Self-energy of an electron bound in a Coulomb field

J. Zamastil and V. Patkóš
Department of Chemical Physics and Optics, Charles University, Faculty of Mathematics and Physics, Ke Karlovu 3, 121 16 Prague 2, Czech Republic

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The evaluation method of the one-loop self-energy of the electron bound in a Coulomb field is described. The method combines the relativistic multipole expansion with the free-particle approximation in the virtual states without breaking any integrations of pieces. The relativistic multipole expansion is based on a single assumption: except for the part of the time component of the electron four-momentum corresponding to the electron rest mass, the exchange of four-momentum between the virtual electron and photon can be treated perturbatively. This assumption holds very well, except for the electron virtual states with very high three-momentum. It is shown that for such virtual states one can always rearrange the pertinent expression in a way that allows the electron to be treated as free. The fraction of the free-particle approximation contained in the relativistic multipole expansion carried out to a given order is precisely determined. Furthermore, it is pointed out that in the virtual states with very large wave numbers the electron ceases to feel the Coulomb force from the nucleus for arbitrarily strong fields. This results in a simple scaling behavior of the integrals over the large electron wave numbers. This in turn enables us to avoid a decomposition of convergent integrals into the sum of divergent integrals encountered earlier. By taking the method up to the ninth order and estimating the remainder of the series, the result obtained for the ground state of the hydrogen atom differs from the other result of comparable accuracy by two parts in 10^9. This amounts to the difference of 18 Hz for $2s$-$1s$ transition in hydrogen. This is by four orders smaller than the uncertainty in determination of the proton radius. With an increasing nuclear charge Z, the rate of convergence of the expansion slows down. Nonetheless, the obtained results are in very good agreement with the results obtained by partial wave expansion up to $Z = 90$.

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I. INTRODUCTION

The Lamb shift in hydrogenlike atoms presents a classic and, up to this time, one of the most precise tests of QED [1–4]. It is customary to write the Lamb shift on general S state as

$$\Delta E_n = \frac{n^3 \Delta E_n - \Delta E_1}{n^3} + \frac{\Delta E_1}{n^3}, \tag{1}$$

where the first and the second terms of the right member will be referred to as the state-dependent and the state-independent parts, respectively. The state-independent part of the self-energy effect for the S states is by far the dominant contribution to the Lamb shift in ordinary atoms [1–4]. Therefore, considerable effort has been devoted to an evaluation of this part of the effect [5–14].

The renormalized expression for the self-energy in the nonrecoil limit reads (for notation and units used, see [15])

$$\Delta E = \langle O - \Delta m \rangle = \langle \psi | \gamma_0 (O - \Delta m) | \psi \rangle, \tag{2}$$

where Δm stands for the electromagnetic mass of the electron. The regularized mass operator O reads

$$O = \frac{\alpha}{\pi} \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2 - \lambda)^2} \gamma_\mu \frac{1}{\gamma \cdot (\Pi - k) - m} \gamma_\mu \tag{3}$$

and the wave function ψ of the reference state is a solution of the stationary Dirac equation with the energy E,

$$(\gamma \cdot \Pi - m)\psi = 0. \tag{4}$$

In the case that only the fine structure of the spectral lines is of interest, the components of physical momentum Π of the particle are taken to be those in the external Coulomb field

$$\Pi = \left(E + \frac{Z\alpha}{R}, \vec{P} \right), \tag{5}$$

where $\vec{P}$ is the canonical three-momentum.

The difficulty in the evaluation of Eq. (2) is usually stated as follows [2,6,7,10]. In the region of short wavelengths of the virtual photon the momentum imparted on the electron is so high that, in the first approximation, the electron can be in the virtual states treated as free. The problem can then be formulated as a manageable problem of radiation correction to multiple scattering of the electron by the external Coulomb field. However, such an approach fails when one integrates over long wavelengths of the virtual photon. In that region, the effect of the binding potential has to be treated nonperturbatively. On the other hand, to a first approximation, the motion of the electron in that region is nonrelativistic and a dipole approximation for the interaction of the electron and photon can be used. The problem with the long wavelengths emerges because of the zero photon mass. Indeed, when the effect of the vacuum polarization is evaluated, the finite electron mass provides a natural cutoff for small momenta of the virtual electron. The potential expansion of the electron propagator can be used without any difficulty. The leading term of the expansion yields Uehling potential. This is, for light atoms, by far the dominant contribution to the effect of vacuum polarization [1,2].

The different treatment of different wavelengths of the virtual photon persists also in a calculation based on the partial wave expansion (PWE) [12,13].

Following [8,9], we multiply $1/[\gamma \cdot (\Pi - k) - m]$ in Eq. (3) by $[\gamma \cdot (\Pi - k) + m]/[\gamma \cdot (\Pi - k) + m]$ from the right. Using the Dirac equation and properties of γ matrices [15] we get

$$\langle O\rangle = -\frac{\alpha}{2\pi}\left\langle \gamma_\mu\left(G_4\Pi_\mu - \frac{m}{2}G\cdot\gamma\gamma_\mu\right)\right\rangle, \tag{6}$$

where

$$G_{4,\nu} = (-4)\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2-\lambda)^2}\frac{(1,k_\nu/m)}{k^2-2k\cdot\Pi+H}. \tag{7}$$

Here the second-order Hamilton operator H [8] reads

$$\begin{aligned} H &= (\gamma\cdot\Pi+m)(\gamma\cdot\Pi-m)\\ &= \Pi\cdot\Pi - m^2 + \tfrac{1}{4}[\Pi_\mu,\Pi_\nu][\gamma_\mu,\gamma_\nu]. \end{aligned} \tag{8}$$

Recently, an expansion of the electron propagator has been suggested [16–18]. This expansion will be referred to as a relativistic generalization of multipole expansion (RME). This expansion is based on a single assumption, namely, that the four-momentum Π of the bound electron in the virtual states is dominated by the four-momentum ε of the electron at rest:

$$\frac{1}{k^2-2k\cdot\varepsilon+H-2k\cdot(\Pi-\varepsilon)} = \frac{1}{z-\tilde{H}_0-\lambda\tilde{H}_1}. \tag{9}$$

Here the propagator is written in a generic form $(z-\tilde{H})^{-1}$, where $\tilde{H} = \tilde{H}_0+\lambda\tilde{H}_1$ is a generic Hamilton operator. Furthermore, λ is a formal perturbation parameter that is eventually set to one,

$$\varepsilon = (m,0,0,0) \tag{10}$$

and

$$z = k^2-2k\cdot\varepsilon,\quad \tilde{H}_0 = -H,\quad \lambda\tilde{H}_1 = 2k\cdot(\Pi-\varepsilon). \tag{11}$$

Once the renormalization of the electron mass is made, each term of the expansion is finite both in the infrared and ultraviolet regions when one integrates over four-momentum k of the virtual photon. From this standpoint, there are two regions that cannot be simultaneously covered by a single approximation, but they are characterized by the electron, not the photon, wave numbers. The squared Hamilton operator H, Eq. (8), with four-momentum Π given by Eq. (5) has for the continuous part of the spectrum eigenvalues [16,19]

$$\begin{aligned} -\frac{H}{m^2} &= (Z\alpha)^2\left[1+k_e^2(l_0+1)^2\right],\quad k_e\in(0,\infty),\\ l_0+1 &= \sqrt{1-(Z\alpha)^2}. \end{aligned} \tag{12}$$

The low- and high-energy regions are given by the discrete part of the spectrum and k_e up to, say, $(Z\alpha)^{-1}$ and by k_e ranging from $(Z\alpha)^{-1}$ to infinity, respectively. In the low-energy region the convergence of the RME is very fast. As discussed in detail in [17], the energy shift for non-S states and the state-dependent part of the S states is determined nearly completely by this low-energy part. Thus, very accurate results can be obtained in these cases just by considering a few terms of RME [17]. *This reduces the problem to the calculation of the ground state* [see Eq. (1)]. In the high-energy region the RME yields, after initially fast convergence, slowly convergent series. However, in this region, a simplification appears. Namely, under the circumstances to be specified later, the free-particle approximation of the electron propagator can be used. As shown in [18] and in a substantially simpler way here, if the RME is truncated after a finite number of terms, one can exactly determine how much of the free-particle result is contained in it. Therefore, the part of RME causing the worst convergence problems can be precisely summed up to the infinite order. When considering the self-energy effect of the light hydrogenlike ions, this is the greatest advantage of the RME over the method used in [12–14] based on PWE.

The paper is organized as follows. In Sec. II we use partial wave expansion to integrate out spinor-angular degrees of freedom. Section III contains the essence of the method. It shows how the individual terms of the RME are generated. The electron propagator is successively expanded in spatial and time components of $\Pi-\varepsilon$. Further, the four-momentum of the virtual photon is integrated out. The only remaining integration is then the integration over the continuous part of the hydrogen spectrum. Furthermore, the relation between RME and $Z\alpha$ expansion is clarified. In Sec. IV the numerical results are presented and discussed. Appendices are devoted to additional technical issues. In Appendix A we determine the contribution of the virtual electron states with very large wave numbers. This is achieved in several steps. First, we use a nonrelativistic model introduced in [18]. Second, we specify the conditions under which a free-particle approximation is allowed. Third, we show how to convert the nonrelativistic model in such a form. Finally, the integration over the photon and electron variables is performed. In Appendix B we discuss further applications of the nonrelativistic model. In Appendix C we show how to obtain an asymptotic expansion of the hypergeometric function needed in Sec. III. In Appendix D, the integration over four-momentum of the virtual photon is described in some detail. Finally, in Appendix E the behavior of the integrands for the large electron wave numbers encountered in integration over the continuous part of the hydrogen spectrum in Sec. III is derived.

II. ANGULAR-SPINOR INTEGRATION

We insert Eq. (7) into Eq. (6) and use the equation

$$\frac{1}{k^2-2k\cdot\Pi+H} = e^{i\vec{k}\cdot\vec{R}}\frac{1}{k^2-2k_0\Pi_0+H+\omega^2}e^{-i\vec{k}\cdot\vec{R}}. \tag{13}$$

The strategy is to separate the radial and spinor-angular degrees of freedom. We do so in the spectral decomposition of the Hamilton operator H, in the action of the momentum operator Π on the reference state function ψ and by decomposition of the plane wave $\exp\{\pm i\vec{k}\cdot\vec{R}\}$ into spherical waves. After this has been done we integrate out angular-spinor variables of the electron and photon.

A. Spectral decomposition of the squared Hamilton operator

First, we use the spectral resolution of the Hamilton operator H, Eq. (8), with Π given by Eq. (5),

$$f(H) = \sum_{\Gamma,K,j,m,l_\Gamma} f\left(H_{l_\Gamma}\right)\frac{|\Gamma,K,j,m\rangle\langle\Gamma,K,j,m|\gamma_0}{\langle\Gamma,K,j,m|\gamma_0|\Gamma,K,j,m\rangle} \tag{14}$$

[see Eq. (45) of [16]]. Here Γ, K, $j(j+1)$, and m denote the eigenvalues of the relativistic generalization of the angular momentum operator [16,19], the relativistic parity operator, and the square and the third component of the total angular momentum, respectively. The eigenvalues Γ and K read [16,19]

$$\Gamma=\rho|\Gamma|,\quad \rho=\pm1,\quad |\Gamma|=\sqrt{(j+1/2)^2-(Z\alpha)^2} \tag{15}$$

and

$$K=\pi|K|,\quad \pi=\pm1,\quad |K|=j+1/2. \tag{16}$$

$|\Gamma,K,j,m\rangle$ are the corresponding eigenvectors. Their explicit form reads

$$|\Gamma,K,j,m\rangle=\begin{pmatrix} c_1\langle\vec{n}|j,m\rangle^{\pi}\\ c_2\langle\vec{n}|j,m\rangle^{-\pi}\end{pmatrix}, \tag{17}$$

where the symbol $\langle\vec{n}|j,m\rangle^{\pi}$ denotes the spherical spinors and

$$c_1=\frac{Z\alpha}{(2|K|)^{1/2}(|K|-\pi\Gamma)},\quad c_2=-\frac{i}{Z\alpha}(K-\Gamma)c_1. \tag{18}$$

The radial Hamiltonians H_{l_Γ} in the right member of Eq. (14) stand for [16,19]

$$H_{l_\Gamma}=E^2-m^2+2\frac{EZ\alpha}{R}-\left(P_R^2+\frac{l_\Gamma(l_\Gamma+1)}{R^2}\right), \tag{19}$$

where the effective orbital quantum number l_Γ reads

$$l_\Gamma=\delta_{\rho,1}(|\Gamma|-1)+\delta_{\rho,-1}|\Gamma|. \tag{20}$$

The eigenvalues of the discrete part of the spectrum of H_{l_Γ} are obtained from Eq. (12) by the substitution $k_e\to -i/n$, where $n=n_r+l_\Gamma+1$, $n_r=0,1,2,\ldots$.

The radial part of the wave function of the ground state reads

$$\langle r|l_0+1,l_0\rangle=C_{l_0+1,l_0}r^{l_0}e^{-r/(l_0+1)}, \tag{21}$$

where l_0 is given by Eq. (12), C_{l_0+1,l_0} is a normalization constant to be explicitly specified below, and r is the electron radial variable in atomic units. The transition from natural to atomic units is

$$R=\frac{r}{EZ\alpha}. \tag{22}$$

The energy E of the ground state reads

$$\frac{E}{m}=\sqrt{1-(Z\alpha)^2}. \tag{23}$$

The subscript 0 on the quantum numbers will refer to the quantum numbers of the ground state,

$$\Gamma_0=\sqrt{1-(Z\alpha)^2},\quad K_0=1,\quad j_0=\tfrac{1}{2},\quad m_0=\pm\tfrac{1}{2}. \tag{24}$$

B. Action of momentum operator on the reference function

The action of the electron four-momentum Π on the wave function ψ of the ground state, $\langle r|\psi\rangle=\langle r|l_0+1,l_0\rangle|\Gamma_0,K_0,j_0,m_0\rangle$, will be written in the form

$$\frac{(\Pi-\varepsilon)_\mu}{m}\psi=\left(O_\mu^0+\frac{O_\mu^{-1}}{r}\right)\psi, \tag{25}$$

where

$$O_\mu^0=\left(\frac{E-m}{m},\frac{iEZ\alpha}{m(l_0+1)}\vec{n}\right) \tag{26}$$

and

$$O_\mu^{-1}=\left(\frac{E}{m}(Z\alpha)^2,\frac{(-i)EZ\alpha}{m}(\vec{\nabla}^n+l_0\vec{n})\right). \tag{27}$$

The angular differential operator $\vec{\nabla}^n$ is given in Eq. (108) of [16]. The action of the space components of the momentum operator was evaluated by means of Eq. (107) of [16] and Eq. (21).

C. Partial wave expansion

We insert Eqs. (7), (13), and (25) into Eq. (6). Writing further

$$\vec{k}=\omega\vec{\eta},$$
$$\int d^4k_F\,f_r(k^2,\omega)f_a(\vec{\eta})=\int\frac{d\Omega_\eta}{4\pi}f_a(\vec{\eta})\int d^4k_F\,f_r(k^2,\omega) \tag{28}$$

and concentrating on the angular part we are to integrate the expressions

$$\int\frac{d\Omega_\eta}{4\pi}\langle O_1\exp\{i\vec{k}\cdot\vec{R}_1\}f(H)O_2\exp\{-i\vec{k}\cdot\vec{R}_2\}r_2^c\rangle \tag{29}$$

and

$$\int\frac{d\Omega_\eta\eta_i}{4\pi}\langle\gamma_0\exp\{i\vec{k}\cdot\vec{R}_1\}f(H)\gamma_i\gamma_0\exp\{-i\vec{k}\cdot\vec{R}_2\}\rangle. \tag{30}$$

In expression (29) O_1 and O_2 are in general the spinor-angular operators whose concrete forms will be considered in the moment. The superscript c on r in (29) is equal to 0 or -1. The actual value depends on the operator O_2 and can be read of Eqs. (6) and (25). The subscripts 1 and 2 on the operators O and R indicate only if these operators appear before (1) or after (2) of the operator function $f(H)$. Inserting Eq. (14) and a decomposition of the plane wave into spherical waves

$$e^{i\vec{k}\cdot\vec{R}}=4\pi\sum_{L=0}^{\infty}i^L j_L(\omega R)\sum_{m_p=-L}^{L}Y_{L,m_p}^*(\vec{n})Y_{L,m_p}(\vec{\eta}) \tag{31}$$

into expressions (29) and (30) we separate the radial and spinor-angular operators

$$(29)=\sum_{L,\rho,j}\langle l_0+1,l_0|j_L(\omega R_1)f\big(H_{l_\Gamma}\big)j_L(\omega R_2)r_2^c|l_0+1,l_0\rangle \times\sum_{\pi}\Theta_{O_1,O_2}(L,j,\rho,\pi) \tag{32}$$

and

$$(30)=\sum_{L,L'=L\pm1,\rho,j}\langle l_0+1,l_0|j_L(\omega R_1)f\big(H_{l_\Gamma}\big)j_{L'}(\omega R_2) \times|l_0+1,l_0\rangle\sum_{\pi}\Theta_{\gamma_0\eta_i,\gamma_i\gamma_0}(L,L',j,\rho,\pi). \tag{33}$$

In more detail, insertion of Eq. (31) and its complex conjugate into expressions (29) and (30) leads to the double summation over L and L'. The integration over the direction of the virtual photon together with orthonormality of spherical harmonics and selection rules for SO(3) vector operators enforces $L'=L$ and $L'=L\pm1$ on the right members of Eqs. (32) and

