Self-energy of a bound electron for excited states

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The method for the evaluation of the self-energy of bound electron is proposed. The integration over four-momenta of virtual photons is done in a way that preserves manifest Lorentz invariance. The resulting expression can then be decomposed into high- and low-energy parts in a Lorentz invariant fashion. The high-energy part depends only on the behavior of the wave function of the reference state in the immediate vicinity of the nucleus and can be calculated analytically. The low-energy part depends on further details of the atomic structure and has to be calculated numerically. The results accurate at least up to $\alpha(Z\alpha)^6$ are obtained for non-S states and normalized difference $n^3\Delta E_n - \Delta E_1$ of the S states. The method is applied to the states with the principal quantum number n ranging from 2 to 10, with the orbital quantum number l ranging from 0 to 3 and with the nuclear charges Z ranging from 1 to 30. In the cases that were already considered in literature a very good agreement with previous calculations is found, especially for the atoms with lower nuclear charges. The advantages of the present method over the previous ones are pointed out.

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I. INTRODUCTION

The renormalized expression for the self-energy in the nonrecoil limit reads (for notation and units used see [1])

$$\Delta E = \langle O - \Delta m \rangle = \langle \psi | \gamma_0 (O - \Delta m) | \psi \rangle, \tag{1}$$

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

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

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

$$(\gamma \cdot \Pi - m)\psi = 0, \tag{3}$$

where Π is the physical four-momentum of the particle in the external time-independent electromagnetic field. The self-energy effect is the dominant contribution to the Lamb shift of the hydrogenlike atoms [2–4]. Therefore,considerable effort has been devoted to the evaluation of Eq. (1) for the case of the Coulomb external field

$$\Pi_0 = E + \frac{Z\alpha}{R}, \quad \vec{\Pi} = \vec{P} \tag{4}$$

for the reference states with different principal and orbital quantum numbers n and l and different nuclear charges Z [5–20]. We multiply $1/[\gamma \cdot (\Pi - k) - m]$ in Eq. (2) by $[\gamma \cdot (\Pi - k) + m]/[\gamma \cdot (\Pi - k) + m]$ from the right. Using Dirac equation and properties of γ matrices [1], we get

$$\langle O \rangle = \frac{\alpha}{\pi} \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2 - \lambda)^2} \times \left\langle \gamma_\mu \frac{1}{k^2 - 2k \cdot \Pi + H} (2\Pi_\mu - k \cdot \gamma \gamma_\mu) \right\rangle. \tag{5}$$

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

$$H = (\gamma \cdot \Pi + m)(\gamma \cdot \Pi - m) = \Pi \cdot \Pi - m^2 + \tfrac{1}{4}[\Pi_\mu, \Pi_\nu][\gamma_\mu, \gamma_\nu]. \tag{6}$$

To evaluate the expression (5) we use the spectral decomposition of the Hamilton operator H. Equation (5) then presents an eleven-dimensional integral: four integrations over variables of virtual photon, three plus three integrations in electron coordinate space when evaluating the matrix elements of γ_μ and $(2\Pi_\mu - k \cdot \gamma \gamma_\mu)$ between reference and intermediate states, and one integration (summation) over continuous (discrete) part of the electron intermediate states. The difficulty in the evaluation of the self-energy effect even for the atoms with low nuclear charges arises from the presence of several important scales. The frequency ω of the virtual photon can be of the order of the electron mass m or of the order of the atomic energies $m(Z\alpha)^2$. The wave number k_e of the electron in the intermediate state can be of the order of the electron mass m or of the order of the atomic momentum $m(Z\alpha)$. Consequently, there are four important regions: the region I, where $\omega \simeq m(Z\alpha)^2$, $k_e \simeq m(Z\alpha)$, the region II, where $\omega \simeq m$, $k_e \simeq m(Z\alpha)$, the region III, where $\omega \simeq m(Z\alpha)^2$, $k_e \simeq m$, and the region IV, where $\omega \simeq m$, $k_e \simeq m$. This can be illustrated on the expansion of the self-energy in powers of $Z\alpha$,

$$\Delta E = \frac{m\alpha(Z\alpha)^4}{\pi n^3} F(Z\alpha), \tag{7}$$

where

$$F(Z\alpha) = A_{41} \ln(Z\alpha)^{-2} + A_{40} + A_{50}(Z\alpha) + (Z\alpha)^2 \times [A_{62} \ln^2(Z\alpha)^{-2} + A_{61} \ln(Z\alpha)^{-2} + A_{60}] + \cdots. \tag{8}$$

