\rangle + \frac{127}{105}Z^2 + Z^2\ln\alpha^{-2}\bigg)\pi Z\delta^3(r_1) - \frac{1}{4}\frac{Z^2}{r_1^4} + \bigg(E_0 + \frac{Z}{r_2} - \frac{1}{r}\bigg)^2\frac{Z}{r_1} \\ + 2\bigg(E_0 + \frac{Z}{r_2} - \frac{1}{r}\bigg)\frac{Z^2}{r_1^2} + \frac{13}{14}\vec{p}_1\,\pi Z\delta^3(r_1)\,\vec{p}_1 - \bigg(E_0 + \frac{Z}{r_2} - \frac{1}{r} - \frac{p_2^2}{2}\bigg)\frac{Z^2}{r_1^2} + \frac{1}{2}\vec{p}_1\,\frac{Z^2}{r_1^2}\,\vec{p}_1 - \frac{1}{2}p_1^2\,\frac{Z}{r_1}\,p_2^2 \\ + p_1^i\,\frac{Z}{r_1\,r}\bigg(\delta^{ij} + \frac{r^i r^j}{r^2}\bigg)\,p_2^j + (1 \leftrightarrow 2)\bigg]\bigg\rangle\bigg\} + \bigg\langle\frac{52}{63}\vec{p}\,\delta^3(r)\,\vec{p} + \bigg(\frac{19}{45} - \frac{\pi^2}{27}\bigg)[Z^3\,\delta^3(r_1) + Z^3\,\delta^3(r_2)]\bigg\rangle. \end{aligned} \tag{187}$$

IX. TWO-LOOP AND THREE-LOOP CONTRIBUTIONS

The two-loop radiative contribution is proportional to the electron-nucleus Dirac δ function and is obtained immediately from the hydrogenic result,

$$E^{(7)}_{\rm rad2} = \frac{Z^2}{\pi}\,\langle\delta^3(r_1) + \delta^3(r_2)\rangle\,B_{50}\,, \tag{188}$$

where the coefficient B_{50} is known only numerically [9,10,23], $B_{50} = -21.554\,47\,(13)$.

After dropping the part contributing to the fine structure, the three-loop radiative correction becomes also proportional to the electron-nucleus Dirac δ function and is given by [24,25]

$$\begin{aligned} E^{(7)}_{\rm rad3} = \frac{Z}{\pi^2}\,\langle\delta^3(r_1) + \delta^3(r_2)\rangle\bigg[-\frac{568\,{\rm a}_4}{9} + \frac{85\,\zeta(5)}{24} \\ - \frac{121\,\pi^2\,\zeta(3)}{72} - \frac{84\,071\,\zeta(3)}{2304} - \frac{71\,\ln^4 2}{27} \\ - \frac{239\,\pi^2\,\ln^2 2}{135} + \frac{4787\,\pi^2\,\ln 2}{108} + \frac{1591\,\pi^4}{3240} \\ - \frac{252\,251\,\pi^2}{9720} + \frac{679\,441}{93\,312}\bigg]\,, \end{aligned} \tag{189}$$

where ${\rm a}_4 = \sum_{n=1}^{\infty} 1/(2^n\,n^4) = 0.517\,479\,061\ldots.$

X. SUMMARY

In this work, we derived the radiative $\alpha^7 m$ QED correction for the triplet states of a two-electron atom. This correction consists of the one-loop self-energy part $E^{(7)}_{\rm SE}$ given by the sum of Eqs. (152) and (156), the one-loop vacuum-polarization part $E^{(7)}_{\rm VP}$ given by Eq. (187), the two-loop part $E^{(7)}_{\rm rad2}$ given by Eq. (188), and the three-loop part $E^{(7)}_{\rm rad3}$ given by Eq. (189).