(33), respectively. By means of Wigner-Eckart theorem and matrix elements of SO(3) vector operators we obtain for the spinor-angular part of the integration

$$\Theta_{\gamma_0,1} = 4\pi \sum_{m,m_p} \frac{\langle \Gamma_0,K_0,j_0,m_0|Y^*_{L,m_p}|\Gamma,K,j,m\rangle\langle\Gamma,K,j,m|\gamma_0 Y_{L,m_p}|\Gamma_0,K_0,j_0,m_0\rangle}{\langle\Gamma,K,j,m|\gamma_0|\Gamma,K,j,m\rangle}$$
$$= \left(\left|c_1^0\right|^2|c_1|^2 - \left|c_2^0\right|^2|c_2|^2\right)\frac{K}{\Gamma}[\delta_{\pi,1}\delta_{j,L+1/2}(L+1) + \delta_{\pi,-1}\delta_{j,L-1/2}L], \quad (34)$$

$$\Theta_{\gamma_i,n_i} = 4\pi \sum_{m,m_p} \frac{\langle \Gamma_0,K_0,j_0,m_0|\gamma_0\gamma_i Y^*_{L,m_p}|\Gamma,K,j,m\rangle\langle\Gamma,K,j,m|\gamma_0 n_i Y_{L,m_p}|\Gamma_0,K_0,j_0,m_0\rangle}{\langle\Gamma,K,j,m|\gamma_0|\Gamma,K,j,m\rangle}$$
$$= -i\frac{Z\alpha}{2}\frac{K}{\Gamma}\left\{\delta_{\pi,1}\left(\delta_{j,L-(1/2)}\frac{(L-1)}{(2L-1)}[L-(\Gamma_0+\Gamma)] + \delta_{j,L+(3/2)}\frac{(L+1)}{(2L+3)}(L+1+\Gamma_0+\Gamma)\right)\right.$$
$$\left. + \delta_{\pi,-1}\left(\delta_{j,L+(1/2)}\frac{(L+2)}{(2L+3)}(L+1+\Gamma_0+\Gamma) + \delta_{j,L-(3/2)}\frac{L}{(2L-1)}[L-(\Gamma_0+\Gamma)]\right)\right\}, \quad (35)$$

$$\Theta_{\gamma_i,\nabla_i^n} = 4\pi \sum_{m,m_p} \frac{\langle \Gamma_0,K_0,j_0,m_0|\gamma_0\gamma_i Y^*_{L,m_p}|\Gamma,K,j,m\rangle\langle\Gamma,K,j,m|\gamma_0 Y_{L,m_p}\nabla_i^n|\Gamma_0,K_0,j_0,m_0\rangle}{\langle\Gamma,K,j,m|\gamma_0|\Gamma,K,j,m\rangle}$$
$$= -i\frac{Z\alpha}{2}\frac{1}{\Gamma}\left\{\delta_{\pi,1}\left(\delta_{j,L-(1/2)}L\left(K-\Gamma+(K_0-\Gamma_0)\frac{L}{(2L-1)}\right) + \delta_{j,L+(3/2)}(K_0-\Gamma_0)\frac{(L+1)(L+2)}{(2L+3)}\right)\right.$$
$$\left. + \delta_{\pi,-1}\left(\delta_{j,L+(1/2)}(L+1)\left(K-\Gamma+(K_0-\Gamma_0)\frac{(L+1)}{(2L+3)}\right) + \delta_{j,L-(3/2)}(K_0-\Gamma_0)\frac{L(L-1)}{(2L-1)}\right)\right\}, \quad (36)$$

$$\Theta_{\gamma_i,\gamma_0\gamma_i} = 4\pi \sum_{m,m_p} \frac{\langle \Gamma_0,K_0,j_0,m_0|\gamma_0\gamma_i Y^*_{L,m_p}|\Gamma,K,j,m\rangle\langle\Gamma,K,j,m|\gamma_i Y_{L,m_p}|\Gamma_0,K_0,j_0,m_0\rangle}{\langle\Gamma,K,j,m|\gamma_0|\Gamma,K,j,m\rangle}$$
$$= \frac{1}{4\Gamma}\left\{\left(3(\Gamma_0+1)(\Gamma-K)L - (\Gamma_0-1)(K+\Gamma)\frac{L(2L+1)}{2L-1}\right)\delta_{j,L-(1/2)}\delta_{\pi,1}\right.$$
$$+ \left(3(\Gamma_0+1)(\Gamma-K)(L+1) - (\Gamma_0-1)(K+\Gamma)\frac{(L+1)(2L+1)}{2L+3}\right)\delta_{j,L+(1/2)}\delta_{\pi,-1}$$
$$\left. - 4(K+\Gamma)(\Gamma_0-1)\left(\frac{(L+1)(L+2)}{2L+3}\delta_{j,L+(3/2)}\delta_{\pi,1} + \frac{L(L-1)}{2L-1}\delta_{j,L-(3/2)}\delta_{\pi,-1}\right)\right\} \quad (37)$$

and

$$-\Theta_{\gamma_0\eta_i,\gamma_i\gamma_0}(L,L') = 4\pi \sum_{m,m_p,m'_p} \int \frac{d\Omega_\eta \eta_i}{4\pi} \frac{\langle \Gamma_0,K_0,j_0,m_0|Y^*_{L,m_p}(\vec{n})Y_{L,m_p}(\vec{\eta})|\Gamma,K,j,m\rangle}{\langle\Gamma,K,j,m|\gamma_0|\Gamma,K,j,m\rangle}$$
$$\times \langle\Gamma,K,j,m|\gamma_i Y_{L',m'_p}(\vec{n})Y^*_{L',m'_p}(\vec{\eta})|\Gamma_0,K_0,j_0,m_0\rangle i^L(-i)^{L'}. \quad (38)$$

Here,

$$-\Theta_{\gamma_0\eta_i,\gamma_i\gamma_0}(L,L'=L-1) = \frac{Z\alpha}{4\Gamma}\left\{\delta_{j,L+(1/2)}\delta_{\pi,1}\frac{2L(L+1)}{(2L+1)}[\Gamma_0-K_0-(\Gamma+K)]\right.$$
$$\left. - \delta_{j,L-(1/2)}\delta_{\pi,-1}L\left(\frac{\Gamma_0-K_0-(\Gamma+K)}{(2L+1)} - (\Gamma-K)+\Gamma_0+K_0\right)\right\}$$

and

$$-\Theta_{\gamma_0\eta_i,\gamma_i\gamma_0}(L,L'=L+1) = -\frac{Z\alpha}{4\Gamma}\left\{\delta_{j,L-(1/2)}\delta_{\pi,-1}\frac{2L(L+1)}{(2L+1)}[\Gamma_0-K_0-(\Gamma+K)]\right.$$
$$\left. + \delta_{j,L+(1/2)}\delta_{\pi,1}(L+1)\left(\frac{\Gamma_0-K_0-(\Gamma+K)}{(2L+1)} + \Gamma-K-(\Gamma_0+K_0)\right)\right\}.$$

In [16] we have found that

$$-\Theta_{\gamma_\mu\eta_i,\gamma_i\gamma_\mu} = -2\Theta_{\gamma_0\eta_i,\gamma_i\gamma_0} \tag{39}$$

so the term $\Theta_{\gamma_j\eta_i,\gamma_i\gamma_j}$ need not be calculated.

III. RELATIVISTIC GENERALIZATION OF MULTIPOLE EXPANSION

The relativistic generalization of multipole expansion consists of expanding the left member of Eq. (9) in space and time components of $\Pi - \varepsilon$. The expansion in the space components is obtained by expanding the right members of Eqs. (32) and (33) where $f(H) = (k^2 - 2k_0\Pi_0 + H + \omega^2)^{-1}$ in powers of ω^2. The expansion in the time components is obtained first by using a spectral decomposition of the operator $(k^2 - 2k_0\Pi_0 + H)^{-1}$ and then expanding in powers of k_0. After these expansions are made one can integrate over four-momentum of the virtual photon and sum the contributions of the electron intermediate states.

A. Expansion in space components

We expand the spherical Bessel functions $j_L(\omega R)$ in powers of ω, thus converting the partial wave expansion into a multipole expansion:

$$j_L(\omega R) = \sum_{q=0}^{\infty}\left(-\frac{1}{2}\right)^q \frac{r^{L+2q}}{q!(2L+2q+1)!!}\left(\frac{\omega}{EZ\alpha}\right)^{L+2q}. \tag{40}$$

This is accompanied by the expansion

$$\frac{1}{k^2 - 2k_0\Pi_0 + H_{l_\Gamma} + \omega^2} = \sum_{q=0}^{\infty}\frac{\omega^{2q}}{q!}\frac{d^q}{d\sigma^q}\frac{1}{k^2 - 2k_0\Pi_0 + H_{l_\Gamma} + \sigma}\bigg|_{\sigma=0}. \tag{41}$$

By inserting Eqs. (40) and (41) into Eqs. (32) and (33) and collecting the terms of order ω^{2v} and ω^{2v-1} we obtain

$$\langle O_1 G_{4,0} O_2\rangle = \sum_{v=0}^{\infty}\sum_{L=0}^{v}\sum_{\rho=\pm1}\sum_{j-(1/2)=0}^{\infty}\sum_{\pi=\pm1}\Theta_{O_1,O_2}(L,j,\rho,\pi)\sum_{p=0}^{v-L}(EZ\alpha)^{-2(p+L)}\left(-\frac{1}{2}\right)^p \times\sum_{q=0}^{p}\frac{1}{q!(2L+2q+1)!!}\frac{1}{(p-q)![2L+2(p-q)+1]!!}\frac{1}{(v-p-L)!}\frac{d^{v-p-L}}{d\sigma^{v-p-L}}U_{4,0}(v,L,l_\Gamma,p,q,c)\bigg|_{\sigma=0} \tag{42}$$

and

$$\langle\gamma_0 G_i\gamma_i\gamma_0\rangle = \sum_{v=0}^{\infty}\sum_{L=0}^{v}\sum_{\rho=\pm1}\sum_{j-(1/2)=0}^{\infty}\sum_{p=0}^{v-L}(EZ\alpha)^{-2(p+L)+1}\left(-\frac{1}{2}\right)^p \times\sum_{q=0}^{p}\sum_{\pi=\pm1}\{\Theta_{\gamma_0 n_i,\gamma_i\gamma_0}(L,L'=L-1,j,\rho,\pi)[2L+2(p-q)+1] - \Theta_{\gamma_0 n_i,\gamma_i\gamma_0}(L,L'=L+1,j,\rho,\pi)2(p-q)\} \times\frac{1}{q!(2L+2q+1)!!}\frac{1}{(p-q)!(2L+2(p-q)+1)!!}\frac{1}{(v-p-L)!}\frac{d^{v-p-L}}{d\sigma^{v-p-L}}U_1(v,L,l_\Gamma,p,q)\bigg|_{\sigma=0}, \tag{43}$$

where

$$U_{4,0}(v,L,l_\Gamma,p,q,c) = (-4)\int_0^{\Lambda^2}d\lambda\int\frac{d^4k_F(1,k_0/m)}{(k^2-\lambda)^2}\langle l_0+1,l_0|r^{L+2q}\frac{\omega^{2v}}{k^2-2k_0\Pi_0+H_{l_\Gamma}+\sigma}r^{L+2(p-q)+c}|l_0+1,l_0\rangle \tag{44}$$

and

$$U_1(v,L,l_\Gamma,p,q) = (-4)\int_0^{\Lambda^2}d\lambda\int\frac{d^4k_F\omega/m}{(k^2-\lambda)^2}\langle l_0+1,l_0|r^{L+2q}\frac{\omega^{2v-1}}{k^2-2k_0\Pi_0+H_{l_\Gamma}+\sigma}r^{L+2(p-q)-1}|l_0+1,l_0\rangle, \tag{45}$$

respectively. In derivation of Eq. (43) we used Eq. (40) twice. In the second time we substituted $L \to L \pm 1$. For $L \to L-1$ this produces the factor $[2L + 2(p-q) + 1]$ multiplying the angular part $\Theta_{\gamma_0 n_i,\gamma_i\gamma_0}(L' = L-1)$. For $L \to L+1$ we shift the summation variable in Eq. (40) by -1. This then produces the factor $(-2)(p-q)$ multiplying the angular part $\Theta_{\gamma_0 n_i,\gamma_i\gamma_0}(L' = L+1)$.

B. Elimination of explicit appearance of $\Pi_0 - m$

The diagonalization of the operator $(k^2 - 2k_0\Pi_0 + H_{l_\Gamma} + \sigma)^{-1}$ yields [see also Eqs. (44)–(51) of [16]]

$$\langle l_0+1,l_0|r^a\frac{1}{k^2-2k_0\Pi_0+H_{l_\Gamma}+\sigma}r^b|l_0+1,l_0\rangle$$
$$=\int_0^\infty dk_e\frac{P_{l_\Gamma}^{a,b}(k_e,\xi)}{k^2-2k\cdot\varepsilon+\Delta[k_e\xi(l_0+1),\xi]+\sigma}+\sum_{n=l_0+2}^{\infty}\frac{P_{l_\Gamma}^{a,b}\left(-\frac{i}{n},\xi\right)}{k^2-2k\cdot\varepsilon+\Delta\left[-\frac{i}{n}\xi(l_0+1),\xi\right]+\sigma}\Bigg|_{\xi=1-\frac{k_0}{E}}, \tag{46}$$

where ε is given by Eq. (10). For the continuum part of the spectrum

$$-\frac{\Delta[k_e\xi(l_0+1),\xi]}{m^2}=(Z\alpha)^2\left\{[(l_0+1)\xi k_e]^2+1+(\xi-1)\frac{2(l_0+1)}{2+l_0}\right\} \tag{47}$$

and

$$P_{l_\Gamma}^{a,b}(k_e,\xi)=\langle l_0+1,l_0|r^a|k_e,l_\Gamma\rangle_\xi(\langle l_0+1,l_0|r^b|k_e,l_\Gamma\rangle_\xi)^*, \tag{48}$$

where [20]

$$\langle l_0+1,l_0|r^a|k_e,l_\Gamma\rangle_\xi=C_{l_0+1,l_0}\Gamma(l_\Gamma+l_0+a+3)\xi^{1/2}(l_0+1)^{l_0+a+2}\frac{2^{l_\Gamma}}{\Gamma(2l_\Gamma+2)}\sqrt{\frac{2}{\pi}}\left|\Gamma\left(l_\Gamma+1-\frac{i}{k_e}\right)\right|$$
$$\times\exp\left(\frac{\frac{\pi}{2}-2\arctan k_e\xi(l_0+1)}{k_e}\right)\left(\frac{\xi(l_0+1)k_e}{1-i\xi k_e(l_0+1)}\right)^{l_\Gamma+1}[1+i\xi k_e(l_0+1)]^{-(l_0+a+2)}$$
$$\times F\left(-\frac{i}{k_e}+l_\Gamma+1,l_\Gamma-l_0-a-1,2l_\Gamma+2,-\frac{2ik_e\xi(l_0+1)}{1-ik_e\xi(l_0+1)}\right). \tag{49}$$

Likewise, for the discrete part of the spectrum

$$-\frac{\Delta\left[-\frac{i}{n}\xi(l_0+1),\xi\right]}{m^2}=(Z\alpha)^2\left\{-\frac{[(l_0+1)\xi]^2}{n^2}+1+(\xi-1)\frac{2(l_0+1)}{2+l_0}\right\} \tag{50}$$

and

$$P_{l_\Gamma}^{a,b}\left(-\frac{i}{n},\xi\right)=\langle l_0+1,l_0|r^a|n,l_\Gamma\rangle_\xi(\langle l_0+1,l_0|r^b|n,l_\Gamma\rangle_\xi)^*, \tag{51}$$

where [20]

$$\langle l_0+1,l_0|r^a|n,l_\Gamma\rangle_\xi=C_{l_0+1,l_0}\Gamma(l_\Gamma+l_0+a+3)C_{n,l_\Gamma}\xi^{(2l_\Gamma+3)/2}\left(\frac{1}{l_0+1}+\frac{\xi}{n}\right)^{-(l_\Gamma+l_0+a+3)}$$
$$\times F\left(-n+l_\Gamma+1,l_\Gamma+l_0+a+3,2l_\Gamma+2,\frac{2\xi/n}{1/(l_0+1)+\xi/n}\right). \tag{52}$$

The normalization constant for the discrete part of the spectrum is

$$C_{n,l_\Gamma}=\frac{2}{n^2}\sqrt{\frac{\Gamma(n+l_\Gamma+1)}{\Gamma(n-l_\Gamma)}}\frac{\left(\frac{2}{n}\right)^{l_\Gamma}}{\Gamma(2l_\Gamma+2)}. \tag{53}$$

C. Expansion in time components

The expansion in time component of $(\Pi-\varepsilon)$ is now obtained by expanding the right member of Eq. (46) in powers of k_0,

$$\int_0^\infty dk_e\frac{P_{l_\Gamma}^{a,b}(k_e,\xi)}{k^2-2k\cdot\varepsilon+\Delta[k_e\xi(l_0+1),\xi]+\sigma}\Bigg|_{\xi=1-(k_0/E)}=\sum_{t=0}^{\infty}\frac{1}{2^t t!}\left(\frac{-2k_0}{E}\right)^t\frac{\partial^t}{\partial\xi^t}\int_0^\infty dk_e\frac{P_{l_\Gamma}^{a,b}(k_e,\xi)}{k^2-2k\cdot\varepsilon+\Delta[k_e\xi(l_0+1),\xi]+\sigma}\Bigg|_{\xi=1} \tag{54}$$

and analogously for the discrete part.