Coefficients A were calculated in Refs. [5–14] and are summarized in several places, e.g. [2,3,17]. It is convenient to write the self-energy effect on the general S state as

$$\Delta E_n = \frac{n^3 \Delta E_n - \Delta E_1}{n^3} + \frac{\Delta E_1}{n^3}, \tag{9}$$

where the first and the second terms on the right member will be referred to as the state-dependent and the state-independent parts, respectively. The difference $n^3\Delta E_n - \Delta E_1$ will be

called the normalized difference of the S states. For the state-independent part of the S states the coefficient A_{41} comes from region I, A_{40} from regions I and II, A_{50} from region IV, A_{62} from region III, A_{61} from regions I and III, and A_{60} from regions I, II, and IV. For the state-dependent part of the S states and non-S states, the situation is considerably simpler: the coefficients A_{41}, A_{50}, and A_{62} vanish, the coefficient A_{61} comes from region I, and the coefficients A_{40} and A_{60} come from regions I and II. Clearly, the contribution of the intermediate electron states with very large electron wave numbers is significantly suppressed in these cases.

In view of the foregoing discussion it appears to be a hopeless task to find a single approximation that would give after a finite number of terms the exact values of the coefficients in Eq. (8). This is indeed the shared wisdom in the field; see, e.g., the discussion in Refs. [3,10]. Therefore, modern approaches [10,12–14] broke up calculation at least into two regions and matched the contributions from these regions.

In Refs. [21,22] we suggested expanding the electron propagator as follows:

$$\begin{aligned}\frac{1}{k^2-2k\cdot\Pi+H} &= \frac{1}{k^2-2k\cdot\varepsilon+H}+\frac{1}{k^2-2k\cdot\varepsilon+H}2k\cdot(\Pi-\varepsilon)\\ &\times\frac{1}{k^2-2k\cdot\varepsilon+H}+\frac{1}{k^2-2k\cdot\varepsilon+H}2k\cdot(\Pi-\varepsilon)\\ &\times\frac{1}{k^2-2k\cdot\varepsilon+H}2k\cdot(\Pi-\varepsilon)\frac{1}{k^2-2k\cdot\varepsilon+H}+\cdots,\end{aligned} \tag{10}$$

where

$$\varepsilon=(m,0,0,0). \tag{11}$$

This expansion has been motivated by the following considerations. First, as shown by Bethe [5], the dominant contribution to the self-energy of the bound electron for low values of nuclear charge comes from the integration over low frequencies of the virtual photon. To get this contribution right, the Hamilton operator H has to be kept at the leading approximation of the propagator. Second, when the wave number k_e of the electron in the intermediate state is of the order of atomic momentum $m(Z\alpha)$, the electron four-momentum Π in the electron propagator is dominated by the rest mass of the electron.

As discussed in [21], for the state-independent part of the S states this single expansion yields after a finite number of terms the exact values of the coefficients A_{41}, A_{40}, A_{62}, and A_{61}. The exact values of coefficients A_{50} and A_{60} are obtained only when an infinite number of the terms are considered [22]. However, a very good approximation to these exact values is obtained just by considering a few terms [22].

The purpose of this paper is to apply the expansion (10) to the evaluation of the self-energy effect for the state-dependent part of the S states and non-S states. We show that in these cases only very few terms of the single expansion (10) have to be considered to get results that are exact at least up to the order $\alpha(Z\alpha)^6$. Furthermore, the suppression of the electron intermediate states with very large wave numbers results in considerable simplification of the calculation and a part of the calculation can be carried out analytically, as noted already in Refs. [12–14].