In order to obtain the complete $\alpha^7 m$ QED correction, we have to add to the above mentioned contributions the nonradiative photon exchange part $E^{(7)}_{\rm exch}$ derived in Ref. [15] and the relativistic correction to the Bethe logarithm $E^{(7)}_L$ from Ref. [14]. More specifically, the photon-exchange correction is

$$E^{(7)}_{\rm exch} = \langle H^{(7)}_{\rm exch}\rangle + 2\Big\langle H^{(4)} \frac{1}{(E_0 - H_0)'} H^{(5)}_{\rm exch}\Big\rangle, \tag{190}$$

where $H^{(7)}_{\rm exch}$ and $H^{(5)}_{\rm exch}$ are given, correspondingly, by Eqs. (156) and (10) of Ref. [15], and the Bethe-logarithm correction is

$$E^{(7)}_L = E^{(7)}_{L1} + E^{(7)}_{L2} + E^{(7)}_{L3}, \tag{191}$$

with $E^{(7)}_{L1}$, $E^{(7)}_{L2}$, and $E^{(7)}_{L3}$ given by Eqs. (14), (20), and (27) of Ref. [14], respectively.

The final step of our project will be the numerical evaluation of all $\alpha^7 m$ QED corrections. The most complicated part of the computation is already accomplished in Ref. [14], where we obtained numerical results for the relativistic corrections to the Bethe logarithm for the $2\,^3S$ and $2\,^3P$ states. A computation of the remaining photon-exchange and radiative contributions looks relatively straightforward. The only additional feature as compared to our previous calculations of higher order QED corrections in helium [6,26] is the appearance of singular operators with $\ln r$, such as $\ln r/r^4$ in Eq. (156). Matrix elements of such operators should be understood in terms of a special limit, as discussed in Appendix E. In particular, the regularized operator $\ln r/r^4$ is defined by Eq. (E3). We are currently working on developing an effective computational scheme for such operators.

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APPENDIX A: ELECTROMAGNETIC FORM FACTORS

The electromagnetic form factors F_1 and F_2 of an electron are defined as

$$\gamma_\mu \to \Gamma_\mu = \gamma_\mu + \gamma_\mu F_1(q_0^2 - q^2) + \frac{i}{2m} F_2(q_0^2 - q^2)\Big(\frac{i}{2}\Big)[\gamma_\mu, \not{q}], \tag{A1}$$

where q is the outgoing photon momentum. The small-q expansion of the one-loop form factors in $D = 4 - 2\epsilon$ is [27]

$$F_1^{(1)}(q^2) = \frac{\alpha}{\pi}\bigg[q^2\Big(-\frac{1}{8} - \frac{1}{6\epsilon} - \frac{1}{2}\epsilon\Big) + q^4\Big(-\frac{11}{240} - \frac{1}{40\epsilon} - \frac{5}{48}\epsilon\Big)\bigg], \tag{A2}$$

$$F_2^{(1)}(q^2) = \frac{\alpha}{\pi}\bigg[\frac{1}{2} + 2\epsilon + q^2\Big(\frac{1}{12} + \frac{5}{12}\epsilon\Big) + q^4\Big(\frac{1}{60} + \frac{11}{120}\epsilon\Big)\bigg]. \tag{A3}$$

APPENDIX B: INTEGRATIONS IN SPHEROIDAL COORDINATES IN *d* DIMENSIONS

To introduce the spheroidal coordinates in d dimensions, we start with the volume element in the spherical coordinates in $d-1$ dimensions, with variable z for the last dimension,

$$dV = r^{d-2} dr\, dz\, \Omega_{d-1}. \tag{B1}$$

Let us define

$$r_1 = \sqrt{r^2 + \Big(z + \frac{a}{2}\Big)^2}, \tag{B2}$$

$$r_2 = \sqrt{r^2 + \Big(z - \frac{a}{2}\Big)^2}, \tag{B3}$$

and introduce spheroidal variables ξ and η as

$$\xi = \frac{r_1 + r_2}{a}, \tag{B4}$$

$$\eta = \frac{r_1 - r_2}{a}. \tag{B5}$$

The following relations hold:

$$z = \frac{\xi\,\eta}{2}, \tag{B6}$$

$$r^2 = \frac{1}{4}(\xi^2 - 1)(1 - \eta^2). \tag{B7}$$

In the new coordinates, the volume element is

$$dV = \Big(\frac{a}{2}\Big)^d \Omega_{d-1}[(\xi^2 - 1)(1 - \eta^2)]^{\frac{d-3}{2}} \times (\xi - \eta)(\xi + \eta)\, d\xi\, d\eta, \tag{B8}$$

and $\eta \in (-1, 1)$, $\xi \in (1, \infty)$.