D. Integration over four-momentum of virtual photon

The integration over four-momentum of the virtual photon yields (see Appendix D)

$$(-4)\int_0^{\Lambda^2}d\lambda\int\frac{d^4k_F\left(1,\frac{k_0}{m}\right)}{(k^2-\lambda)^2}\frac{(2\omega)^{2v}(-2k_0)^t}{k^2-2k\varepsilon+\Delta+\sigma}=(-1)^v(2v+1)!!\Phi_{4,0}^{2v,t}(\Delta+\sigma)m^{2v+t}, \tag{55}$$

where

$$\Phi_{4,0}^{2v,t}(\Delta+\sigma) = 2^v(-1)^t \frac{\partial^t}{\partial(\varepsilon_0)^t}\int_0^1 dy\, y^v(1,y\varepsilon_0)\int_0^{-(\Delta+\sigma)/m^2} d^{v+t}w\, \ln\left(\frac{\varepsilon_0^2 y + w}{y}\right)\Bigg|_{\varepsilon_0=1} \tag{56}$$

and

$$(-4)\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F\,\frac{\omega}{m}}{(k^2-\lambda)^2}\frac{(2\omega)^{2v-1}(-2k_0)^t}{k^2-2k\varepsilon+\Delta+\sigma} = (-1)^v(2v+1)!!\frac{1}{2}\Phi_4^{2v,t}(\Delta+\sigma)m^{2v-1+t}. \tag{57}$$

The symbol $d^n w$ in Eq. (56) henceforth stands for n iterated integration over the parameter w:

$$\int_0^a d^n w\, f(w) = \int_0^a dw_n \cdots \int_0^{w_3} dw_2 \int_0^{w_2} dw_1\, f(w_1) = \frac{1}{(n-1)!}\int_0^a dw(a-w)^{(n-1)} f(w). \tag{58}$$

The contribution to the electromagnetic mass of the electron, Eq. (80) of [16], was subtracted from the left members of Eqs. (55) and (57) and the terms proportional to negative powers of cutoff Λ neglected. Henceforth, m stands for the measurable mass of the electron. This is the renormalization of the electron mass.

The insertion of Eqs. (46) and (55) into Eq. (44) yields

$$U_{4,0}(v,L,l_\Gamma,p,q,c) = (-1)^v\frac{(2v+1)!!}{2^{2v}}m^{2v}\sum_{t=0}^{\infty}\left(\frac{m}{E}\right)^t\frac{1}{2^t t!}\frac{\partial^t}{\partial\xi^t}\left\{\int_0^\infty dk_e\, P_{l_\Gamma}^{L+2q,L+2(p-q)+c}(k_e,\xi)\,\Phi_{4,0}^{2v,t}\{\Delta[k_e\xi(l_0+1),\xi]+\sigma\}\right.$$
$$\left.+\sum_{n=l_0+2}^{\infty}P_{l_\Gamma}^{L+2q,L+2(p-q)+c}\left(-\frac{i}{n},\xi\right)\Phi_{4,0}^{2v,t}\left\{\Delta\left[-\frac{i}{n}\xi(l_0+1),\xi\right]+\sigma\right\}\right\}_{\xi=1}. \tag{59}$$

A similar result is obtained for U_1 by inserting Eqs. (46) and (57) into Eq. (45),

$$U_1(v,L,l_\Gamma,p,q) = \frac{1}{m}U_4(v,L,l_\Gamma,p,q,c=-1). \tag{60}$$

E. Contribution of the virtual electron states with very large wave numbers

For very large electron wave numbers k_e, the overlap integrals (48) behave as

$$P_{l_\Gamma}^{a,b}(k_e,\xi) \to \xi(l_0+1)P_{l_\Gamma,\infty}^{a,b}[k_e\xi(l_0+1),\xi], \tag{61}$$

where

$$P_{l_\Gamma,\infty}^{a,b}[k_e\xi(l_0+1),\xi] = A_{l_\Gamma}^{a,b}B_{l_\Gamma,\infty}^{a,b}[k_e\xi(l_0+1)]\left(1+\frac{c_{1,0}+c_{1,1}\xi}{k_e\xi(l_0+1)}+\frac{c_{2,0}+c_{2,1}\xi+c_{2,2}\xi^2}{\left[k_e(l_0+1)\xi\right]^2}+\cdots\right), \tag{62}$$

$$A_{l_\Gamma}^{a,b} = \left|C_{l_0+1,l_0}\right|^2\frac{2}{\pi}\left(\frac{\Gamma(l_\Gamma+1)}{\Gamma(2l_\Gamma+2)}\right)^2 2^{2l_\Gamma}(l_0+1)^{2l_0+a+b+3}\Gamma(l_\Gamma+l_0+a+3)\Gamma(l_\Gamma+l_0+b+3)$$
$$\times F(l_\Gamma+1,l_\Gamma-l_0-a-1,2l_\Gamma+2,2)F^*(l_\Gamma+1,l_\Gamma-l_0-b-1,2l_\Gamma+2,2) \tag{63}$$

and

$$B_{l_\Gamma,\infty}^{a,b}[k_e(l_0+1)\xi] = [1+i\xi(l_0+1)k_e]^{-a-l_0-2}[1-i\xi(l_0+1)k_e]^{-b-l_0-2}\frac{[k_e(l_0+1)\xi]^{2l_\Gamma+2}}{\{1+[k_e(l_0+1)\xi]^2\}^{l_\Gamma+1}}. \tag{64}$$

To obtain the expansion (62) from Eqs. (48) and (49) one needs an asymptotic expansion of the hypergeometric functions appearing in Eq. (49). This is described in Appendix C. For actual evaluation we write

$$\int_0^\infty dk_e\, P_l^{a,b}(k_e,\xi)\Phi_{4,0}^{2v,t}\{\Delta[k_e\xi(l_0+1),\xi]+\sigma\}$$
$$= \int_0^\infty dk_e\left[P_l^{a,b}(k_e,\xi)-\xi(l_0+1)P_{l,\infty}^{a,b}(k_e\xi(l_0+1),\xi)\right]\Phi_{4,0}^{2v,t}\{\Delta[k_e\xi(l_0+1),\xi]+\sigma\}$$
$$+\int_0^\infty dk_e\, P_{l,\infty}^{a,b}(k_e,\xi)\Phi_{4,0}^{2v,t}[\Delta(k_e,\xi)+\sigma], \tag{65}$$

where in the second term on the right member we made the substitution

$$k_e \to \frac{k_e}{\xi(l_0+1)}. \tag{66}$$

This is advantageous for the following reason. The integral over the electron wave numbers k_e on the right member of Eq. (59) is convergent. However, *before* we carry out a numerical integration over the electron wave numbers k_e, we have to differentiate it with respect to ξ. In general for $t > 1$ we then get a convergent integral as a sum of divergent integrals. Since we have to integrate numerically, this has to be avoided. Therefore, we take as many terms in the asymptotic expansion in Eq. (62) as to get the integral in the first term on the right member of Eq. (65) after differentiation with respect to ξ as a sum of convergent integrals. When we differentiate with respect to ξ, the second term on the right member of Eq. (65) also yields a convergent integral; insertion of the second term on the right member of Eq. (65) into Eqs. (42) and (59) leads to the expression

$$m^{2v}(EZ\alpha)^{-2(p+L)}\frac{1}{t!}\frac{\partial^t}{\partial\xi^t}\int_0^\infty dk_e\, P_{l_\Gamma,\infty}^{L+2q,L+2(p-q)+c}(k_e,\xi)\frac{d^{v-p-L}}{d\sigma^{v-p-L}}\Phi_{4,0}^{2v,t}\Big|_{\sigma=0}\Big|_{\xi=1}. \quad (67)$$

As shown in detail in Appendix E,

$$(67) \simeq (Z\alpha)^{2t-[t]}c_{t,t}A_{l_\Gamma}^{L+2q,L+2(p-q)+c}\left(\frac{E}{m}\right)^{-2(p+L)}([t]-1)!!2^{v+[t]/2}\int_0^1 dy\, y^{v+[t]/2}(1,y)\int_0^1 d^{L+p+t-[t]/2}w$$
$$\times\int_0^\infty dk_e\frac{(1+k_e^2)^{t-[t]/2}}{k_e^t}\left(\frac{k_e^2}{1+k_e^2}\right)^{l_\Gamma+1}(1+k_e^2)^{-l_0-2}(1-ik_e)^{-c}\ln\left[y+w(Z\alpha)^2(k_e^2+1)\right]+\cdots, \quad (68)$$

where

$$[t] = t \pm \frac{(-1)^t-1}{2}. \quad (69)$$

Here $+$ and $-$ signs hold for $\Phi_4^{2v,t}$ and $\Phi_0^{2v,t}$, respectively. Recall that c is equal to 0 or -1 and it is present just for the terms with $\Phi_4^{2v,t}$. We are thus coming to the important conclusion that when integrating over the electron wave numbers k_e, the integrand never behaves for large k_e worse than $k_e^{-2l_0-3}\ln k_e$. Thus, the integrals converge rather fast.

A natural question then arises as to why we do not make the substitution (66) already in Eq. (59). The reason is that if we look at Eq. (49), we see that differentiation of $P_{l_\Gamma}^{a,b}(k_e,\xi)$ with respect to ξ involves, among other things, also differentiation of the hypergeometric functions $F(-\frac{i}{k_e}+l_\Gamma+1,l_\Gamma-l_0-a-1,2l_\Gamma+2,-\frac{2ik_e\xi(l_0+1)}{1-ik_e\xi(l_0+1)})$. This is easily done. On the other hand, after the substitution (66) we would need to differentiate with respect to ξ the hypergeometric functions $F(-\frac{i\xi(l_0+1)}{k_e}+l_\Gamma+1,l_\Gamma-l_0-a-1,2l_\Gamma+2,-\frac{2ik_e}{1-ik_e})$. This is a much more difficult task even for modern computer languages for symbolic calculation.

The difficulty in evaluating the integrals over k_e on the right member of Eq. (59) has been noticed already in [16]. In fact it was incorrectly concluded that these integrals diverge. The solution proposed there follows. Instead of the partition (11), consider the partition

$$z = k^2, \quad \tilde{H}_0 = 2k\cdot\bar{\varepsilon} - H, \quad \lambda\tilde{H}_1 = -2k\cdot(\Pi-\bar{\varepsilon}), \quad (70)$$

where

$$\bar{\varepsilon} = \left(\frac{H+m^2}{E},0,0,0\right). \quad (71)$$

The solution proposed here is, however, significantly better than the one proposed in [16]. First, the generation of the individual terms of the expansion based on the partition (70) is somewhat more involved than the one based on the partition (11). Second, and more importantly, the convergence of the expansion based on the partition (11) is much faster than the one based on the partition (70).

F. Formula for ΔE

As in the previous papers [16,18], we order the individual terms according to naive counting of powers of $Z\alpha$:

$$\Delta E = m\frac{\alpha}{\pi}(Z\alpha)^4\sum_{v=1}^\infty F_v \quad (72)$$

$$-2(Z\alpha)^4F_v = \sum_{t=0}^v\Big\langle\gamma_0G_4^{2(v-t),t}+\gamma_\mu G_4^{2(v-t-1),t}\frac{(\Pi-\varepsilon)_\mu}{m} + \gamma_0G_0^{2(v-t),t}+\gamma_0G_i^{2(v-t)-1,t}\gamma_i\gamma_0 + \left(-\frac{1}{2}\right)\gamma_\mu\left[G_0^{2(v-t-3),t},\gamma_0\gamma_\mu\right]\Big\rangle. \quad (73)$$

This naive counting follows from transition (22) from natural to atomic units: each additional power of spatial and time components of $\Pi-\varepsilon$ contributes the additional factors of $Z\alpha$ and $(Z\alpha)^2$, respectively. As already discussed in the previous papers [16,18], this counting holds only in the low-energy region. Nonetheless, the expansion in time components of $\Pi-\varepsilon$ produces at least the factor $Z\alpha$ in the high-energy region [see Eq. (68)]. As discussed further, the expansion in space components of $\Pi-\varepsilon$ leads in the high-energy region to convergent series [see Eq. (78) below].

The spinor-angular part of the integration of $\langle\gamma_\mu G_4(\Pi-\varepsilon)_\mu\rangle/m$ and $\langle\gamma_0G_i\gamma_i\gamma_0\rangle$ is by the factor $(Z\alpha)^2$ smaller than the spinor-angular part of the integration of $\langle\gamma_0G_{4,0}\rangle$. Likewise, the spinor-angular part of $\langle(-\frac{1}{2})\gamma_\mu[G_0,\gamma_0\gamma_\mu]\rangle$ is by the factor $(Z\alpha)^6$ smaller. This is the reason for a shift of the first superscript on G's in the second, fourth, and fifth terms on the right member of Eq. (73).

G. Series in $Z\alpha$

It is well known that the self-energy has expansion in powers of $Z\alpha$,

$$\Delta E = \frac{m\alpha(Z\alpha)^4}{\pi N^3 s^3} F(Z\alpha,N,l_j), \tag{74}$$

where [7–11]

$$\begin{aligned} F(Z\alpha) = {} & A_{41} \ln s(Z\alpha)^{-2} + A_{40} + A_{50}(Z\alpha) \\ & + (Z\alpha)^2[A_{62} \ln^2 s(Z\alpha)^{-2} + A_{61} \ln s(Z\alpha)^{-2} + A_{60}] \\ & + (Z\alpha)^3[\ln s(Z\alpha)^{-2} A_{71} + A_{70}] + \cdots , \end{aligned} \tag{75}$$

and $s = 1$ in the nonrecoil limit. Setting $s = 1 + m_e/m_n$, where m_e/m_n is a ratio of the electron and nuclear masses, one takes into account the dominant part of the nuclear recoil effect [1,2]. The coefficients $A = A(N,l_j)$ are summarized, e.g., in [1,13]. With the exception of the coefficients A_{60} and A_{71} the coefficients were calculated more than once. The analytic form of the coefficient A_{70} is unknown and even the form of the series beyond the $\alpha(Z\alpha)^7$ term is not known.

A question then arises as to the relation of the series (72) to (75). As argued in [16–18] the coefficients A_{41}, A_{40}, and A_{62} are contained in $F_1 + F_2$ and the coefficient A_{61} and a sufficiently great part of the A_{60} coefficient is contained in $F_1 + F_2 + F_3$. (See Tables 2 and 3 of [18] for the precise meaning of "sufficiently great part.") The coefficient A_{50} is contained in the complete sum (72). This coefficient is entirely determined by the electron virtual states with very high wave numbers k_e and short wavelengths of the virtual photon. It is for these states that the assumption underlying the RME breaks down. Fortunately, as shown in detail in Appendix A, one can always rearrange the appropriate expression for these states in such a way that the electron can be in these states treated as free. Writing

$$A_{50} = \sum_{v=1}^{\infty} A_{50}^{(v)}, \tag{76}$$

where $A_{50}^{(v)}$ is the part of the A_{50} coefficient contained in F_v one obtains (see Appendix A)

$$A_{50}^{(v)} = -2^3 \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(v-\frac{5}{2}\right)(16v^4 - 32v^3 + 296v^2 + 8v - 267)}{\pi\Gamma(v)(2v+5)(2v+3)(2v+1)^2(2v-3)}. \tag{77}$$

This result implicitly appeared already in [18]. However, the formulas given there are so complicated that the dependence of $A_{50}^{(v)}$ on v is rather obscured. For large v Eq. (77) behaves as

$$A_{50}^{(v)} \simeq -\frac{4}{\pi^{1/2}} v^{-7/2}. \tag{78}$$

The complete coefficient A_{50} is [7–10]

$$A_{50} = 4\pi\left(\frac{139}{128} - \frac{\ln 2}{2}\right). \tag{79}$$

For the self-energy function $F(Z\alpha)$, Eq. (74), we write

$$F(Z\alpha) = (Z\alpha)A_{50} + \sum_{v=1}^{\infty} S_v, \tag{80}$$

where

$$S_v = F_v - (Z\alpha)A_{50}^{(v)}. \tag{81}$$

IV. RESULTS AND DISCUSSION

A. Computational details

Up to the summation and integration over discrete and continuous parts of the hydrogen spectrum the calculation is analytic. We wrote two independent routines in MAPLE and MATHEMATICA. For each expansion of the functions G in $2v$ spatial and t time components of $(\Pi - \varepsilon)$ the calculation was done in symbolic form up to the very end. Thus, there is just one summation and one integration performed for given v and t.

For the discrete part of the spectrum we took the partial sums up to $n = 35$ and then used Richardson extrapolation (see, e.g., [21]) on the interval of n from 20 to 35. For the continuous part of the spectrum we broke the interval $k_e \in (0,\infty)$ into several regions, much in the same way as in [16]. As discussed in [16], the functions Φ became unstable for very small and very large values of k_e. In these regions the asymptotic expansions of Φ in Δ and $1/\Delta$ have to be used. The form of the functions Φ used in the actual calculation is given in the Appendix D.

B. Truncation of the expansion

There are some considerable simplifications when evaluating the terms (73) of the series (72) for light hydrogenlike ions. First, as noted in the previous papers [16,17] the contribution of the terms $\langle\gamma_\mu[G_0,\gamma_0\gamma_\mu]\rangle$ is for the S states exceedingly small (see the first three rows of Table I). Second, the contribution of the higher temporal multipoles is highly suppressed. More precisely, the contribution of the terms $\langle\gamma_0 G_{4,0}^{2v,t}\rangle$ for $t > 3$ and $\langle\gamma_0 G_i^{2v-1,t}\gamma_i\gamma_0\rangle$, $\langle\gamma_\mu G_4^{2v,t}(\Pi - \varepsilon)_\mu\rangle/m$ for $t > 2$ is very small. In Table I the contributions of the first two spatial multipoles for $\langle\gamma_0 G_{4,0}^{2v,4}\rangle$, $\langle\gamma_0 G_i^{2v-1,3}\gamma_i\gamma_0\rangle$ and $\langle\gamma_\mu G_4^{2v,3}(\Pi - \varepsilon)_\mu\rangle/m$ are displayed. Third, as noted in [16] the terms $\langle\gamma_\mu G_4^{2v,t} O_\mu^{-1}\rangle$ are by the factor of $(Z\alpha)^2$ smaller than the terms $\langle\gamma_\mu G_4^{2v,t} O_\mu^{0}\rangle$. For given t and sufficiently large v the contribution of the terms $\langle\gamma_\mu G_4^{2v,t} O_\mu^{-1}\rangle$ becomes completely negligible compared to that of $\langle\gamma_\mu G_4^{2v,t} O_\mu^{0}\rangle$. In particular, the values $\langle\gamma_\mu G_4^{2v,3}(\Pi - \varepsilon)_\mu\rangle/m$ given in Table I were obtained by omitting the terms $\langle\gamma_\mu G_4^{2v,3} O_\mu^{-1}\rangle$ completely.