The paper is organized as follows. In Sec. II the integration over four-momentum of virtual photon is performed. Operator expression resulting from the integration is further simplified and put into computationally useful form in Sec. III. The results obtained are discussed in Sec. IV; Sec. V contains conclusions. Most of the derivations needed in Sec. III are skipped in the main text and left to Appendixes A and B. Appendix A also contains details needed for practical evaluation of the expression given in Sec. III. Appendix C contains derivation of the coefficients A_{41} and A_{61} in Eq. (8).

II. INTEGRATION OVER FOUR-MOMENTUM OF VIRTUAL PHOTON

First we introduce some convenient notation and rewrite Eq. (10) as follows:

$$\begin{aligned}\frac{1}{k^2-2k\cdot\Pi+H} &= \frac{1}{k^2-2k\cdot\varepsilon+H}+\frac{2k\cdot(\Pi-\varepsilon)_1}{(k^2-2k\cdot\varepsilon+H_{01})(k^2-2k\cdot\varepsilon+H_{12})}\\ &+\frac{2k\cdot(\Pi-\varepsilon)_1 2k\cdot(\Pi-\varepsilon)_2}{(k^2-2k\cdot\varepsilon+H_{01})(k^2-2k\cdot\varepsilon+H_{12})(k^2-2k\cdot\varepsilon+H_{23})}+\cdots.\end{aligned} \tag{12}$$

The components of the operators $(\Pi-\varepsilon)$ do not mutually commute. The subscripts of these operators then indicate the ordering in which they act on a bra-vector. The Hamilton operator H does not commute with the operators $(\Pi-\varepsilon)$. The subscript of this operator then indicates where the operator appears with respect to the operators $(\Pi-\varepsilon)$. For example, in the last displayed term on the right member of Eq. (12) H_{01} acts on a bra-vector before the two operators $(\Pi-\varepsilon)$, H_{12} acts between the two operators $(\Pi-\varepsilon)$, and H_{23} acts after the two operators $(\Pi-\varepsilon)$. Clearly, by endowing the Hamilton operators H with the subscripts, we keep the track of their position with respect to the operators $(\Pi-\varepsilon)$. Thus the operators H with the subscripts can be treated as numbers.

For an integration over four-momentum of virtual photon it is advantageous to rearrange the expansion (12) as follows:

$$\begin{aligned}\frac{1}{k^2-2k\cdot\Pi+H} &= \frac{1}{k^2-2k\cdot\varepsilon+H}-2k\cdot(\Pi-\varepsilon)_1 D_1\left[\frac{1}{k^2-2k\cdot\varepsilon+H}\right]\\ &+2k\cdot(\Pi-\varepsilon)_1 2k\cdot(\Pi-\varepsilon)_2 D_2\left[\frac{1}{k^2-2k\cdot\varepsilon+H}\right]+\cdots,\end{aligned} \tag{13}$$

where

$$D_1[f(H)] = \frac{f(H_{01})}{H_{01}-H_{12}} + \frac{f(H_{12})}{H_{12}-H_{01}}, \tag{14}$$

$$D_2[f(H)] = \frac{f(H_{01})}{(H_{01}-H_{12})(H_{01}-H_{23})} + \frac{f(H_{12})}{(H_{12}-H_{01})(H_{12}-H_{23})} + \frac{f(H_{23})}{(H_{23}-H_{01})(H_{23}-H_{12})} \tag{15}$$

and so on. Further, by means of the identities [see Sec. 4.5, Eqs. (71)–(73) of Ref. [21] for a detailed discussion]

$$-\frac{2k_\mu}{k^2-2k\cdot\varepsilon+H} = H\int_0^1 dw\frac{\partial}{\partial\varepsilon_\mu}\frac{1}{k^2-2k\cdot\varepsilon+wH}, \tag{16}$$

$$\frac{2k_\mu 2k_\nu}{k^2-2k\cdot\varepsilon+H} = H^2\int_0^1 dw(1-w)\frac{\partial^2}{\partial\varepsilon_\mu\partial\varepsilon_\nu}\times\frac{1}{k^2-2k\cdot\varepsilon+wH}, \tag{17}$$

and so on, we convert calculation of all the integrals over photon variables k arising in the expansion (10) to the calculation of the only integral [see, e.g., Eq. (74) of Ref. [21]],

$$\int_0^{\Lambda^2} d\lambda\int\frac{d^4k_F}{(k^2-\lambda)^2}\frac{(1,k_\nu)}{k^2-2k\cdot\varepsilon+wH} = -\frac{1}{4}\int_0^1 dy(1,y\varepsilon_\nu)\{\ln(\varepsilon^2y-wH)-\ln[\Lambda^2(1-y)/y]\}. \tag{18}$$

Note that the expressions (16), (17) appear inside the expressions (14), (15). Therefore, H enters the expressions (16), (17) with the subscripts and can be treated as a number.