We now consider the integral of the form

$$\begin{aligned}\int d^d k\, f\Big(\Big|\vec{k} + \frac{\vec{a}}{2}\Big|, \Big|\vec{k} - \frac{\vec{a}}{2}\Big|\Big) &= \int d^d k\, f(r_1, r_2) \\ &= \Big(\frac{a}{2}\Big)^d \Omega_{d-1} \int d\xi\, d\eta\, [(\xi^2 - 1)(1 - \eta^2)]^{\frac{d-3}{2}} \\ &\quad \times (\xi - \eta)(\xi + \eta)\, f\Big(a\frac{(\xi + \eta)}{2}, a\frac{(\xi - \eta)}{2}\Big).\end{aligned} \tag{B9}$$

In spheroidal coordinates, it is just a two-dimensional integral over ξ and η.

The particular case of such an integral with integer powers i and j

$$J_{ij} = \int d^d k \, \frac{1}{\left|\vec{k}+\frac{\vec{q}}{2}\right|^i} \frac{1}{\left|\vec{k}-\frac{\vec{q}}{2}\right|^j} \frac{1}{\left|\vec{k}+\frac{\vec{q}}{2}\right|+\left|\vec{k}-\frac{\vec{q}}{2}\right|} \tag{B10}$$

can be transformed to the spheroidal coordinates as

$$J_{ij} = q^{d-i-j-1}\, 2^{i+j-d}\, \Omega_{d-1} \int_1^\infty d\xi \int_{-1}^1 d\eta \times [(\xi^2-1)(1-\eta^2)]^{\frac{d-3}{2}} (\xi-\eta)^{1-j}(\xi+\eta)^{1-i}\, \frac{1}{\xi}. \tag{B11}$$

The integrations over ξ and η can now be performed for each particular i and j, yielding results in agreement with those from Appendix C of Ref. [15]. The advantage of using the spheroidal coordinates, however, is that this approach can be applied also to noninteger values of i and j, in particular, for the case when they are equal to d, which is needed in the evaluation of the middle-energy contribution.

APPENDIX C: CANCELATION OF THE λ DEPENDENCE

In this section, we demonstrate that the sum of all $\alpha^7 m$ terms depending on the intermediate momentum cutoff λ vanishes. The dimensionless cutoff parameter λ appears when the integral over the photon momentum k is divided into the $k < \Lambda$ and $k > \Lambda$ regions, $\Lambda = \alpha^2\lambda$; see Eq. (23). In order to cancel the λ-dependent terms, we need to add the radiative contribution calculated in this work, the nonradiative photon-exchange contribution from Ref. [15], and the Bethe-logarithm correction from Ref. [14].

We first address the λ-dependent part of the radiative correction from Eqs. (55) and (85). Denoting it as $E^\lambda_{\rm rad}$, we have

$$\begin{aligned} E^\lambda_{\rm rad} = \ln\lambda \Bigg\{ &-\frac{2}{3\pi}\left\langle H_R' \frac{1}{(E_0-H_0)'} H_R\right\rangle + \langle\phi|\frac{1}{\pi}\bigg\{\pi Z\delta^d(r_1)\bigg[-\frac{2}{15}\left(-E_0+\frac{1-11Z}{r_2}+\frac{11}{2}p_2^2\right)-\frac{2}{3}\left\langle\frac{1}{r}\right\rangle\bigg] \\ &-\frac{1}{2}\frac{Z^2}{r_1^4}+\frac{5}{3}\frac{Z\vec{r}_1}{r_1^3}\cdot\frac{\vec{r}}{r^3}-\frac{11}{15}p_1^i\,\pi Z\delta^d(r_1)\,p_1^i-\frac{2}{3}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}\right)^2\frac{Z}{r_1}-\frac{4}{3}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}\right)\frac{Z^2}{r_1^2} \\ &+\frac{1}{3}p_1^2\frac{Z}{r_1}p_2^2+\frac{4}{3}E_0E^{(4)}-\frac{2}{3}E^{(4)}\left\langle\frac{1}{r}\right\rangle+\frac{2}{3}Y_1-\frac{2}{3}p_1^i\frac{Z}{r_1 r}\left(\delta^{ij}+\frac{r^ir^j}{r^2}\right)p_2^j+(1\leftrightarrow 2)\bigg\} \\ &-\frac{8}{3}\vec{P}_1\cdot\vec{P}_2-\frac{16}{15}q^2-\frac{4}{3}\frac{[(\vec{P}_1-\vec{P}_2)\cdot\vec{q}]^2}{q^2}-\frac{2q^2}{9}\sigma_1\cdot\sigma_2+\frac{10\pi}{3}q|\phi\rangle\Bigg\}. \end{aligned} \tag{C1}$$