Taking into account the above simplifications, instead of Eq. (73) we considered

$$\begin{aligned} -2(Z\alpha)^4 F_v \simeq \Bigg\langle \gamma_0 \sum_{t=0}^{T}\left(G_4^{2(v-t),t} + G_0^{2(v-t),t}\right) & \\ + \sum_{t=0}^{T-1}\Bigg(\gamma_\mu G_4^{2(v-t-1),t}\frac{(\Pi - \varepsilon)_\mu}{m} & \\ + \gamma_0 G_i^{2(v-t)-1,t}\gamma_i\gamma_0\Bigg)\Bigg\rangle, & \end{aligned} \tag{82}$$

where $T = 3$. The convergence of the series (80) is displayed in Table III. For the complete self-energy function F we

TABLE I. Some of the smaller contributions to Eq. (73) justifying the neglect of the terms $(-\frac{1}{2})\langle\gamma_\mu[G_0^{2v,t},\gamma_0\gamma_\mu]\rangle$ and the terms with higher number of time components. The contributions are multiplied by the factor $[-2(Z\alpha)^4]^{-1}$.

Term	$Z=1$	$Z=5$	$Z=10$	$Z=20$
$(-\frac{1}{2})\langle\gamma_\mu[G_0^{0,0},\gamma_0\gamma_\mu]\rangle$	0.790×10^{-7}	0.812×10^{-5}	0.547×10^{-4}	0.340×10^{-3}
$(-\frac{1}{2})\langle\gamma_\mu[G_0^{2,0},\gamma_0\gamma_\mu]\rangle$	-0.697×10^{-8}	-0.588×10^{-6}	-0.268×10^{-5}	0.454×10^{-6}
$(-\frac{1}{2})\langle\gamma_\mu[G_0^{0,1},\gamma_0\gamma_\mu]\rangle$	-0.27×10^{-9}	-0.143×10^{-6}	-0.187×10^{-5}	-0.211×10^{-4}
$\langle\gamma_\mu G_4^{0,3}(\Pi-\varepsilon)_\mu\rangle$	-0.18×10^{-9}	-0.694×10^{-6}	-0.917×10^{-5}	-0.836×10^{-4}
$\langle\gamma_\mu G_4^{2,3}(\Pi-\varepsilon)_\mu\rangle$		-0.483×10^{-7}	-0.174×10^{-5}	-0.361×10^{-4}
$\langle\gamma_0 G_i^{1,3}\gamma_i\gamma_0\rangle$	-0.180×10^{-7}	-0.542×10^{-5}	-0.547×10^{-4}	-0.489×10^{-3}
$\langle\gamma_0 G_i^{3,3}\gamma_i\gamma_0\rangle$	0.5×10^{-10}	-0.106×10^{-6}	-0.339×10^{-5}	-0.774×10^{-4}
$\langle\gamma_0 G_0^{0,4}\rangle$	0.691×10^{-8}	0.249×10^{-5}	0.285×10^{-4}	0.304×10^{-3}
$\langle\gamma_0 G_0^{2,4}\rangle$	-0.257×10^{-9}	-0.102×10^{-6}	-0.120×10^{-5}	-0.667×10^{-5}
$\langle\gamma_0 G_4^{0,4}\rangle$	-0.248×10^{-7}	-0.651×10^{-5}	-0.600×10^{-4}	-0.480×10^{-3}
$\langle\gamma_0 G_4^{2,4}\rangle$	0.70×10^{-9}	0.177×10^{-6}	0.354×10^{-6}	-0.281×10^{-4}

write

$$F(Z\alpha)=A_{50}(Z\alpha)+\sum_{v=1}^{V}S_v+F_{\text{rem}}+F_{\text{small}}. \qquad (83)$$

The coefficients S_v are calculated from Eq. (81), where F_v are taken from Eq. (82). F_{small} is the contribution of smaller terms not included in Eq. (82). Their contribution is estimated by summing the terms displayed in Table I. V is the number of explicitly calculated terms (81). F_{rem} stands for the remainder of the series

$$(-2)(Z\alpha)^4F_{\text{rem}}=\sum_{v=V+1}^{\infty}S_v. \qquad (84)$$

It is seen from Table II that with increasing v the ratios S_v/S_{v-1} approach the ratios $A_{50}^{(v)}/A_{50}^{(v-1)}$. For $v>V$ this offers the possibility to estimate the remainder of the series by replacing the ratios S_v/S_{v-1} by the ratios $A_{50}^{(v)}/A_{50}^{(v-1)}$; then

$$F_{\text{rem}}\simeq\frac{S_V}{A_{50}^{(V)}}\sum_{v=V+1}^{\infty}A_{50}^{(v)}=\frac{S_V}{A_{50}^{(V)}}\left(A_{50}-\sum_{v=1}^{V}A_{50}^{(v)}\right). \qquad (85)$$

It is reassuring that this appears also for higher nuclear charges: though the coefficients S_v differ for different Z in the magnitude significantly, their ratios tend to be very close to each other (compare Tables II and III).

Table IV displays preliminary results obtained by means of series (72) for higher nuclear charges $Z>20$. Instead of evaluating the full expression (73), we again made the approximation (82), where we took $T=4$. To this we added

$$(-2)(Z\alpha)^4F_{\text{spin}}=\left(-\frac{1}{2}\right)\sum_{v=0}^{1}\sum_{t=0}^{v}\langle\gamma_\mu[G_0^{2(v-t),t},\gamma_0\gamma_\mu]\rangle. \qquad (86)$$

Further we made an approximation $\langle\gamma_\mu G_4^{2v,3}(\Pi-\varepsilon)_\mu\rangle/m\simeq\langle\gamma_\mu G_4^{2v,3}O_\mu^0\rangle$. Furthermore, the terms $\langle\gamma_0 G_{0,4}^{2v,4}\rangle$ with $v>1$ were omitted for $Z=30$ and with $v>2$ for $Z=40$; the terms $\langle\gamma_\mu G_4^{6,3}O_\mu^0\rangle$ and $\langle\gamma_0 G_i^{7,3}\gamma_i\gamma_0\rangle$ were omitted for $Z=30$ and $Z=40$. Some of these approximations could not be completely justified. Thus, the agreement between RME and PWE for high nuclear charges, $Z>60$, is likely to result from cancellation of the uncalculated terms. Further, the error committed by the free-particle approximation in the electron virtual states is too large for higher nuclear charges. For example, for $Z=30$ the free-particle approximation yields for the terms $\langle\gamma_0 G_4^{2v,2}\rangle$ typically just about 10% of the whole effect; compare this with the results for $Z=1$ in Table V. Therefore, for $Z>20$ we did not try to supplement RME by free-particle result.

C. Discussion

The result for hydrogen ($Z=1$) is of greatest interest. The error of the present calculation due to the sum of uncalculated contributions and the rounding errors of the calculated ones for hydrogen is estimated to be 0.7×10^{-8}. The only other calculation of comparable accuracy to the one presented here is given in [13]. In that paper, several millions of partial waves were considered. For each partial wave there is a three-dimensional integration to be performed

TABLE II. Comparison of the ratios $A_{50}^{(v)}/A_{50}^{(v-1)}$ and S_v/S_{v-1} for different nuclear charges.

v	$A_{50}^{(v)}/A_{50}^{(v-1)}$	$Z=1$	$Z=5$	$Z=10$	$Z=20$
5	0.2645	0.1907	0.1958	0.1989	0.2078
6	0.3921	0.3466	0.3481	0.3431	0.3225
7	0.4868	0.4625	0.4643	0.4570	0.4265
8	0.5577	0.5404	0.5404	0.5351	
9	0.6119	0.6110	0.6057		

TABLE III. The convergence of RME with the infinite order summation of $\alpha(Z\alpha)^5$ terms. The terms S_v are calculated from Eq. (81). "Lead" stands for the sum $S_1 + S_2 + A_{50}(Z\alpha)$. "rem" is the estimate of the remainder of the series obtained from Eq. (85). "small" is the sum of the contributions displayed in Table I. "other" is the result of PWE taken from [13] for $Z = 1$ and $Z = 5$ and from [12] for $Z = 10$ and $Z = 20$. "r.d." is the relative difference between "Total" and "Other."

	$Z = 1$	$Z = 5$	$Z = 10$	$Z = 20$
Lead	10.315870916	6.238382304	4.615985057	3.143785475
S_3	0.891183×10^{-3}	0.1252179×10^{-2}	0.3552640×10^{-2}	0.9320166×10^{-1}
S_4	0.23509×10^{-4}	0.537629×10^{-3}	0.1992039×10^{-2}	0.720546×10^{-2}
S_5	0.4484×10^{-5}	0.105272×10^{-3}	0.396161×10^{-3}	0.149713×10^{-2}
S_6	0.1554×10^{-5}	0.36643×10^{-4}	0.135912×10^{-3}	0.48289×10^{-3}
S_7	0.719×10^{-6}	0.17011×10^{-4}	0.62117×10^{-4}	0.20594×10^{-3}
S_8	0.388×10^{-6}	0.9192×10^{-5}	0.33240×10^{-4}	
S_9	0.237×10^{-6}	0.5568×10^{-5}		
sum	10.316792992	6.251615412	4.654130926	3.246378550
rem	0.648×10^{-6}	0.1519×10^{-4}	0.7583×10^{-4}	0.37690×10^{-3}
small	0.36×10^{-7}	-0.283×10^{-5}	-0.5123×10^{-4}	-0.57784×10^{-3}
Total	10.316793675(7)	6.2516278(7)	4.654156(9)	3.24618(9)
Other	10.316793650(1)	6.251627078(1)	4.6541622(2)	3.2462556(1)
r.d.	0.24×10^{-8}	0.11×10^{-6}	0.14×10^{-5}	0.24×10^{-4}

numerically (for details see [12,13]). These two completely independent calculations, the present one and the one in [13] agree with each other on the fractional level of two parts in 10^9, although the difference is slightly greater than the estimated errors of the calculations. This difference leads to the shift of 18 Hz for the $2s$-$1s$ transition in hydrogen. This uncertainty is smaller by the order of magnitude than the one found in [17] for the state-dependent part of the S states. Altogether, such an agreement between different, completely independent approaches definitely excludes the possibility that the discrepancy in the determination of the proton radius from the comparison of the theory and experiment in ordinary [1] and muonic [22] hydrogen has anything to do with the calculation of the one-loop self-energy.

Reference [14] is an attempt to substantially reduce the number of partial waves to be taken into account in comparison with [13]. Nonetheless, the result obtained there for the hydrogen atom is worse than the result of the present method taken up to the third order, that is, by considering the terms of the expansion (81) up to $v = 3$.

The relative difference between the series (75) truncated after the $\alpha(Z\alpha)^6$ term and the numerical result is three parts in 10^6 even for $Z = 1$. This difference is significantly higher than the current experimental accuracy [23]. In view of the complexity of the calculation of the A_{60} coefficient [10], there is no hope of achieving significantly better accuracy with the approach based purely on the series (75). Clearly, such an approach is not sufficient anymore. As has been pointed out in [18], the result obtained by means of the series (75) for low Z is reproduced by the present method taken up to the third order.

The results obtained by the present method up to $Z = 20$ are in very good agreement with the results obtained by PWE in [12,13]. This agreement definitely excludes the possibility that the excellent agreement between RME and PWE found for $Z = 1$ is accidental. Understandably, the convergence of RME slows down with the increasing nuclear charge. Also, the importance of higher temporal multipoles rises with an increasing nuclear charge (see Tables I and III).

The results for nuclear charges $Z > 20$ displayed in Table IV illustrate the remarkable fact that although RME was primarily aimed to obtain accurate results for light hydrogenlike ions, its domain of applicability is not restricted to weak external fields (see also discussion in [16]). However,

TABLE IV. The convergence of RME for the hydrogenlike atoms with higher nuclear charges. "Lead" stands for the sum $F_1 + F_2$. "Spin" is given by Eq. (86). "Other" is the result of PWE taken from [12]. "r.d." is the relative difference between "Total" and "Other."

Z	30	40	50	60	70	80	90
Lead	2.572289	2.141568	1.85198	1.6476	1.4999	1.3925	1.3145
F_3	−0.014237	−0.004437	0.00691	0.0194	0.0332	0.0481	0.0634
F_4	−0.003527	−0.000598	0.00457	0.0129	0.0261	0.0471	0.0813
F_5	−0.001720	−0.001668	−0.00145	−0.0011	−0.0004	−0.0001	−0.0017
F_6	−0.000793	−0.001006	−0.00115				
F_7	−0.000413	−0.000008					
Spin	0.000927	0.001999	0.00373	0.0064	0.0107	0.0177	0.0299
Total	2.5525(5)	2.1358(6)	1.8646(10)	1.6853(30)	1.5694(50)	1.5053(60)	1.4874(100)
Other	2.5520151(1)	2.1352284(1)	1.8642743(2)	1.6838358(3)	1.5674075(4)	1.5027775(4)	1.4875419(4)
r.d.	0.20×10^{-3}	0.29×10^{-3}	0.17×10^{-3}	0.89×10^{-3}	0.12×10^{-2}	0.17×10^{-2}	0.9×10^{-4}

TABLE V. The comparison of the exact calculation, nonrelativistic approximation, and free-particle approximation contributing at the order $(Z\alpha)^5$ for the terms $\langle\gamma_0 G_4^{2v,2}\rangle$. The contributions are multiplied by $-[2(Z\alpha)^4]^{-1}$; $B_v = \frac{2^4\Gamma(\frac{3}{2})(-1)^v(v-1)}{\Gamma(\frac{7}{2}-v)\Gamma(v)(v-\frac{3}{2})(v-\frac{1}{2})(v+\frac{1}{2})}$ [see Eq. (A80)]. The relative error of the nonrelativistic and free-particle approximations with respect to the exact result are displayed in parentheses in the third and fourth columns, respectively.

v	$\langle\gamma_0 G_4^{2v,2}\rangle$	$\langle G_4^{2v,2}\rangle_0$	$(Z\alpha)^5 B_v$
1	0.294962×10^{-2}	0.294948×10^{-2} (0.47×10^{-4})	0.222396×10^{-2} (0.25)
2	0.230441×10^{-3}	0.230090×10^{-3} (0.15×10^{-2})	0.185330×10^{-3} (0.20)
3	0.514669×10^{-4}	0.514055×10^{-4} (0.12×10^{-2})	0.421204×10^{-4} (0.18)
4	0.172584×10^{-4}	0.172376×10^{-4} (0.12×10^{-2})	0.141751×10^{-4} (0.18)

to obtain the results of similar accuracy as that in [12], further refinement of the present method of calculation of the contributions of higher temporal multipoles for high nuclear charges is needed.

V. CONCLUSION

The presented method has a number of advantages. Once the renormalization of the electron mass is made, all the integrals over either photon or electron variables are finite both at the lower and upper bounds of the integrations. Thus, no separation of any of the integrations is necessary. The terms of RME are generated very easily. In fact, by means of computer languages for symbolic calculation like MAPLE or MATHEMATICA they can be generated automatically. The only integrals to be performed numerically are one-dimensional integrals over the electron wave numbers of the continuous part of the spectrum. These integrals converge very fast. The contribution of the terms with very large wave numbers can be precisely summed up to the infinite order.

The most difficult part of the computation is numerical integration, more precisely, the evaluation of the pertinent hypergeometric functions. This requires nearly all computer time needed for calculation of the terms of the expansion (72). Further, we encountered difficulties when calculating higher spatial multipoles, $v > 9$, for low temporal multipoles, $t < 4$, and generally the contributions from higher temporal multipoles, $t \geqslant 4$. This is probably the consequence of severe numerical cancellations. Thus, there is still room for further improvement of the method. Until the puzzle of the proton radius is resolved, there is no need for further refinement of the present method for light hydrogenlike ions. Otherwise, such refinement could also become desirable when the precise independent check of the results obtained in [12] for higher nuclear charges is sought.

There is a number of other problems the present method can be extended to. These include calculations of the two-loop corrections [24–26], radiative recoil corrections [27], self-energy correction to hyperfine splitting and g-factor of a bound electron [28], radiation corrections to transitions amplitudes, both ordinary [29] and parity violating [30], and so on.