Furthermore, for an arbitrary function f depending only on ε^2 and function N depending on the components of ε linearly, we have

$$\frac{\partial(Nf)}{\partial\varepsilon_\lambda} = N2\varepsilon_\lambda\frac{\partial f}{\partial\varepsilon^2}+\frac{\partial N}{\partial\varepsilon_\lambda}f, \tag{19}$$

$$\frac{\partial^2(Nf)}{\partial\varepsilon_\lambda\partial\varepsilon_\rho} = \left(\frac{\partial N}{\partial\varepsilon_\lambda}\varepsilon_\rho+\frac{\partial}{\partial\varepsilon_\rho}(\varepsilon_\lambda N)\right)2\frac{\partial f}{\partial\varepsilon^2}+4\varepsilon_\lambda\varepsilon_\rho N\frac{\partial^2 f}{\partial(\varepsilon^2)^2}, \tag{20}$$

and so on. After we insert Eqs. (13)–(20) into Eq. (5), subtract from the expression (5) the contribution to the electromagnetic mass of the electron [see, e.g., Eq. (80) of [21]]

$$\Delta m\langle 1\rangle = -\frac{\alpha}{2\pi}\int_0^1 dy\left\langle\gamma_\mu\{\ln(m^2y)-\ln[\Lambda^2(1-y)/y]\}\times\left(\Pi_\mu-\frac{y}{2}\Pi\cdot\gamma\gamma_\mu\right)\right\rangle, \tag{21}$$

and identify m with the observable mass of the electron, the observable effect of the self-energy can then be written as

$$\Delta E = -\frac{\alpha}{2\pi}\left\langle\gamma_\mu\left(G_4\Pi_\mu-\frac{m}{2}G\cdot\gamma\gamma_\mu\right)\right\rangle, \tag{22}$$

where

$$G_4 = \phi_0(H)+(\Pi-\varepsilon)_{1\lambda}\varepsilon_\lambda D_1[\phi_2'(H)]+(\Pi-\varepsilon)_{1\lambda}\times(\Pi-\varepsilon)_{2\lambda}D_2[\phi_2(H)]+\cdots \tag{23}$$

and

$$G_\nu = \varepsilon_\nu\phi_1'(H)+(\Pi-\varepsilon)_{1\nu}D_1[\phi_1(H)]+\varepsilon_\mu\varepsilon_\nu(\Pi-\varepsilon)_{1\mu}\times D_1\{[\phi_3(H)]''\}+\cdots. \tag{24}$$

Here the prime denotes differentiation with respect to H and the functions ϕ are given as

$$\phi_{2q}(H) = \frac{2^qH^{2q}}{(2q-1)!}\int_0^1 dw(1-w)^{2q-1}\frac{\partial^q}{\partial(\varepsilon^2)^q}\times\int_0^1 dy[\ln(\varepsilon^2y-wH)-\ln(m^2y)]\Big|_{\varepsilon^2=m^2} = m^{2q}h^{2q}\frac{2^q(-1)^{q-1}(q-1)!}{(2q-1)!}\int_0^1 dw(1-w)^{2q-1}\times\int_0^1 dy\frac{y^q}{(y+wh)^q} \tag{25}$$

and

$$\phi_{2q+1}(H) = \frac{2^qH^{2q+1}}{m(2q)!}\int_0^1 dw(1-w)^{2q}\frac{\partial^q}{\partial(\varepsilon^2)^q}\times\int_0^1 dy\,y[\ln(\varepsilon^2y-wH)-\ln(m^2y)]\Big|_{\varepsilon^2=m^2} = m^{2q+1}h^{2q+1}\frac{2^q(-1)^{q-1}(q-1)!}{(2q)!}\int_0^1 dw(1-w)^{2q}\times\int_0^1 dy\frac{y^{q+1}}{(y+wh)^q} \tag{26}$$