Second, we need to account for the λ-dependent part of the nonradiative photon-exchange correction derived in our previous paper [15]. It is

$$\begin{aligned} E^\lambda_{\rm exch} = \ln\lambda\Bigg\langle &\bigg\{\frac{8}{15}\left[p_1^i,\left[\frac{Z}{r_1},p_1^j\right]\right]\left(-4\delta^{ij}+\frac{q^iq^j}{q^2}\right)\frac{1}{q^2}-\frac{7}{15\pi}\frac{Z\vec{r}_1}{r_1^3}\cdot\frac{\vec{r}}{r^3}+(1\leftrightarrow 2)\bigg\}+\frac{4}{5}(\vec{P}_1-\vec{P}_2)^2 \\ &+\frac{16}{15}q^2+\frac{8}{3}\vec{P}_1\cdot\vec{P}_2+\frac{4}{3}\frac{[(\vec{P}_1-\vec{P}_2)\cdot\vec{q}]^2}{q^2}+\frac{2q^2}{9}\sigma_1\cdot\sigma_2-\frac{6\pi}{5}q\Bigg\rangle. \end{aligned} \tag{C2}$$

It is advantageous to use this form of the expression in the momentum representation and not the final formula in the coordinate representation presented in Ref. [15] because of strong cancellation of the electron-electron terms in the sum with Eq. (C1). Adding the two contributions and then transforming this result into the coordinate representation with help of formulas from Appendix G, we obtain for $E^\lambda = E^\lambda_{\rm exch} + E^\lambda_{\rm rad}$ the result

$$\begin{aligned} E^\lambda = \ln\lambda\Bigg\{ &-\frac{2}{3\pi}\left\langle H_R'\frac{1}{(E_0-H_0)'}H_R\right\rangle+\langle\phi|\frac{1}{\pi}\bigg\{\pi Z\delta^d(r_1)\bigg[-\frac{2}{15}\left(-E_0-\frac{41}{3r_2}-\frac{11Z}{r_2}+\frac{11}{2}p_2^2\right) \\ &-\frac{2}{3}\left\langle\frac{1}{r}\right\rangle\bigg]-\frac{1}{2}\frac{Z^2}{r_1^4}+\frac{6}{5}\frac{Z\vec{r}_1\cdot\vec{r}}{r_1^3r^3}-\frac{11}{15}p_1^i\,\pi Z\delta^d(r_1)\,p_1^i-\frac{2}{3}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}\right)^2\frac{Z}{r_1}-\frac{4}{3}\left(E_0+\frac{Z}{r_2}-\frac{1}{r}\right)\frac{Z^2}{r_1^2} \\ &+\frac{1}{3}p_1^2\frac{Z}{r_1}p_2^2+\frac{4}{3}E_0E^{(4)}-\frac{2}{3}E^{(4)}\left\langle\frac{1}{r}\right\rangle+\frac{2}{3}Y_1-\frac{2}{3}p_1^i\frac{Z}{r_1r}\left(\delta^{ij}+\frac{r^ir^j}{r^2}\right)p_2^j+\frac{Z}{15}\frac{\left(\delta^{ij}r_1^2-3\,r_1^ir_1^j\right)}{r_1^3}\frac{r^ir^j}{r^3} \\ &+(1\leftrightarrow 2)\bigg\}+\frac{8}{5}\vec{p}\,\delta^d(r)\,\vec{p}-\frac{32}{15\pi}\frac{1}{r^4}|\phi\rangle\Bigg\}. \end{aligned} \tag{C3}$$