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APPENDIX A: CONTRIBUTION OF VIRTUAL STATES WITH VERY LARGE WAVE NUMBERS FOR LOW NUCLEAR CHARGES

1. Nonrelativistic approximation

The contribution of the terms $\alpha(Z\alpha)^5$ is determined by the double limit of small $Z\alpha$ and large k_e. The former is obtained by taking a nonrelativistic approximation to the spinor-angular part of the integration and by the replacement of l_Γ and l_0 in the radial integrals $\langle l_0+1,l_0|r^a|k_e,l_\Gamma\rangle\langle k_e,l_\Gamma|r^b|l_0+1,l_0\rangle$ by their nonrelativistic values. For small $Z\alpha$ the quantum number $|\Gamma|$ approaches $j+\frac{1}{2}$ [see Eq. (15)]. Then $l_\Gamma \simeq \delta_{\rho,1}(j-\frac{1}{2})+\delta_{\rho,-1}(j+\frac{1}{2})$ [see Eq. (20)]. With this replacement the leading terms of the asymptotic expansion (62) generally vanish and one has to consider the subleading terms in Eq. (62). Thus, to obtain the desired double limit is far from trivial. In [18] we found this limit to be

$$\langle\gamma_\mu G_4 \varepsilon_\mu\rangle \simeq \left\langle G_4 + \frac{(Z\alpha)^2}{4}\bar{G}_4\right\rangle_0, \tag{A1}$$

$$\frac{\langle\gamma_\mu G_4(\Pi-\varepsilon)_\mu\rangle}{m} \simeq \left\langle -\frac{1}{2m^2}P_i(G_4+\tilde{G}_4)P_i + \tilde{G}_4\frac{\Pi_0-m}{m}\right\rangle_0, \tag{A2}$$

$$-\frac{1}{2}\langle\gamma_\mu G_0\gamma_0\gamma_\mu\rangle \simeq \left\langle G_0 + \frac{(Z\alpha)^2}{4}\bar{G}_0\right\rangle_0, \tag{A3}$$

and

$$\frac{1}{2}\langle\gamma_\mu G_i\gamma_i\gamma_\mu\rangle \simeq \left\langle -\frac{1}{2m}\{G_i,P_i\}\right\rangle_0, \tag{A4}$$

where $\tilde{G}_4$ and $\bar{G}_{4,0}$ are given by Eqs. (23) and (D.17) of [18],

$$\tilde{G}_4 = (-4)\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2-\lambda)^2}\frac{1}{k^2-2k\cdot\Pi+H}\frac{1}{1-\frac{k_0}{m}} \tag{A5}$$

and

$$\langle \bar{G}_{4,0} \rangle_0 = (-4) \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F(1,k_0/m)}{(k^2-\lambda)^2} \sum_{L=0}^{\infty} \Big\langle \frac{(L+1)^2-1}{L+1} j_{L+1}(\omega R) \frac{1}{k^2-2k_0\Pi_0+H_L+\omega^2} j_{L+1}(\omega R) + \frac{L^2-1}{L} j_{L-1}(\omega R) \frac{1}{k^2-2k_0\Pi_0+H_L+\omega^2} j_{L-1}(\omega R) \Big\rangle_0, \quad \text{(A6)}$$

respectively. Furthermore,

$$\langle O \rangle_0 = \langle \psi_0 | O | \psi_0 \rangle, \quad \text{(A7)}$$

where ψ_0 is the Schrödinger wave function of the hydrogen,

$$\psi_0(\vec{r}) = \langle \vec{n}|0,0\rangle\langle r|1,0\rangle, \quad \psi_0(\mu\vec{r}) = \frac{2\mu^{3/2}}{\sqrt{4\pi}} e^{-\mu r} \quad \text{(A8)}$$

and Hamilton operator H is replaced by the nonrelativistic limit H_0,

$$H_0 = 2m(\Pi_0 - m) - \vec{P}^2. \quad \text{(A9)}$$

Thus, the G's appearing on the right members of Eqs. (A1)–(A4) differ from those appearing on the left members by the replacement of H by H_0 in Eq. (7). Also, the radial Hamiltonians H_L in Eq. (A6) read

$$H_L = 2m(\Pi_0 - m) - \left(P_R^2 - \frac{L(L+1)}{R^2} \right). \quad \text{(A10)}$$

By inserting these approximations into Eq. (6), we obtain

$$\langle O \rangle \simeq -m \frac{\alpha}{2\pi} \Big\langle G_4 + \frac{(Z\alpha)^2}{4} \bar{G}_4 - \frac{1}{2m^2} P_i (G_4 + \tilde{G}_4) P_i + \tilde{G}_4 \frac{\Pi_0 - m}{m} + G_0 + \frac{(Z\alpha)^2}{4} \bar{G}_0 - \frac{1}{2m}\{G_i, P_i\} \Big\rangle_0. \quad \text{(A11)}$$

2. The matrix elements of the operators between the ground and continuum states for very large electron and photon wave numbers

Using the method described in [20] one gets

$$\int \frac{dV}{r} (\psi_{\vec{p}}^-)^* e^{-i\vec{q}\cdot\vec{r}} \psi_0(\mu\vec{r}) = \mu^{3/2} \sqrt{\frac{2}{\pi^2}} e^{\pi/2p} \left(\frac{(\vec{q}+\vec{p})^2 + \mu^2}{(\mu - ip)^2 + q^2} \right)^{i/p} \frac{\Gamma\left(1 - \frac{i}{p}\right)}{\mu^2 + (\vec{q}+\vec{p})^2}, \quad \text{(A12)}$$

where $\psi_{\vec{p}}^-$ is the solution of the Schrödinger equation for hydrogen atom that behaves at infinity as the plane wave with momentum $\vec{p}$ [20]. In the nonrelativistic limit the electron energy E in Eq. (22) is replaced by the electron mass m. Then $\vec{p}$ is related to $\vec{P}$ by

$$\vec{P} = (mZ\alpha)\vec{p}. \quad \text{(A13)}$$

The eigenvalues of the Hamilton operator (A9) in the basis of the states $\psi_{\vec{p}}^-$ are

$$H_0 = 2m(E - m) - \vec{P}^2. \quad \text{(A14)}$$

From the integral (A12) one obtains additional integrals by parametric differentiation, e.g.,

$$\int dV\, n_i (\psi_{\vec{p}}^-)^* e^{-i\vec{q}\cdot\vec{r}} \psi_0(\mu\vec{r}) = i \frac{\partial}{\partial q_i} \int \frac{dV}{r} (\psi_{\vec{p}}^-)^* e^{-i\vec{q}\cdot\vec{r}} \psi_0(\mu\vec{r}), \quad \text{(A15)}$$

$$\int dV (\psi_{\vec{p}}^-)^* e^{-i\vec{q}\cdot\vec{r}} \psi_0(\mu\vec{r}) = -\mu^{3/2} \frac{\partial}{\partial\mu} \int \frac{dV}{r} (\psi_{\vec{p}}^-)^* e^{-i\vec{q}\cdot\vec{r}} \psi_0(\mu\vec{r}) \mu^{-3/2}, \quad \text{(A16)}$$

and so on. For large p and q one has

$$\left| \int \frac{dV}{r} (\psi_{\vec{p}}^-)^* e^{-i\vec{q}\cdot\vec{r}} \psi_0(\mu\vec{r}) \right|^2 \to \frac{1}{(2\pi)^3} \left| \int \frac{dV}{r} e^{-i\vec{p}\cdot\vec{r}} e^{-i\vec{q}\cdot\vec{r}} \psi_0(\mu\vec{r}) \right|^2 \to \frac{2}{\pi^2} \frac{\mu^3}{\mu^2 + (\vec{q}+\vec{p})^2}, \quad \text{(A17)}$$

$$\left| \int dV\, n_i (\psi_{\vec{p}}^-)^* e^{-i\vec{q}\cdot\vec{r}} \psi_0(\mu\vec{r}) \right|^2 \to \frac{1}{(2\pi)^3} \left| \int dV\, n_i e^{-i\vec{p}\cdot\vec{r}} e^{-i\vec{q}\cdot\vec{r}} \psi_0(\mu\vec{r}) \right|^2 \to \frac{2^3}{\pi^2} \frac{\mu^3}{\mu^2 + (\vec{q}+\vec{p})^2}, \quad \text{(A18)}$$

and

$$\left| \int dV (\psi_{\vec{p}}^-)^* e^{-i\vec{q}\cdot\vec{r}} \psi_0(\vec{r}) \right|^2 \simeq \frac{2^3\mu^3}{\pi^2} \left| 1 - \frac{(\vec{p}+\vec{q})^2}{(\vec{p}^2 - \vec{q}^2)} \right|^2 \frac{1}{(\vec{p}+\vec{q})^4}. \quad \text{(A19)}$$

Now, it is important to note that while Eqs. (A17) and (A18) depend for large p and q only on the sum $\vec{p}+\vec{q}$ and the exact wave function of the hydrogen $\psi_{\vec{p}}^-$ can be for large p and q replaced by free-particle wave function $\exp\{-i\vec{p}\cdot\vec{r}\}/(2\pi)^{3/2}$, this is clearly not true for Eq. (A19). This is not surprising at all. The states $\psi_{\vec{p}}^-$ and ψ_0 are orthogonal for arbitrarily large p. Thus, for $q = 0$ the integral (A19) has to be zero for all p. This clearly cannot be achieved when the exact wave function is replaced by the free-particle wave function. Fortunately, when calculating the contribution of the order $\alpha(Z\alpha)^5$, we do not have to deal with the integrals (A16) at all. By means of identities

$$\left\langle \frac{1}{k^2-2k\cdot\Pi+H}(\Pi-\varepsilon)_\mu \right\rangle = \frac{1}{k^2-2k\cdot\varepsilon}\langle(\Pi-\varepsilon)_\mu\rangle + \frac{1}{k^2-2k.\varepsilon}\left\langle 2k\cdot(\Pi-\varepsilon)\frac{1}{k^2-2k\cdot\Pi+H}(\Pi-\varepsilon)_\mu \right\rangle, \quad \text{(A20)}$$

$$\left\langle \frac{1}{k^2-2k\cdot\Pi+H} \right\rangle = \frac{1}{k^2-2k\cdot\varepsilon}\langle 1\rangle + \frac{1}{(k^2-2k\cdot\varepsilon)^2}\langle 2k\cdot(\Pi-\varepsilon)\rangle + \frac{1}{(k^2-2k\cdot\varepsilon)^2}\left\langle 2k\cdot(\Pi-\varepsilon)\frac{1}{k^2-2k\cdot\Pi+H}2k\cdot(\Pi-\varepsilon)\right\rangle \quad \text{(A21)}$$

we always transform the integrals (A16) to the integrals (A12) or (A15). These identities follow from the identity

$$\begin{aligned}\frac{1}{k^2-2k\cdot\Pi+H} &= \frac{1}{k^2-2k\cdot\varepsilon+H} + \frac{1}{k^2-2k\cdot\varepsilon+H}2k\cdot(\Pi-\varepsilon)\frac{1}{k^2-2k\cdot\Pi+H}\\ &= \frac{1}{k^2-2k\cdot\varepsilon+H} + \frac{1}{k^2-2k\cdot\varepsilon+H}2k\cdot(\Pi-\varepsilon)\frac{1}{k^2-2k\cdot\varepsilon+H}\\ &\quad + \frac{1}{k^2-2k\cdot\varepsilon+H}2k\cdot(\Pi-\varepsilon)\frac{1}{k^2-2k\cdot\Pi+H}2k\cdot(\Pi-\varepsilon)\frac{1}{k^2-2k\cdot\varepsilon+H}\end{aligned}$$

and the fact that H, operating on the reference wave function, yields zero. The first term on the right member of Eq. (A20) and the first two terms on the right member of Eq. (A21) are either removed by the renormalization of the electron mass or do not contribute at the order $\alpha(Z\alpha)^5$. Thus, they will not be considered further.

3. Elimination of explicit appearance of $\Pi_0 - m$

In the case of Coulomb potential, the interaction term $-2k_0(\Pi_0-m)$ can be eliminated from the electron propagator as follows:

$$\begin{aligned}&\left\langle (\Pi-\varepsilon)_\mu \frac{1}{k^2-2k\cdot\varepsilon+u\,[2k\cdot(\Pi-\varepsilon)+H]}(\Pi-\varepsilon)_\nu \right\rangle\\ &= \left\langle (\Pi-\varepsilon)_\mu e^{i\vec{k}\cdot\vec{R}} \frac{1}{k^2-2k\cdot\varepsilon+u[2k_0(\Pi-\varepsilon)_0+H+\omega^2]} e^{-i\vec{k}\cdot\vec{R}}(\Pi-\varepsilon)_\nu \right\rangle\\ &= \xi^2\left\langle (\Pi-\varepsilon)_\mu e^{i\vec{k}\cdot\frac{\vec{R}}{\xi}} \frac{1}{k^2-2k\cdot\varepsilon+u[2(\xi-1)(m^2-Em)+(\xi-1)^2(m^2-E^2)+H\xi^2+\omega^2]} e^{-i\vec{k}\cdot(\vec{R}/\xi)}(\Pi-\varepsilon)_\nu \right\rangle_\xi\\ &= \xi^2\left\langle (\Pi-\varepsilon)_\mu \frac{1}{k^2-2k\cdot P_u+u\Delta}(\Pi-\varepsilon)_\nu \right\rangle_\xi, \end{aligned} \quad \text{(A22)}$$

where

$$\xi = 1-\frac{k_0}{E}, \quad \text{(A23)}$$

$$P_u = (m\varepsilon_0, \vec{P}u\xi), \quad \text{(A24)}$$

$$\Delta = 2(\xi-1)(m^2-Em)+(\xi-1)^2(m^2-E^2)+H_0\xi^2, \quad \text{(A25)}$$

and

$$\langle O\rangle_\xi = \int\!\!\int d^3\vec{r}\,d^3\vec{r}\,'\psi^+\left(\frac{\vec{r}}{\xi}\right)O(\vec{r},\vec{r}\,')\psi\left(\frac{\vec{r}\,'}{\xi}\right). \quad \text{(A26)}$$

The first equality in Eq. (A22) follows from Eq. (13). The second equality follows from Eq. (46) where the substitution $r\to r/\xi$ is made. The last equality follows again from Eq. (13) but this time used in the reversed way. Furthermore, in the second equality we used an approximation

$$(\Pi-\varepsilon)_0 = \Pi_0 - m \simeq m\frac{(Z\alpha)^2}{r}. \quad \text{(A27)}$$

Using Eqs. (A17) and (A18), we can write for large P,

$$(A22) \to \xi^2\int d^3\vec{p}\left\langle (\Pi-\varepsilon)_\mu \frac{|\vec{p}\rangle\langle\vec{p}|}{k^2-2k\cdot P_u+u\Delta(\vec{P})}(\Pi-\varepsilon)_\nu \right\rangle_\xi, \quad \text{(A28)}$$

where from Eqs. (A14) and (A25) we have

$$\Delta(\vec{P}) = 2(\xi-1)(m^2-Em) + (\xi-1)^2(m^2-E^2) + [2m(E-m)-\vec{P}^2]\xi^2 = -\vec{P}^2\xi^2 + \xi(Z\alpha)^2. \tag{A29}$$

In the last equality we made an approximation

$$\frac{E}{m} \simeq 1 - \frac{(Z\alpha)^2}{2}. \tag{A30}$$

Armed with Eq. (A22) and Feynman parameters, we can rewrite the last terms on the right members of Eqs. (A20) and (A21):

$$\frac{1}{k^2-2k\cdot\varepsilon}\left\langle 2k\cdot(\Pi-\varepsilon)\frac{1}{k^2-2k\cdot\Pi+H}(\Pi-\varepsilon)_\mu\right\rangle = \xi^2\left\langle(\Pi-\varepsilon)_\nu\frac{\partial}{\partial(P_u)_\nu}\int_0^1 du\frac{1}{k^2-2k\cdot P_u+u\Delta}(\Pi-\varepsilon)_\mu\right\rangle_\xi \tag{A31}$$

and

$$\frac{1}{(k^2-2k\cdot\varepsilon)^2}\left\langle 2k\cdot(\Pi-\varepsilon)\frac{1}{k^2-2k\cdot\Pi+H}2k\cdot(\Pi-\varepsilon)\right\rangle = \xi^2\left\langle(\Pi-\varepsilon)_\nu\frac{\partial^2}{\partial(P_u)_\nu\partial(P_u)_\mu}\int_0^1 du\frac{(1-u)}{k^2-2k\cdot P_u+u\Delta}(\Pi-\varepsilon)_\mu\right\rangle_\xi. \tag{A32}$$

4. Expansion in time components

As in Eq. (54), the expansion in time component of $(\Pi-\varepsilon)$ is now obtained by expanding the electron propagator in powers of k_0,

$$\xi^2\left\langle(\Pi-\varepsilon)_\nu\frac{1}{k^2-2k\cdot P_u+u\Delta}(\Pi-\varepsilon)_\mu\right\rangle_\xi\Bigg|_{\xi=1-(k_0/E)}$$
$$= \sum_t\left(\frac{-2k_0}{E}\right)^t\frac{1}{2^t}\frac{1}{t!}\frac{\partial^t}{\partial\xi^t}\xi^2\left\langle(\Pi-\varepsilon)_\nu\frac{1}{k^2-2k\cdot P_u+u\Delta}(\Pi-\varepsilon)_\mu\right\rangle_\xi\Bigg|_{\xi=1}. \tag{A33}$$

5. Integration over four-momentum of the virtual photon

As discussed in Appendix D, the integration over four-momentum of the virtual photon yields

$$(-4)\int_0^{\Lambda^2}d\lambda\int\frac{d^4k_F(1,k_\nu/m)}{(k^2-\lambda)^2}\frac{(-2k_0/E)^t}{k^2-2k\cdot P_u+u\Delta(\vec{P})} = \left(\frac{m}{E}\right)^t\int_0^1 dy\int_{(\Lambda^2/m^2)[(1-y)/y]}^0 d^{t+1}\lambda(-1)^t\,\frac{\partial^t}{\partial\varepsilon_0^t}\,\frac{\left(1,\frac{(P_u)_\nu}{m}y\right)}{D_u(\vec{P})}\Bigg|_{\varepsilon_0=1}, \tag{A34}$$

where

$$D_u(\vec{P}) = \frac{P_u^2}{m^2}y - \frac{\Delta(\vec{P})}{m^2}u + \lambda. \tag{A35}$$

By inserting Eq. (A34) into Eq. (A33) and setting $E\simeq m$, we obtain

$$\left\langle(\Pi-\varepsilon)_\rho G_{4,\nu}(\Pi-\varepsilon)_\mu\right\rangle_0 = \sum_{t=0}^{\infty}\int_0^1 dy\int_{(\Lambda^2/m^2)[(1-y)/y]}^0 d^{t+1}\lambda(-1)^t\frac{\partial^t}{\partial\varepsilon_0^t}\frac{1}{2^t}\frac{1}{t!}\frac{\partial^t}{\partial\xi^t}\xi^2\left\langle(\Pi-\varepsilon)_\rho\frac{\left(1,\frac{(P_u)_\nu}{m}y\right)}{D_u(\vec{P})}(\Pi-\varepsilon)_\mu\right\rangle_\xi\Bigg|_{\varepsilon_0=\xi=1}. \tag{A36}$$

We will show in a moment that as far as the terms of the order $(Z\alpha)^5$ are concerned, the expression $\xi^2\langle(\Pi-\varepsilon)_\rho\frac{(1,\frac{(P_u)_\nu}{m}y)}{D_u(\vec{P})}(\Pi-\varepsilon)_\mu\rangle_\xi$ is independent of ξ. Thus, the contribution of the order $(Z\alpha)^5$ is determined just by the zeroth term of the sum on the right member of Eq. (A36).