for $q>0$ and

$$\phi_0 = h\int_0^1 dy\int_0^1 dw\frac{1}{y+wh} \tag{27}$$

and

$$\phi_1 = -mh^2\int_0^1 dy\,y\int_0^1 dw\frac{1-w}{y+wh} \tag{28}$$

for $q=0$. Here the scaled Hamilton operator

$$h = -\frac{H}{m^2} \tag{29}$$

has been introduced.

III. INTEGRATION OVER ELECTRON VARIABLES

A. Covariant separation into low- and high-energy parts

In the case of the greatest interest, that of the Coulomb external field, Eq. (4), the second-order Hamilton operator H is at least of the order $(Z\alpha)^2$, see Eqs. (A26) and (A37) below, so it is tempting to consider the expansion of the functions ϕ in powers of H:

$$\phi_2 = \frac{H^2}{m^2}+\tilde\phi_2,\quad \phi_4 = -\frac{H^4}{6m^4}+\tilde\phi_4, \tag{30}$$

$$\phi_1 = -\frac{H^2}{2m^3}+\tilde\phi_1,\quad \phi_3 = \frac{H^3}{6m^3}+\frac{H^4}{12m^5}+\tilde\phi_3, \tag{31}$$

$$\phi_6 \simeq \frac{H^6}{45m^6}, \quad \phi_5 \simeq -\frac{H^5}{60m^5} - \frac{H^6}{90m^7}, \quad \phi_7 \simeq \frac{H^7}{630m^7}. \tag{32}$$

By virtue of the identities

$$\begin{aligned} &D_1[H] = 1, \quad D_1[H^2] = H_{01} + H_{12}, \quad D_2[H^2] = 1, \\ &D_2[H^3] = H_{01} + H_{12} + H_{23} \end{aligned} \tag{33}$$

or, more generally,

$$D_n[H^n] = 1, \quad D_n[H^{n+1}] = \sum_{j=0}^{n} H_{j,j+1} \tag{34}$$

following from the definitions (14), (15), the terms involving only the powers of H can be evaluated rather simply. For example, we have

$$\begin{aligned} &\varepsilon_\mu\varepsilon_\nu(\Pi-\varepsilon)_{1\mu}D_1\left[\left(\frac{H^3}{6m^3}+\frac{H^4}{12m^5}\right)''\right] + (\varepsilon_\lambda g_{\mu\nu}+\varepsilon_\mu g_{\lambda\nu}+\varepsilon_\nu g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}D_2\left[\left(\frac{H^3}{6m^3}+\frac{H^4}{12m^5}\right)'\right] \\ &\quad + (g_{\lambda\rho}g_{\mu\nu}+g_{\mu\rho}g_{\lambda\nu}+g_{\nu\rho}g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}(\Pi-\varepsilon)_{3\rho}D_3\left[\frac{H^3}{6m^3}+\frac{H^4}{12m^5}\right] \\ &= \varepsilon_\mu\varepsilon_\nu(\Pi-\varepsilon)_{1\mu}\left(\frac{1}{m^3}+\frac{H_{01}+H_{12}}{m^5}\right) + (\varepsilon_\lambda g_{\mu\nu}+\varepsilon_\mu g_{\lambda\nu}+\varepsilon_\nu g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}\left(\frac{1}{2m^3}+\frac{H_{01}+H_{12}+H_{23}}{3m^5}\right) \\ &\quad + (g_{\lambda\rho}g_{\mu\nu}+g_{\mu\rho}g_{\lambda\nu}+g_{\nu\rho}g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}(\Pi-\varepsilon)_{3\rho}\left(\frac{1}{6m^3}+\frac{H_{01}+H_{12}+H_{23}+H_{34}}{12m^5}\right) = \frac{\overline{\tilde\Pi^2\Pi_\nu}}{6m^3}+\frac{\overline{\Pi_\nu\tilde\Pi^2 H}}{12m^5}. \end{aligned} \tag{35}$$

Here, we introduced notation

$$\tilde\Pi^2 = \Pi\cdot\Pi - m^2 \tag{36}$$

and the bar denotes the sum over all possible permutations of the orderings of the operators involved.