E^λ has to be combined with the λ-dependent part of the relativistic correction to the Bethe logarithm, which will be denoted as $E^\lambda_{\rm Bethe}$. It is given by the sum of the contributions induced by the asymptotic coefficients given in Eqs. (A7), (A10), (B7), (B9), (C21), and (C24) of Ref. [14], which is

$$E^{\lambda}_{\rm Bethe} = \ln\lambda\biggl\{\frac{2}{3\pi}\biggl\langle H'_R\frac{1}{(E_0-H_0)'}H_R\biggr\rangle + \langle\phi|\frac{1}{\pi}\biggl\{\pi Z\delta^d(r_1)\biggl[-\frac{2}{15}\biggl(E_0+\frac{41}{3r_2}+\frac{11Z}{r_2}-\frac{11}{2}p_2^2\biggr) + \frac{2}{3}\biggl\langle\frac{1}{r}\biggr\rangle\biggr] - \frac{6}{5}\frac{Z\vec r_1\cdot\vec r}{r_1^3r^3} + \frac{11}{15}p_1^i\,\pi Z\delta^d(r_1)\,p_1^i + \frac{2}{3}\biggl(E_0+\frac{Z}{r_2}-\frac{1}{r}\biggr)^2\frac{Z}{r_1} + \frac{4}{3}\biggl(E_0+\frac{Z}{r_2}-\frac{1}{r}\biggr)\frac{Z^2}{r_1^2} - \frac{Z^3}{r_1^3} - \frac{1}{3}\,p_1^2\frac{Z}{r_1}\,p_2^2 - \frac{4}{3}E_0\,E^{(4)} + \frac{2}{3}E^{(4)}\biggl\langle\frac{1}{r}\biggr\rangle - \frac{5}{3}Y_1 + \frac{2}{3}\,p_1^i\,\frac{Z}{r_1\,r}\biggl(\delta^{ij}+\frac{r^ir^j}{r^2}\biggr)p_2^j - \frac{Z}{15}\frac{\bigl(\delta^{ij}r_1^2-3\,r_1^ir_1^j\bigr)}{r_1^3}\frac{r^ir^j}{r^3} + (1\leftrightarrow 2)\biggr\} - \frac{8}{5}\vec p\,\delta^d(r)\,\vec p + \frac{32}{15\pi}\frac{1}{r^4}|\phi\rangle\biggr\}. \tag{C4}$$

We now take into account the identity

$$\frac{Z^2}{r_1^4} = -2\frac{Z^3}{r_1^3} - 2Y_1 - 12Z^3\pi\,\delta^d(r_1)\,, \tag{C5}$$

where we should drop the second term on the right-hand side, in accordance with the procedure of omitting all the electron-nucleus δ-like contributions at this stage of the derivation. Therefore, we find that $E^{\lambda}+E^{\lambda}_{\rm Bethe}=0$.

The cancellation of the λ-dependent terms proportional to the pure electron-nucleus Dirac δ function is demonstrated in Appendix D. After we checked that all λ-dependent terms vanish as they should, we can just set $\lambda\to 1$ in all final formulas.

APPENDIX D: CANCELATION OF THE λ DEPENDENCE IN THE HYDROGENIC LIMIT

In Appendix C, we proved that all λ-dependent $\alpha^7 m$ terms vanish, with the exception of pure electron-nucleus Dirac-δ contributions, which were omitted in the derivation. The δ-like contribution was restored in Sec. VII A by matching our results against the known hydrogenic limit. Here we will show that the λ-dependent terms proportional to the electron-nucleus Dirac δ function in the hydrogenic limit vanish as well.