Further, we leave out the terms contributing to the renormalization of the electron mass. The cutoff Λ can then be taken to the infinity. Equation (A36) then acquires the form of

$$\langle(\Pi-\varepsilon)_\rho G_{4,\nu}(\Pi-\varepsilon)_\mu\rangle_0 \simeq \xi^2\int_0^1 dy\int_\infty^0 d\lambda\left\langle(\Pi-\varepsilon)_\rho\frac{\left(1,\frac{(P_u)_\nu}{m}y\right)}{D_u(\vec{P})}(\Pi-\varepsilon)_\mu\right\rangle_\xi. \tag{A37}$$

Applying this equation on Eq. (A32), Eq. (A31) for $\mu = 0$ and Eq. (A31) for $\mu = i$, we obtain

$$\int_0^1 du(1-u)\left\langle(\Pi-\varepsilon)_\nu \frac{\partial^2}{\partial(P_u)_\nu\partial(P_u)_\mu} G_{4,0}(\Pi-\varepsilon)_\mu\right\rangle_0 = \xi^2\int_\infty^0 d\lambda\int_0^1 dy\int_0^1 du(1-u)\left\langle(\Pi-\varepsilon)_\nu \frac{\partial^2}{\partial(P_u)_\nu\partial(P_u)_\mu}\frac{(1,\varepsilon_0 y)}{D_u}(\Pi-\varepsilon)_\mu\right\rangle_\xi, \tag{A38}$$

$$\frac{1}{m}\int_0^1 du\left\langle(\Pi_0-m)\frac{\partial}{\partial(P_u)_\nu}\tilde{G}_4(\Pi-\varepsilon)_\nu\right\rangle_0 = \frac{\xi}{m}\int_\infty^0 d\lambda\int_0^1 dy\int_0^1 du\left\langle(\Pi_0-m)\frac{\partial}{\partial(P_u)_\nu}\frac{1}{D_u}(\Pi-\varepsilon)_\nu\right\rangle_\xi, \tag{A39}$$

and

$$-\frac{1}{m^2}\int_0^1 du\left\langle P_i\frac{\partial}{\partial(P_u)_\nu}G_i(\Pi-\varepsilon)_\nu\right\rangle_0 = (-1)\frac{\xi^2}{m^2}\int_\infty^0 d\lambda\int_0^1 dy\int_0^1 du\left\langle P_i\frac{\partial}{\partial(P_u)_\nu}\frac{(P_u)_i y}{D_u}(\Pi-\varepsilon)_\nu\right\rangle_\xi, \tag{A40}$$

respectively. Furthermore, for $\langle\bar{G}_{4,0}\rangle_0$ given by Eq. (A6) we have found by numerology

$$\frac{(Z\alpha)^2}{4}\langle\bar{G}_{4,0}\rangle_0 = -\frac{4\xi^2}{m^2}\int_\infty^0 d\lambda\int_0^1 dy\int_0^1 du(1-u)\left\langle(\Pi_0-m)(1,y\varepsilon_0)\frac{\partial}{\partial\varepsilon_0^2}\frac{1}{D_u}(\Pi_0-m)\right\rangle_\xi. \tag{A41}$$

6. Parametric differentiation

Using equations

$$\frac{\partial}{\partial(P_u)_i}\frac{1}{D_u} = \frac{(-2)(P_u)_i}{m^2}\frac{\partial}{\partial\varepsilon_0^2}\frac{1}{D_u} \tag{A42}$$

and

$$\frac{\partial^2}{\partial(P_u)_i\partial(P_u)_j}\frac{1}{D_u} = \frac{(-2)\delta_{ij}}{m^2}\frac{\partial}{\partial\varepsilon_0^2}\frac{1}{D_u} + \frac{4(P_u)_i(P_u)_j}{m^4}\frac{\partial^2}{\partial\left(\varepsilon_0^2\right)^2}\frac{1}{D_u} \tag{A43}$$

following from Eqs. (A24) and (A35) and using further Schrödinger equation

$$\xi^2\vec{P}^2\psi_0\left(\frac{\vec{r}}{\xi}\right) = \xi 2m(\Pi_0-m)\psi_0\left(\frac{\vec{r}}{\xi}\right), \tag{A44}$$

we obtain from Eq. (A38) separating explicitly the time and space components.

$$\int_0^1 du(1-u)\left\langle P_i\frac{\partial^2}{\partial(P_u)_i\partial(P_u)_j}G_{4,0}P_j\right\rangle_0 = \frac{\xi^2}{m^2}\int_\infty^0 d\lambda\int_0^1 dy\int_0^1 du(1-u)\left\langle -2P_i\frac{\partial}{\partial\varepsilon_0^2}\frac{(1,y)}{D_u}P_i + 16u^2(\Pi_0-m)\frac{\partial^2}{\partial\left(\varepsilon_0^2\right)^2}\frac{(1,y)}{D_u}(\Pi_0-m)\right\rangle_\xi, \tag{A45}$$

$$2\int_0^1 du(1-u)\left\langle(\Pi_0-m)\frac{\partial^2}{\partial(P_u)_0\partial(P_u)_i}G_{4,0}P_i\right\rangle_0 = \frac{\xi^2}{m^2}\int_\infty^0 d\lambda\int_0^1 dy\int_0^1 du(1-u)(-8u)\left\langle(\Pi_0-m)\frac{\partial}{\partial\varepsilon_0}\left[(1,\varepsilon_0 y)\frac{\partial}{\partial\varepsilon_0^2}\frac{1}{D_u}\right](\Pi_0-m)\right\rangle_\xi, \tag{A46}$$

and

$$\int_0^1 du(1-u)\left\langle(\Pi_0-m)\frac{\partial^2}{\partial(P_u)_0\partial(P_u)_0}G_{4,0}(\Pi_0-m)\right\rangle_0 = \frac{\xi^2}{m^2}\int_\infty^0 d\lambda\int_0^1 dy\int_0^1 du(1-u)\left\langle(\Pi_0-m)\frac{\partial^2}{\partial\varepsilon_0^2}\frac{(1,\varepsilon_0 y)}{D_u}(\Pi_0-m)\right\rangle_\xi. \tag{A47}$$

Likewise, by inserting Eq. (A42) into Eq. (A39) and using Eq. (A44) we obtain

$$\int_0^1 du\frac{1}{m}\left\langle(\Pi_0-m)\frac{\partial}{\partial(P_u)_i}\tilde{G}_4 P_i\right\rangle_0 = \frac{\xi}{m^2}\int_\infty^0 d\lambda\int_0^1 dy\int_0^1 du(-4u)\left\langle(\Pi_0-m)\frac{\partial}{\partial\varepsilon_0^2}\frac{1}{D_u}(\Pi_0-m)\right\rangle_\xi \tag{A48}$$

and

$$\frac{1}{m}\int_0^1 du\left\langle(\Pi_0-m)\frac{\partial}{\partial(P_u)_0}\tilde{G}_4(\Pi_0-m)\right\rangle_0=\frac{\xi}{m^2}\int_\infty^0 d\lambda\int_0^1 dy\int_0^1 du\left\langle(\Pi_0-m)\frac{\partial}{\partial\varepsilon_0}\frac{1}{D_u}(\Pi_0-m)\right\rangle_\xi. \tag{A49}$$

Finally, by inserting equation

$$\frac{\partial}{\partial(P_u)_j}\frac{(P_u)_i}{D_u}=\frac{\delta_{ij}}{D_u}-\frac{2(P_u)_i(P_u)_j}{m^2}\frac{\partial}{\partial\varepsilon_0^2}\frac{1}{D_u} \tag{A50}$$

into Eq. (A40) and using Eq. (A44) we obtain

$$-\frac{1}{m^2}\int_0^1 du\left\langle P_i\frac{\partial}{\partial(P_u)_j}G_iP_j\right\rangle_0=\frac{\xi^2}{m^2}\int_\infty^0 d\lambda\int_0^1 dyy\int_0^1 du\left\langle -P_i\frac{1}{D_u}P_i+8u^2(\Pi_0-m)\frac{\partial}{\partial\varepsilon_0^2}\frac{1}{D_u}(\Pi_0-m)\right\rangle_\xi \tag{A51}$$

and

$$-\frac{1}{m^2}\int_0^1 du\left\langle P_i\frac{\partial}{\partial(P_u)_0}G_i(\Pi_0-m)\right\rangle_0=-\frac{\xi^2}{m^2}\int_\infty^0 d\lambda\int_0^1 dy\,y\int_0^1 du\,2u\left\langle(\Pi_0-m)\frac{\partial}{\partial\varepsilon_0}\frac{1}{D_u}(\Pi_0-m)\right\rangle_\xi. \tag{A52}$$

7. Integration over three-momentum of the virtual electron

Using Eqs. (A17), (A18), and (A28) we get

$$\frac{\xi^2}{m^2}\left\langle(\Pi_0-m)\frac{1}{D_u}(\Pi_0-m)\right\rangle_\xi \to\frac{(Z\alpha)^2}{\xi}\frac{2}{\pi^2}\int d^3\vec{p}\,\frac{1}{D_u(\vec{p})}\frac{1}{(\xi^{-2}+\vec{p}^2)^2} \tag{A53}$$

and

$$\frac{\xi^2}{m^2}\left\langle P_i\frac{1}{D_u}P_i\right\rangle_\xi\to\frac{(Z\alpha)^2}{\xi^3}\frac{2^3}{\pi^2}\int d^3\vec{p}\,\frac{1}{D_u(\vec{p})}\frac{1}{(\xi^{-2}+\vec{p}^2)^3}, \tag{A54}$$

where in Eq. (A53) the approximation (A27) was used. From Eqs. (A13), (A24), (A29), and (A35) we have

$$D_u(\vec{p})=\varepsilon_0^2y+\vec{p}^2(\xi Z\alpha)^2u(1-yu)+\xi u(Z\alpha)^2+\lambda. \tag{A55}$$

Integrating now over the three-momentum of the virtual electron and keeping only the leading term in $(Z\alpha)$ leads to

$$\text{(A53)}\to(Z\alpha)^5(-2^2)\frac{[u(1-yu)]^{1/2}}{\left(\varepsilon_0^2y+\lambda\right)^{3/2}}, \tag{A56}$$

$$\text{(A54)}\to(Z\alpha)^5 2^4\frac{[u(1-yu)]^{3/2}}{\left(\varepsilon_0^2y+\lambda\right)^{5/2}}. \tag{A57}$$

Performing integrations over λ we get

$$\int_\infty^0 d\lambda\frac{1}{\left(\varepsilon_0^2y+\lambda\right)^{3/2}}=-2\left(\varepsilon_0^2y\right)^{-1/2},\qquad \int_\infty^0 d\lambda\frac{1}{\left(\varepsilon_0^2y+\lambda\right)^{5/2}}=-\frac{2}{3}\left(\varepsilon_0^2y\right)^{-3/2}. \tag{A58}$$

By combining this result with Eqs. (A56) and (A57) we obtain

$$\frac{\xi^2}{m^2}\int_\infty^0 d\lambda\left\langle(\Pi_0-m)\frac{1}{D_u}(\Pi_0-m)\right\rangle_\xi \to\frac{2^3[u(1-yu)]^{1/2}}{\left(\varepsilon_0^2y\right)^{1/2}}(Z\alpha)^5 \tag{A59}$$

and

$$\frac{\xi^2}{m^2}\int_\infty^0 d\lambda\left\langle P_i\frac{1}{D_u}P_i\right\rangle_\xi\to-\frac{2^5[u(1-yu)]^{3/2}}{3\left(\varepsilon_0^2y\right)^{3/2}}(Z\alpha)^5. \tag{A60}$$

As announced above, the result is independent of ξ. This *a posteriori* justifies the replacement of Eq. (A36) by Eq. (A37).

8. The terms contributing at the order $\alpha(Z\alpha)^5$

In the following part the superscript t on $G_{4,\nu}^t$ denotes the number of expanded powers of Π_0-m.

When comparing Eqs. (7) and (A5), apparently $\tilde{G}_4^0=G_4^0$. Then from Eq. (A60) for $u=1$ and $\varepsilon_0=1$ one has

$$-\frac{1}{2m^2}\left\langle P_i\left(G_4^0+\tilde{G}_4^0\right)P_i\right\rangle_0\simeq(Z\alpha)^5\int_0^1 dy\frac{2^5(1-y)^{3/2}}{3y^{3/2}}. \tag{A61}$$

From Eqs. (A41) and (A59)

$$\frac{(Z\alpha)^2}{4}\left\langle\bar{G}_{4,0}^0\right\rangle_0\simeq-(Z\alpha)^5 2^5\int_0^1 dy\int_0^1 du[u(1-yu)]^{1/2}\times\frac{\partial}{\partial\varepsilon_0^2}\frac{(1,y)}{\left(\varepsilon_0^2y\right)^{1/2}}. \tag{A62}$$

It follows from Eqs. (A21) and (A32) that

$$\left\langle G_{4,0}^0\right\rangle_0=\int_0^1 du(1-u)\left\langle P_i\frac{\partial^2}{\partial(P_u)_i\partial(P_u)_j}G_{4,0}P_j\right\rangle_0, \tag{A63}$$

$$\left\langle G_{4,0}^1\right\rangle_0=2\int_0^1 du(1-u)\left\langle(\Pi_0-m)\frac{\partial^2}{\partial(P_u)_0\partial(P_u)_i}G_{4,0}P_i\right\rangle_0, \tag{A64}$$

and

$$\langle G_{4,0}^2\rangle_0 = \int_0^1 du(1-u) \times \left\langle (\Pi_0 - m)\frac{\partial^2}{\partial(P_u)_0\partial(P_u)_0}G_{4,0}(\Pi_0 - m)\right\rangle_0. \quad \text{(A65)}$$

Inserting successively Eqs. (A45), (A46), and (A47) into Eqs. (A63), (A64), and (A65) and using Eqs. (A59) and (A60) one gets

$$\text{(A63)} \simeq (Z\alpha)^5 \int_0^1 dy \int_0^1 du \left[\frac{2^6}{3}\frac{[u(1-yu)]^{3/2}}{y^{3/2}}\frac{\partial}{\partial\varepsilon_0^2}\frac{(1,y)}{(\varepsilon_0^2)^{3/2}} + 2^7\frac{\partial^2}{\partial(\varepsilon_0^2)^2}\frac{[u(1-uy)]^{1/2}(1,y)}{(\varepsilon_0^2 y)^{1/2}}\right], \quad \text{(A66)}$$

$$\text{(A64)} \simeq (Z\alpha)^5 \int_0^1 dy \int_0^1 du(-2^6 u)\frac{\partial}{\partial\varepsilon_0}(1,\varepsilon_0 y) \times \frac{\partial}{\partial\varepsilon_0^2}\frac{[u(1-uy)]^{1/2}}{(\varepsilon_0^2 y)^{1/2}}, \quad \text{(A67)}$$

and

$$\text{(A65)} \simeq (Z\alpha)^5 \int_0^1 dy \int_0^1 du 2^3 \frac{\partial^2}{\partial\varepsilon_0^2}(1,\varepsilon_0 y)\frac{[u(1-uy)]^{1/2}}{(\varepsilon_0^2 y)^{1/2}}. \quad \text{(A68)}$$

Similarly, it follows from Eqs. (A20) and (A31)

$$\frac{1}{m}\langle \tilde{G}_4^0(\Pi_0 - m)\rangle_0 = \int_0^1 du \frac{1}{m}\left\langle (\Pi_0 - m)\frac{\partial}{\partial(P_u)_i}\tilde{G}_4 P_i\right\rangle_0, \quad \text{(A69)}$$

$$-\frac{1}{2m}\langle\{G_i^0, P_i\}\rangle_0 = -\frac{1}{m^2}\int_0^1 du \left\langle P_i \frac{\partial}{\partial(P_u)_j}G_i P_j\right\rangle_0, \quad \text{(A70)}$$

and

$$-\frac{1}{2m}\langle\{G_i^1, P_i\}\rangle_0 = -\frac{1}{m^2}\int_0^1 du \left\langle P_i \frac{\partial}{\partial(P_u)_0}G_i(\Pi_0 - m)\right\rangle_0. \quad \text{(A71)}$$

Inserting successively Eqs. (A48), (A51), and (A52) into Eqs. (A69), (A70), and (A71) and using further Eqs. (A60) and (A59) yields

$$\text{(A69)} \simeq -(Z\alpha)^5 \int_0^1 dy \int_0^1 du\, 2^5 u \frac{\partial}{\partial\varepsilon_0^2}\frac{[u(1-uy)]^{1/2}}{(\varepsilon_0^2 y)^{1/2}}, \quad \text{(A72)}$$

$$\text{(A70)} \simeq (Z\alpha)^5 \int_0^1 dy \int_0^1 du\, 2^5 y \left[\frac{1}{3}\frac{[u(1-yu)]^{3/2}}{y^{3/2}} + 2\frac{\partial}{\partial\varepsilon_0^2}(1,\varepsilon_0 y)\frac{[u(1-uy)]^{1/2}u^2}{(\varepsilon_0^2 y)^{1/2}}\right], \quad \text{(A73)}$$

and

$$\text{(A71)} \simeq -(Z\alpha)^5 \int_0^1 dy \int_0^1 du\, 2^4 uy \frac{\partial}{\partial\varepsilon_0}\frac{[u(1-uy)]^{1/2}}{(\varepsilon_0^2 y)^{1/2}}. \quad \text{(A74)}$$

The sum

$$-\frac{1}{2m^2}\langle P_i(\tilde{G}_4^t)P_i\rangle_0 + \frac{1}{m}\langle \tilde{G}_4^t(\Pi_0 - m)\rangle_0$$

is not independent of ξ, but does not contribute at the order $\alpha(Z\alpha)^5$ for $t > 0$. The contributions of individual terms mutually cancel out.

In Eqs. (A61) and (A66) the divergence appears at the lower bound of the integration over the parameter y. This is merely a consequence of the approximation (A57), where the term $\xi u(Z\alpha)^2$ in Eq. (A55) has been neglected. Had we included this term, the integrals over y would be finite at the lower bound. The integration would produce a term of the order $(Z\alpha)^4$ that is now of no interest for us. Thus, the divergence can be safely ignored.

9. Final result and its relation to RME

The remaining integrals over Feynman parameters y and u are calculated more easily if we make a substitution

$$y = \frac{v}{u} \quad \text{(A75)}$$

from y to v. Furthermore, we write

$$A_{50} = \sum A_{50}^v, \quad \text{(A76)}$$

where A_{50}^v is the contribution of the order $(Z\alpha)$ contained in F_v, Eq. (73). To get this contribution, we have to count the powers of $\vec{P}^2$ in the equations of the previous section that are not contained in the zeroth order of RME. Such a counting is provided by the factor yu in parentheses $(1-yu)$ in the second term on the right member of Eq. (A55). In the following part we multiply it by δ. Additional powers of $\vec{P}^2$ are supplied by the identities (A20) and (A21).

It follows from Eqs. (A2), (A61), and (A69)

$$-\frac{1}{2m}\langle\gamma_\mu G_4^0(\Pi-\varepsilon)_\mu\rangle \to -\frac{(Z\alpha)^5}{2}\delta\left(\int_0^1 dy \frac{2^5}{3}\frac{(1-\delta y)^{3/2}}{y^{3/2}} + \delta 2^4 \int_0^1 du\, u \int_0^u dv \frac{(1-v\delta)^{1/2}}{v^{1/2}}\right)$$
$$= \left(8 - \frac{7}{4}\right)\pi(Z\alpha)^5 = (Z\alpha)^5 \sum_v \delta^v \frac{2^3\Gamma\left(\frac{5}{2}\right)(-1)^v}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v-\frac{3}{2}\right)\left(v+\frac{1}{2}\right)}. \quad \text{(A77)}$$

The exact result is obtained by setting $\delta = 1$. The series in δ is obtained by the application of the generalized binomial theorem

$$(1-v\delta)^a = \sum_{v=0}^{\infty}\frac{\Gamma(a+1)}{\Gamma(v+1)\Gamma(a-v+1)}(-v\delta)^v$$

and trivial integrations. In a similar vein, it follows from Eqs. (A1), (A62), and (A66)

$$-\frac{1}{2}\langle\gamma_0 G_4^0\rangle$$
$$\to -\frac{(Z\alpha)^5}{2}\delta\int_0^1 du(1-u)\int_0^u dv\left\{-2^5u^2\left(\frac{(1-v\delta)^{3/2}}{v^{3/2}}-3\delta\frac{(1-v\delta)^{1/2}}{v^{1/2}}\right)+2^4\frac{(1-v\delta)^{1/2}}{v^{1/2}}\right\}=\left(-\frac{121}{32}-\frac{5}{4}\right)\pi(Z\alpha)^5$$
$$=(Z\alpha)^5\sum_v\delta^v\left\{\frac{2^5\Gamma\left(\frac{5}{2}\right)\left(v-\frac{1}{2}\right)(-1)^{v-1}}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v-\frac{3}{2}\right)\left(v+\frac{3}{2}\right)\left(v+\frac{5}{2}\right)}+\frac{2^3\Gamma\left(\frac{3}{2}\right)\left(v-\frac{5}{2}\right)(-1)^{v-1}}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v-\frac{1}{2}\right)\left(v+\frac{1}{2}\right)\left(v+\frac{3}{2}\right)}\right\}, \tag{A78}$$

from Eqs. (A1) and (A67)

$$-\frac{1}{2}\langle\gamma_0 G_4^1\rangle\to-\frac{(Z\alpha)^5}{2}\delta^2(-3)2^5\int_0^1 du(1-u)\int_0^u dv\,u\frac{(1-v\delta)^{1/2}}{v^{1/2}}$$
$$=\frac{25}{8}\pi(Z\alpha)^5=(Z\alpha)^5\sum_v\delta^v\frac{2^5\Gamma\left(\frac{5}{2}\right)(-1)^v(v-1)}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v-\frac{3}{2}\right)\left(v+\frac{1}{2}\right)\left(v+\frac{3}{2}\right)}, \tag{A79}$$

from Eqs. (A1) and (A68)

$$-\frac{1}{2}\langle\gamma_0 G_4^2\rangle\to-\frac{(Z\alpha)^5}{2}\delta^2 2^4\int_0^1 du(1-u)\int_0^u dv\frac{(1-v\delta)^{1/2}}{v^{1/2}}$$
$$=-\frac{5}{4}\pi(Z\alpha)^5=(Z\alpha)^5\sum_v\delta^v\frac{2^3\Gamma\left(\frac{3}{2}\right)(-1)^{v-1}(v-1)}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v-\frac{3}{2}\right)\left(v-\frac{1}{2}\right)\left(v+\frac{1}{2}\right)}, \tag{A80}$$

from Eqs. (A4) and (A73)

$$-\frac{1}{2}\langle\gamma_0 G_i^0\gamma_i\gamma_0\rangle\to-\frac{(Z\alpha)^5}{2}\delta\int_0^1 du\,u\int_0^u dv\left\{\frac{2^5}{3}\frac{(1-v\delta)^{3/2}}{v^{1/2}}-2^5\delta(1-v\delta)^{1/2}v^{1/2}\right\}$$
$$=-\frac{\pi}{4}(Z\alpha)^5=(Z\alpha)^5\sum_v\delta^v\frac{2^4\Gamma\left(\frac{3}{2}\right)(-1)^v}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v+\frac{3}{2}\right)}, \tag{A81}$$

from Eqs. (A4) and (A74)

$$-\frac{1}{2}\langle\gamma_0 G_i^1\gamma_i\gamma_0\rangle\to-\frac{(Z\alpha)^5}{2}\delta^2 2^4\int_0^1 du\int_0^u dv(1-v\delta)^{1/2}v^{1/2}$$
$$=-\frac{\pi}{2}(Z\alpha)^5=(Z\alpha)^5\sum_v\delta^v\frac{2^3\Gamma\left(\frac{3}{2}\right)(-1)^{v-1}(v-1)}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v-\frac{1}{2}\right)\left(v+\frac{1}{2}\right)}, \tag{A82}$$

from Eqs. (A3) and (A66)

$$-\frac{1}{2}\langle\gamma_0 G_0^0\rangle\to-\frac{(Z\alpha)^5}{2}\delta\int_0^1 du(1-u)\int_0^u dv\left\{-2^5u\left(\frac{(1-v\delta)^{3/2}}{v^{1/2}}-3\delta(1-v\delta)^{1/2}v^{1/2}\right)+2^4u^{-1}(1-v\delta)^{1/2}v^{1/2}\right\}$$
$$=\left(\frac{3}{8}+1-2\ln 2\right)\pi(Z\alpha)^5$$
$$=(Z\alpha)^5\sum_v\delta^v\left\{\frac{2^5\Gamma\left(\frac{5}{2}\right)(-1)^{v-1}}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v+\frac{3}{2}\right)\left(v+\frac{5}{2}\right)}-\frac{2^3\Gamma\left(\frac{3}{2}\right)(-1)^{v-1}(v-1)}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v-\frac{3}{2}\right)\left(v+\frac{1}{2}\right)\left(v+\frac{3}{2}\right)}\right\}, \tag{A83}$$

and finally from Eqs. (A3) and (A67)

$$-\frac{1}{2}\langle\gamma_0 G_0^1\rangle\to-\frac{(Z\alpha)^5}{2}\delta^2(-2^6)\int_0^1 du(1-u)\int_0^u dv(1-v\delta)^{1/2}v^{1/2}$$
$$=\frac{5}{8}\pi(Z\alpha)^5=(Z\alpha)^5\sum_v\delta^v\frac{2^5\Gamma\left(\frac{3}{2}\right)(-1)^v(v-1)}{\Gamma\left(\frac{7}{2}-v\right)\Gamma(v)\left(v-\frac{1}{2}\right)\left(v+\frac{1}{2}\right)\left(v+\frac{3}{2}\right)}. \tag{A84}$$

Equations (77) for $A_{50}^{(v)}$ and (79) for A_{50} are obtained by collecting the terms of the powers δ^v from the equations above and summing the above equations, respectively.

TABLE VI. The comparison of the exact calculation and nonrelativistic approximation for the terms $\langle\gamma_0 G_4^{2v,3}\rangle$, $\langle\gamma_0 G_0^{2v,2}\rangle$, $\langle\gamma_0 G_0^{2v,3}\rangle$, and $\langle\gamma_0 G_i^{2v-1,2}\gamma_i\gamma_0\rangle$. The contributions are multiplied by $-[2(Z\alpha)^4]^{-1}$. The relative error of the nonrelativistic approximation with respect to the exact result is displayed in parentheses.

v	$\langle\gamma_0 G_4^{2v,3}\rangle$	$\langle G_4^{2v,3}\rangle_0$	v	$\langle\gamma_0 G_0^{2v,2}\rangle$	$\langle G_0^{2v,2}\rangle 0$
0	-0.140506×10^{-3}	-0.140496×10^{-3} (0.71×10^{-4})	1	0.987415×10^{-4}	0.987814×10^{-4} (0.40×10^{-3})
1	-0.739838×10^{-5}	-0.739063×10^{-5} (0.10×10^{-2})	2	0.998692×10^{-5}	0.998068×10^{-5} (0.62×10^{-3})
2	-0.127661×10^{-5}	-0.127565×10^{-5} (0.75×10^{-3})	3	0.235166×10^{-5}	0.235087×10^{-5} (0.34×10^{-3})
3	-0.376911×10^{-6}	-0.376646×10^{-6} (0.70×10^{-3})	4	0.830516×10^{-6}	0.830290×10^{-6} (0.27×10^{-3})
v	$\langle\gamma_0 G_0^{2v,3}\rangle$	$\langle G_0^{2v,3}\rangle_0$	v	$\langle\gamma_0 G_i^{2v-1,2}\gamma_i\gamma_0\rangle$	$-\langle\{G_i^{2v-1,2},P_i\}\rangle_0/(2m)$
0	0.640844×10^{-4}	0.640770×10^{-4} (0.12×10^{-3})	1	-0.132412×10^{-3}	-0.132397×10^{-3} (0.11×10^{-3})
1	0.224290×10^{-5}	0.223871×10^{-5} (0.19×10^{-2})	2	-0.114446×10^{-4}	-0.114301×10^{-4} (0.12×10^{-2})
2	0.416739×10^{-6}	0.416348×10^{-6} (0.94×10^{-3})	3	-0.307593×10^{-5}	-0.307365×10^{-5} (0.74×10^{-3})
3	0.129357×10^{-6}	0.129288×10^{-6} (0.53×10^{-3})	4	-0.124072×10^{-5}	-0.123992×10^{-5} (0.64×10^{-3})

APPENDIX B: NONRELATIVISTIC APPROXIMATION

The nonrelativistic model defined by Eq. (A11) was used in Appendix A to determine the contribution of the order $\alpha(Z\alpha)^5$. It can also be used for an estimate of the terms that do not contribute to the order $\alpha(Z\alpha)^5$. These are the terms $\langle\gamma_0 G_4^{2(v-t),t}\rangle$ for $t>2$, $\langle\gamma_0 G_0^{2(v-t),t}\rangle$ for $t>1$, $\langle\gamma_0 G_i^{2(v-t)-1,t}\gamma_i\gamma_0\rangle$ for $t>1$ and $\langle\gamma_\mu G_4^{2(v-t-1),t}(\Pi-\varepsilon)_\mu/m\rangle$ for $t>0$. The advantage of the nonrelativistic model lies in the fact that for integer l_0 and l_Γ (it actually suffices for the difference $l_\Gamma - l_0$ to be an integer) the hypergeometric function in Eq. (49) reduces to polynomial. This tremendously simplifies the calculation of the hypergeometric function. This in turn enables us to make the substitution (66) right at the exact expression (49). The calculation of the terms like $\langle\gamma_0 G_{4,0}^{2(v-t),t}\rangle$ for higher t is then substantially simpler than the one described in Sec. III. In Tables V and VI, the comparison between the exact and nonrelativistic results for the terms with higher temporal multipoles $t>1$ is displayed. This is an important check of the calculation as the exact and nonrelativistic results are obtained by somewhat different methods. Further, it enables us to calculate the contributions of higher spatial multipoles for $t>1$ by the nonrelativistic approximation with sufficient accuracy. This leads to a substantial simplification of the calculation.

APPENDIX C: ASYMPTOTIC EXPANSION OF THE HYPERGEOMETRIC FUNCTION

The hypergeometric function possesses series

$$F(a,b,c,z)=\sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{(c)_n}\frac{z^n}{n!}, \tag{C1}$$

where, for example, $(c)_n$ stands for Pochhammer symbol

$$(c)_n=\frac{\Gamma(c+n)}{\Gamma(c)}. \tag{C2}$$

The series (C1) converges for $|z|<1$. The hypergeometric function in Eq. (49) goes for large k_e to $z=2$. To be able to obtain an asymptotic expansion of the function for large k_e, we use the formula (see, e.g., [20])

$$\begin{aligned}
&F\left(\frac{i}{k_e}+l+1,l-l_0-p-1,2l+2,\frac{2ik_ex}{-1+ik_ex}\right)\\
&=\frac{\Gamma(2l+2)\Gamma\left(-l_0-p-2-\frac{i}{k_e}\right)}{\Gamma(l-l_0-p-1)\Gamma\left(l+1-\frac{i}{k_e}\right)}\left(\frac{2ik_ex}{1-ik_ex}\right)^{-l-1}\left(\frac{2ik_ex}{1+ik_ex}\right)^{-l_0-p-2}\left(\frac{1+ik_ex}{1-ik_ex}\right)^{-i/k_e}\\
&\quad\times F\left(l_0+p+2-l,l_0+p+3+l,l_0+p+3+\frac{i}{k_e},\frac{-1+ik_ex}{2ik_ex}\right)+\frac{\Gamma(2l+2)\Gamma\left(l_0+p+2+\frac{i}{k_e}\right)}{\Gamma(l+l_0+p+3)\Gamma\left(l+1+\frac{i}{k_e}\right)}\\
&\quad\times\left(\frac{2ik_ex}{1-ik_ex}\right)^{-l+l_0+p+1}F\left(l-l_0-p-1,-l_0-l-p-2,-1-l_0-p-\frac{i}{k_e},\frac{-1+ik_ex}{2ik_ex}\right),
\end{aligned} \tag{C3}$$

where

$$x=(l_0+1)\xi. \tag{C4}$$

The argument z of the hypergeometric functions on the right member of Eq. (C3) goes for large k_e to $z = 1/2$. The needed asymptotic expansion is thus obtained by first using Eq. (C3) and then using the expansion (C1) for the functions on the right member. Finally, in Eqs. (C1) and (C3) the expansion of the Γ function

$$\Gamma(c_0 + c_1) = \Gamma(c_0)\left(1 + \psi(c_0)c_1 + \frac{c_1^2}{2}\left[\psi(1,c_0) + \psi^2(c_0)\right] + \cdots\right) \tag{C5}$$

is used.