Let us return to the λ-dependent part of the relativistic correction to the Bethe logarithm from Ref. [14], now keeping the δ-like terms. Performing the hydrogenic limit and taking only terms contributing to S states, we have

$$E^{\lambda}_{\rm Bethe}\,({\rm hydr}) = \ln\lambda\,\biggl(\frac{2}{3\pi}\biggl\langle H'_R\frac{1}{(E_0-H_0)'}H_R\biggr\rangle + \langle\phi|\frac{1}{\pi}\biggl\{\pi Z\delta^d(r)\biggl[Z^2\biggl(-\frac{12}{5}+\frac{10}{3}\ln 2-\ln\lambda\biggr)-\frac{2}{15}E_0\biggr] + \frac{11}{15}p^i\,\pi Z\delta^d(r)\,p^i - \frac{4}{3}E_0^3 - \frac{1}{3}E_0\frac{Z^2}{r^2} - \frac{Z^3}{r^3} + \frac{5}{6}\vec p\,\frac{Z^2}{r^2}\,\vec p - \frac{8}{3}E_0\,E^{(4)}\biggr\}|\phi\rangle\biggr). \tag{D1}$$

Using results for the matrix elements from Appendix F, we obtain for the $1S$ state

$$E^{\lambda}_{\rm Bethe}({\rm hydr},\,1S) = -\ln^2\lambda + \ln\lambda\biggl(\frac{5}{3}+\frac{22}{3}\ln 2\biggr). \tag{D2}$$

Switching to the same cutoff Λ as in F_H from Eq. (146), $\Lambda=\alpha^2\lambda$, we see that all cutoff-dependent terms cancel in the sum $E^{\lambda}_{\rm Bethe}({\rm hydr},\,1S)+F_H$.

APPENDIX E: EXPECTATION VALUES OF SINGULAR OPERATORS

In our derivation, we encounter expectation values of several singular operators, which need to be evaluated in the coordinate representation. These expectation values should be understood in the sense of a distribution. Specifically, the expectation values of the operators $1/r^3$, $1/r^4$, and $\ln r/r^4$ are defined by the following limits:

$$\langle\phi|\frac{1}{r^3}|\psi\rangle \equiv \lim_{a\to 0}\int d^3r\,\phi^*(\vec r)\psi(\vec r)\biggl[\frac{1}{r^3}\Theta(r-a)+4\pi\,\delta^3(r)(\gamma+\ln a)\biggr] = \lim_{a\to 0}\int_a^\infty dr\,\frac{f(r)}{r} + f(0)\,(\gamma+\ln a)\,, \tag{E1}$$

$$\langle\phi|\frac{1}{r^4}|\psi\rangle \equiv \lim_{a\to 0}\int_a^\infty dr\,\frac{f(r)}{r^2} - \frac{f(0)}{a} + f'(0)\,(\gamma+\ln a)\,, \tag{E2}$$

$$\langle\phi|\frac{\ln r}{r^4}|\psi\rangle \equiv \lim_{a\to 0}\int_a^\infty dr\,\frac{f(r)\,\ln r}{r^2} - f(0)\,\frac{(1+\ln a)}{a} + f'(0)\,\frac{\ln^2 a}{2}\,, \tag{E3}$$

where

$$f(r) = \int d\Omega\, \phi^*(\vec{r})\, \psi(\vec{r})\,. \tag{E4}$$

APPENDIX F: HYDROGENIC EXPECTATION VALUES

Here we list the expectation values of various $\alpha^7\, m$ operators for the hydrogenic S states. They are

$$E_0 = -\frac{Z^2}{2n^2}\,, \tag{F1}$$

$$E^{(4)} = Z^4\bigg(\frac{3}{8n^4} - \frac{1}{2n^3}\bigg), \tag{F2}$$

$$\frac{Z^2}{r^4} = \frac{8Z^6}{n^3}\bigg[-\frac{5}{3} + \frac{1}{2n} + \frac{1}{6n^2} + \gamma + \Psi(n) - \ln\frac{n}{2Z}\bigg], \tag{F3}$$

$$\frac{Z^3}{r^3} = \frac{4Z^6}{n^3}\bigg[\frac{1}{2} - \frac{1}{2n} - \gamma - \Psi(n) + \ln\frac{n}{2Z}\bigg], \tag{F4}$$

$$\frac{Z^2}{r^2} = \frac{2Z^4}{n^3}\,, \tag{F5}$$

$$\vec{p}\,\frac{Z^2}{r^2}\,\vec{p} = Z^6\bigg(-\frac{2}{3n^5} + \frac{8}{3n^3}\bigg), \tag{F6}$$