APPENDIX D: INTEGRATION OVER THE FOUR-MOMENTUM OF THE VIRTUAL PHOTON AND THE FUNCTIONS Φ

1. Derivation of Eqs. (55) and (57)

The integrals (55) and (57) look divergent even for finite Λ. As discussed in [16], the integrands are determined up to an arbitrary polynomial of the $(2v + t - 1)$-th order in $\Delta + \sigma$. This is enough to make the integrals (55) and (57) convergent [16]. The integrands in Eqs. (55) and (57) can be written as

$$\frac{(2\omega)^{2v}}{k^2 - 2k\varepsilon + \Delta} = \int_0^\Delta d^{2v}w \frac{d^{2v}}{dw^{2v}} \frac{(2\omega)^{2v}}{k^2 - 2k\varepsilon + w} = \int_0^\Delta d^{2v}w \left(\frac{\partial^2}{\partial\varepsilon_i\partial\varepsilon_i}\right)^v \frac{1}{k^2 - 2k\varepsilon + w}\bigg|_{\varepsilon_i=0} \tag{D1}$$

and

$$\frac{(2\omega)^{2v-1}}{k^2 - 2k\varepsilon + \Delta} = \int_0^\Delta d^{2v-1}w \left(\frac{\partial^2}{\partial\varepsilon_i\partial\varepsilon_i}\right)^{v-1} \frac{-2\omega}{(k^2 - 2k\varepsilon + w)^2}\bigg|_{\varepsilon_i=0}. \tag{D2}$$

Thus the only integrals over four-momentum of the virtual photon to be performed explicitly are integrals

$$\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2 - \lambda)^2} \frac{(1,k_v)}{k^2 - 2k\cdot\varepsilon + w} = -\frac{1}{4}\int_0^1 dy(1,y\varepsilon_v)\left[\ln\left(\frac{\varepsilon^2 y - w}{m^2 y}\right) - \ln\left(\frac{\Lambda^2(1-y)}{m^2 y}\right)\right] \tag{D3}$$

and

$$\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2 - \lambda)^2} \frac{2\omega^2}{(k^2 - 2k\cdot\varepsilon + w)^2} = \frac{1}{4}\int_0^1 dy \frac{\partial}{\partial\varepsilon_i}\varepsilon_i y\left[\ln\left(\frac{\varepsilon^2 y - w}{m^2 y}\right) - \ln\left(\frac{\Lambda^2(1-y)}{m^2 y}\right)\right]. \tag{D4}$$

Here the terms proportional to the inverse powers of the cut-off Λ^2 have been neglected. Equations (D3) and (D4) follow from the introduction of Feynman parameter y,

$$\frac{1}{ab^2} = \int_0^1 dy \frac{2(1-y)}{[ay + b(1-y)]^3}, \quad \frac{1}{(ab)^2} = \int_0^1 dy \frac{3!y(1-y)}{[ay + b(1-y)]^4}, \tag{D5}$$

integration over d^4k,

$$\int \frac{d^4k_F(1,k_v)}{(k^2 - 2k\varepsilon y - L)^3} = \frac{1}{8}\frac{(1,\varepsilon_v y)}{(\varepsilon y)^2 + L}, \tag{D6}$$

$$\int \frac{d^4k_F k_i k_i y}{(k^2 - 2k\varepsilon y - L)^4} = -\frac{1}{3!}\frac{\partial}{\partial\varepsilon_i}\int \frac{d^4k_F k_i}{(k^2 - 2k\varepsilon y - L)^3} = -\frac{1}{3!8}\frac{\partial}{\partial\varepsilon_i}\frac{\varepsilon_i y}{(\varepsilon y)^2 + L}, \tag{D7}$$

and integration over λ. Equation (D6) can be found, for example, in the original Feynman papers cited in Ref. [15]. Further, we use formula

$$\left(\frac{\partial^2}{\partial\varepsilon_i\partial\varepsilon_i}\right)^v \phi(\varepsilon^2 y + w)\bigg|_{\varepsilon_i=0} = (-1)^v(2v+1)!!2^v \frac{\partial^v}{\partial(\varepsilon^2)^v}\phi(\varepsilon^2 y + w) = (-1)^v(2v+1)!!2^v y^v \frac{\partial^v}{\partial w^v}\phi(\varepsilon^2 y + w). \tag{D8}$$

Particular cases of this formula are given by Eqs. (76) and (78) of [16]. In a similar way we treat the integrals with powers of k_0,

$$\frac{(-2k_0)^t}{k^2 - 2k\varepsilon + \Delta} = \int_0^\Delta d^t w \frac{d^t}{dw^t}\frac{(-2k_0)^t}{k^2 - 2k\varepsilon + w} = \int_0^\Delta d^t w \frac{\partial^t}{\partial\varepsilon_0^t}\frac{1}{k^2 - 2k\varepsilon + w}\bigg|_{\varepsilon_0=m}. \tag{D9}$$

Finally, when integrating over the parameter w, we make the substitution

$$w \to -m^2 w.$$

By inserting Eqs. (D1), (D3), (D8), and (D9) into the left member of Eq. (55), we obtain the right member of that equation. The second terms in the square brackets on the right members of Eqs. (D3) and (D4) contribute to the electromagnetic mass of the electron. Their contribution is canceled by the counterterm $-\Delta m$ in Eq. (2). Likewise, from Eqs. (D2), (D4), and

$$\frac{d}{dw}2\varepsilon_i y \ln(\varepsilon^2 y - w) = \frac{\partial}{\partial\varepsilon_i}\ln(\varepsilon^2 y - w) \tag{D10}$$

one arrives at

$$\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F}{(k^2 - \lambda)^2}\frac{(2\omega)^{2v-1}\omega}{k^2 - 2k.\varepsilon + \Delta} = \frac{1}{2}\int_0^1 dy \int_0^\Delta d^{2v-1}w \left(\frac{\partial^2}{\partial\varepsilon_i\partial\varepsilon_i}\right)^{v-1}\frac{\partial}{\partial\varepsilon_j}2\varepsilon_j y \times \left[\ln\left(\frac{\varepsilon^2 y - w}{m^2 y}\right) - \ln\left(\frac{\Lambda^2(1-y)}{m^2 y}\right)\right]\bigg|_{\varepsilon_i=\varepsilon_j=0}$$

$$= \frac{1}{2}\int_0^1 dy \int_0^\Delta d^{2v}w \left(\frac{\partial^2}{\partial\varepsilon_i\partial\varepsilon_i}\right)^v \left[\ln\left(\frac{\varepsilon^2 y - w}{m^2 y}\right) - \ln\left(\frac{\Delta^2(1-y)}{m^2 y}\right)\right]\Bigg|_{\varepsilon_i=0}. \quad \text{(D11)}$$

Equation (57) follows from the last equation and Eqs. (D8) and (55).

2. Derivation of Eq. (A34)

A slightly different procedure is used for the evaluation of the integrals on the left member of Eq. (A34). Using the Feynman parametrization (D5), we get

$$(-4)\int_0^{\Lambda^2} d\lambda \int \frac{d^4k_F(1,k_v/m)}{(k^2-\lambda)^2}\frac{(-2k_0/E)^t}{k^2-2k\cdot P_u+u\Delta(\vec{P})}$$
$$= (-8)\int_0^1 dy(1-y)\int_0^{\Lambda^2} d\lambda \times \int \frac{d^4k_F(1,k_v/m)(-2k_0/E)^t}{[k^2-2k\cdot P_u y+yu\Delta(\vec{P})-\lambda(1-y)]^3}. \quad \text{(D12)}$$

Now

$$\frac{\partial}{\partial\lambda}f(D) = -(1-y)\frac{\partial}{\partial D}f(D) \quad \text{(D13)}$$

and

$$\frac{\partial}{\partial(P_u)_0}f(D) = -2k_0 y\frac{\partial}{\partial D}f(D), \quad \text{(D14)}$$

where

$$D = k^2 - 2k\cdot P_u y + yu\Delta(\vec{P}) - \lambda(1-y). \quad \text{(D15)}$$

Thus

$$\text{(D12)} = (-8)\int_0^1 dy\frac{(1-y)^{t+1}}{y^t}\frac{1}{E^t}\frac{\partial^t}{\partial(P_u)_0^t}\int_0^{\Lambda^2} d^{t+1}\lambda \times \int\frac{d^4k_F(1,k_v/m)}{[k^2-2k\cdot P_u y+yu\Delta(\vec{P})-\lambda(1-y)]^3}. \quad \text{(D16)}$$

The integration over four-momentum k according to Eq. (D6) yields

$$\int\frac{d^4k_F(1,k_v/m)}{[k^2-2k\cdot P_u y+yu\Delta(\vec{P})-\lambda(1-y)]^3} = \frac{\left(1,\frac{(P_u)_v}{m}y\right)}{D_u(\vec{P})}, \quad \text{(D17)}$$

where $D_u(\vec{P})$ is given by Eq. (A35). By inserting the last equation into Eq. (D16) and making the substitution $\lambda' = \frac{\lambda}{m^2}\frac{1-y}{y}$, we obtain the right member of Eq. (A34).

3. The functions Φ

Had we been able to calculate the right member of Eq. (59) exactly, we could use the form of the functions Φ given by Eq. (56) in the actual calculation. Since we calculate the right member of Eq. (59) numerically, that is, approximately, the actual form of the functions Φ presents the balance between two opposite requirements. On the one hand, the integrals over the electron wave numbers k_e have to be finite. On the other hand, the functions Φ are multiplied by the inverse powers of $(Z\alpha)$ [see Eqs. (42) and (43)]. This enhances the contribution of the terms with small powers of Δ. In principle Φ's are determined up to a polynomial of the $(2v+t-1)$ order in Δ. This polynomial has to cancel out in the complete expressions, Eqs. (42) and (43). However, such a cancellation is always imperfect in numerical calculations. Thus, the functions Φ should contain the smallest number of the power terms in Δ in order to keep the integrals over k_e convergent. The functions Φ meeting such a requirement follow.

We rewrite Eq. (56) into the form

$$\Phi_{4,0}^{2v,t}(\Delta+\sigma) = 2^v(-1)^t\frac{\partial^t}{\partial(\varepsilon_0)^t}\int_0^1 dy\, y^v(1,y\varepsilon_0) \times\phi\left(-\frac{\Delta+\sigma}{m^2},y\right)\Bigg|_{\varepsilon_0=1}. \quad \text{(D18)}$$

In the case we calculate $\langle\gamma_0 G_4\rangle$ and $\langle\gamma_\mu G_4 O_\mu^0\rangle$, we set

$$\phi(x,y) = \int_0^x d^{v+t}w\,\ln\left(\frac{\varepsilon_0^2 y + w}{y}\right) \quad \text{(D19)}$$

for $t=2$, or for $v=0,\ t=0;\ v=0,\ t=1;$ and $v=1,\ t=0$,

$$\phi(x,y) = \int_0^x d^{v+t}w\,\ln\left(\frac{\varepsilon_0^2 y + w}{\varepsilon_0^2 y}\right) \quad \text{(D20)}$$

for $t=1$ except for $v=0$,

$$\phi(x,y) = \int_0^x d^{v+t+1}w\left[\frac{1}{\varepsilon_0^2 y+w}-\frac{1}{\varepsilon_0^2 y}\right] \quad \text{(D21)}$$

for $t=0$ except for $v=1$,

$$\phi(x,y) = \int_0^x d^{v+t-1}w(\varepsilon_0^2 y+w)\left[\ln\left(\varepsilon_0^2 y+w\right)-1\right] \quad \text{(D22)}$$

for $t=3$, and

$$\phi(x,y) = \int_0^x d^{v+t-1}w\,2\varepsilon_0 y\,\ln\left(\varepsilon_0^2 y+w\right) \quad \text{(D23)}$$

for $t=4$. In the case we calculate $\langle\gamma_\mu G_4 O_\mu^{-1}\rangle$ and $\langle\gamma_0 G_i\gamma_i\gamma_0\rangle$, we use Eq. (D19) for $t<3$ and Eq. (D22) for $t=3$. In all these cases we use the functions $\Phi_4^{2v,t}$. When we calculate $\langle\gamma_0 G_0\rangle$ we use the functions $\Phi_0^{2v,t}$. In such a case we use Eq. (D19) for $t=2$ or for $v=0,\ t=1;\ v=1,\ t=0$, Eq. (D20) for $t=1$ except for $v=0$, and Eq. (D21) for $t=0$ except for $v=1$. Furthermore, we set

$$\phi(x,y) = \int_0^x d^{v+t}w\,\ln\left(\varepsilon_0^2 y+w\right) \quad \text{(D24)}$$

for $t=3$ and

$$\phi(x,y) = \int_0^x d^{v+t-1}w\left(3\varepsilon_0 y+w\varepsilon_0^{-1}\right)\ln\left(\varepsilon_0^2 y+w\right) \quad \text{(D25)}$$

for $t=4$.

In the case we apply nonrelativistic approximation, we use Eqs. (D20) and (D24) when calculating $\langle G_{4,0}^{2v,2}\rangle_0$ and $\langle G_4^{2v,3}\rangle_0$, respectively. When calculating $\langle G_0^{2v,3}\rangle_0$ and $\langle\{G_i^{2v-1,2},P_i\}\rangle_0$, we use the same functions as when calculating the exact expressions $\langle G_0^{2v,3}\rangle$ and $\langle\gamma_0 G_i^{2v-1,2}\gamma_i\gamma_0\rangle$, respectively.

APPENDIX E: DERIVATION OF EQ. (68)

After substituting into Eq. (62) for $a = L + 2q$ and $b = L + 2(p - q) + c$ [see Eq. (44)] one gets

$$P_{l_\Gamma,\infty}^{L+2q,L+2(p-q)+c}(k_e,\xi) = A_{l_\Gamma}^{L+2q,L+2(p-q)+c}\left(\frac{k_e^2}{1+k_e^2}\right)^{l_\Gamma+1}\left(\frac{1+ik_e}{1-ik_e}\right)^{p-2q}\left(1+k_e^2\right)^{-l_0-2-L-p}(1-ik_e)^{-c} \times\left(1+\frac{c_{1,0}+c_{1,1}\xi}{k_e}+\frac{c_{2,0}+c_{2,1}\xi+c_{2,2}\xi^2}{k_e^2}+\cdots\right). \tag{E1}$$

From Eq. (56) we get

$$\left.\frac{d^{v-p-L}}{d\sigma^{v-p-L}}\Phi_{4,0}^{2v,t}\right|_{\sigma=0} = m^{-2(v-L-p)}2^v(-1)^t\,\frac{\partial^t}{\partial(\varepsilon_0)^t}\int_0^1 dy\, y^v(1,y\varepsilon_0)\int_0^{-\Delta/m^2} d^{L+p+t}w\,\ln\left.\left(\frac{\varepsilon_0^2 y+w}{y}\right)\right|_{\varepsilon_0=1}. \tag{E2}$$

Performing now the parametric differentiation with respect to ε_0, we get [recall the definition (69)]

$$\left.\frac{\partial^t}{\partial(\varepsilon_0)^t}(1,y\varepsilon_0)\ln(\varepsilon_0^2 y+w)\right|_{\varepsilon_0=1} \simeq (1,y)([t]-1)!!(2y)^{[t]/2}\frac{\partial^{[t]/2}}{\partial w^{[t]/2}}\ln(y+w)+\cdots. \tag{E3}$$

For large k_e, the other terms on the right member of Eq. (E3) are negligible, compared to the first one. From Eqs. (E2) and (E3) we have

$$\left.\frac{d^{v-p-L}}{d\sigma^{v-p-L}}\Phi_{4,0}^{2v,t}\right|_{\sigma=0} \simeq m^{-2(v-L-p)}2^{v+[t]/2}(-1)^t\int_0^1 dy y^{v+[t]/2}(1,y)\int_0^{-\Delta(k_e,\xi)/m^2} d^{L+p+t-[t]/2}w\,\ln(y+w). \tag{E4}$$

Every differentiation of Eq. (E4) with respect to ξ produces an extra factor of $(Z\alpha)^2$ and lowers the number of integration with respect to the parameter w. This in turn supplies the factor k_e^{-2} for large k_e. Thus, the dominant contribution from the differentiations of the product of Eqs. (E1) and (E4) with respect to ξ in Eq. (67) comes from the differentiation of Eq. (E1). The differentiation of Eq. (E1) with respect to ξ yields for large k_e,

$$\left.\frac{d^t}{t!d\xi^t}P_{l_\Gamma,\infty}^{L+2q,L+2(p-q)+c}(k_e,\xi)\right|_{\xi=1} \simeq A_{l_\Gamma}^{L+2q,L+2(p-q)+c}\left(\frac{k_e^2}{1+k_e^2}\right)^{l_\Gamma+1}\left(\frac{1+ik_e}{1-ik_e}\right)^{p-2q}\left(1+k_e^2\right)^{-l_0-2-L-p}(1-ik_e)^{-c}\frac{c_{t,t}}{k_e^t}. \tag{E5}$$

By the substitution $w \to w(-\frac{\Delta(k_e,\xi=1)}{m^2})$, the integral over the parameter w on the right member of Eq. (E4) can be rewritten into the form

$$\int_0^{-\Delta(k_e,\xi=1)/m^2} d^{L+p+t-[t]/2}w\,\ln(y+w) = \left(-\frac{\Delta(k_e,\xi=1)}{m^2}\right)^{L+p+t-[t]/2}\int_0^1 d^{L+p+t-[t]/2}w\,\ln\left(y-w\frac{\Delta(k_e,\xi=1)}{m^2}\right). \tag{E6}$$

Here we substitute from Eq. (47)

$$-\frac{\Delta(k_e,\xi=1)}{m^2} = (Z\alpha)^2\left[k_e^2+1\right]. \tag{E7}$$

From Eqs. (E4)–(E7) we finally get Eq. (68).

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[15] The following notation is used: d^4k_F stands for $i(2\pi)^{-2}d^4k$ and k stands for the four-momentum of the virtual photon. We use the summation convention $A \cdot B = A_\nu B_\nu = A_0 B_0 - \vec{A} \cdot \vec{B}$. In particular, $k^2 = k_0^2 - \omega^2, \omega^2 = \vec{k} \cdot \vec{k}$. The Dirac γ matrices are defined by the anticommutation relation $\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu}$, where $g_{0\mu} = \delta_{0\mu}$ and $g_{ij} = -\delta_{ij}$. Here δ has the usual meaning of the Kronecker symbol. Well-known Dirac-Pauli realization of γ matrices is used. When integrating over k_0 in Eq. (3) we replace the electron mass m by $m - i\eta$ and take the limit $\eta \to 0$ from above. This is the same notation and the same way of integration as the one used by Feynman in his original papers in Phys. Rev. **76**, 749 (1949); **76**, 769 (1949). The natural units ($\hbar = c = 1$) are used throughout the paper. Symbol α stands for the fine-structure constant. In actual calculation we took the value 1/137.03599911 given in [3].

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