$$\vec{p}\,\pi Z\delta^d(r)\,\vec{p} = 0\,, \tag{F7}$$

$$\pi Z\delta^d(r_1) = \frac{Z^4}{n^3}\,, \tag{F8}$$

where $\Psi(n) = \Gamma'(n)/\Gamma(n)$. The expectation value of Z^3/r^3 and Z^2/r^4 were calculated according to the definitions in Appendix E. Note that the terms with $\ln Z$ originate from the rescaling $r \to Z^{-1}\, r$, which was needed for the correct matching of our results with the hydrogenic limit; see discussion under Eq. (145).

The hydrogenic limit of the second-order correction is

$$\bigg\langle H'_R \frac{1}{(E_0 - H_0)'} H_R \bigg\rangle = Z^6\bigg(-\frac{1}{n^6} - \frac{4}{3n^5} + \frac{3}{n^4} + \frac{7}{3n^3}\bigg), \tag{F9}$$

where the operators H_R and H'_R act on ket states as

$$H_R|\phi\rangle = \bigg[-\frac{1}{2}\bigg(E_0 + \frac{Z}{r}\bigg)^2 - \frac{Z}{4}\frac{\vec{r}\cdot\vec{\nabla}}{r^3}\bigg]|\phi\rangle\,, \tag{F10}$$

$$H'_R|\phi\rangle = -2Z\frac{\vec{r}\cdot\vec{\nabla}}{r^3}|\phi\rangle\,. \tag{F11}$$

APPENDIX G: FOURIER TRANSFORM

Here we list the formulas needed to transform our formulas from momentum space into the coordinate representation. The results are [15]

$$\int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot\vec{r}}\, \frac{4\pi}{q^2} = \frac{1}{r}\,, \tag{G1}$$

$$\int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot\vec{r}}\, 4\pi\, \frac{q^i}{q^2} = i\frac{r^i}{r^3}\,, \tag{G2}$$

$$\int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot\vec{r}}\, 4\pi\, \frac{q^iq^j - \frac{\delta^{ij}}{3}q^2}{q^2} = \frac{\delta^{ij}r^2 - 3r^ir^j}{r^5}\,, \tag{G3}$$

$$\int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot\vec{r}}\, 4\pi\, \frac{q^iq^j}{q^4} = \frac{1}{2r^3}(\delta^{ij}r^2 - r^ir^j). \tag{G4}$$

The transformation of singular operators $1/r^4$ and $\ln r/r^4$ is more complicated. Here we present results valid for triplet states [15]

$$\begin{aligned}\int d^3r\, e^{i\vec{q}\cdot\vec{r}}\,\frac{1}{r^4} &= \lim_{\varepsilon\to 0}\int d^3r\, e^{i\vec{q}\cdot\vec{r}}\left[\frac{1}{r^4}\theta(r-\varepsilon) - 4\pi\,\delta^3(r)\,\frac{1}{\varepsilon}\right]\\ &= \lim_{\varepsilon\to 0} 2\pi\int_{-1}^{1}dx\int_{\varepsilon}^{\infty}\frac{dr}{r^2}\,e^{iqrx} - \frac{4\pi}{\varepsilon}\\ &= -\pi^2\,q \end{aligned} \tag{G5}$$

and

$$\begin{aligned}\int d^3r\, e^{i\vec{q}\cdot\vec{r}}\,\frac{\ln r}{r^4} &= \lim_{\varepsilon\to 0}\int d^3r\, e^{i\vec{q}\cdot\vec{r}}\left[\frac{\ln r}{r^4}\,\theta(r-\varepsilon) - 4\pi\,\delta^3(r)\,\frac{1+\ln\varepsilon}{\varepsilon}\right]\\ &= \lim_{\varepsilon\to 0} 2\pi\int_{-1}^{1}dx\int_{\varepsilon}^{\infty}\frac{dr}{r^2}\,\ln r\, e^{iqrx} - 4\pi\,\frac{1+\ln\varepsilon}{\varepsilon}\\ &= \pi^2\left(-\frac{3}{2}+\gamma+\ln q\right)q\,. \end{aligned} \tag{G6}$$

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