Following the nomenclature used in Refs. [10,12–14] we shall call the contribution of the terms in Eqs. (30)–(32) containing only the power terms of H the high-energy part. This contribution comes from the hard photon region. As shown later, it depends only on the behavior of the reference wave function ψ in the immediate vicinity of the nucleus. It can be evaluated in the closed form.

The contribution of ϕ_0 and the remaining terms in Eqs. (30) and (31), those denoted generically as $\tilde\phi$, will be called the low-energy part. As discussed in detail below, it is sensitive to the details of the atomic structure. It has to be evaluated numerically by using spectral decomposition of the second-order Hamilton operator H.

Further, the terms in Eq. (22) can be rewritten into the form

$$\langle\gamma_\mu G_4\Pi_\mu\rangle = \tfrac{1}{2}\langle\gamma_\mu G_4\Pi_\mu + \Pi_\mu G_4\gamma_\mu\rangle = m\langle G_4\rangle - \tfrac{1}{2}\langle[\Pi_\mu,[\gamma_\mu,G_4]]\rangle \tag{37}$$

and

$$-\tfrac{1}{2}\langle\gamma_\mu G\cdot\gamma\gamma_\mu\rangle = -\tfrac{1}{4}\langle\gamma_\mu\{G_\nu,\gamma_\nu\}\gamma_\mu\rangle = \tfrac{1}{2}\langle\{G_\nu,\gamma_\nu\}\rangle - \tfrac{1}{8}\langle\{\gamma_\nu,[\gamma_\mu,[\gamma_\mu,G_\nu]]\}\rangle. \tag{38}$$

The second terms in these equations are in the case of the Coulomb field (4) by the factor $(Z\alpha)^2$ smaller than the first. By inserting Eqs. (30)–(32) and Eqs. (37) and (38) into Eqs. (22)–(24) we obtain the self-energy in the form

$$\Delta E = \Delta E_{\rm low} + \Delta E_{\rm high}. \tag{39}$$

The low-energy part reads

$$\begin{aligned} \Delta E_{\rm low} = -\frac{\alpha}{2\pi}\Big\langle &\gamma_\mu(\phi_0 + (\Pi-\varepsilon)_{1\lambda}\varepsilon_\lambda D_1[\tilde\phi_2'] + (\Pi-\varepsilon)_{1\lambda}(\Pi-\varepsilon)_{2\lambda}D_2[\tilde\phi_2])\Pi_\mu + m(\varepsilon_\mu\varepsilon_\nu(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\nu}D_2[\tilde\phi_4'] \\ &+ (\varepsilon_\lambda g_{\mu\nu}+\varepsilon_\mu g_{\lambda\nu}+\varepsilon_\nu g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}(\Pi-\varepsilon)_{3\nu}D_3[\tilde\phi_4'] + (g_{\lambda\rho}g_{\mu\nu}+g_{\mu\rho}g_{\lambda\nu}+g_{\nu\rho}g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu} \\ &\times(\Pi-\varepsilon)_{2\lambda}(\Pi-\varepsilon)_{3\rho}(\Pi-\varepsilon)_{4\nu}D_4[\tilde\phi_4]) - \frac{1}{8}\{\gamma_\nu,[\gamma_\mu,[\gamma_\mu,\varepsilon_\nu\tilde\phi_1' + (\Pi-\varepsilon)_{1\nu}D_1[\tilde\phi_1]]]\} + \gamma_\nu(\varepsilon_\nu\tilde\phi_1' + (\Pi-\varepsilon)_{1\nu}D_1[\tilde\phi_1] \\ &+ \varepsilon_\mu\varepsilon_\nu(\Pi-\varepsilon)_{1\mu}D_1[\tilde\phi_3''] + (\varepsilon_\lambda g_{\mu\nu}+\varepsilon_\mu g_{\lambda\nu}+\varepsilon_\nu g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}D_2[\tilde\phi_3'] \\ &+ (g_{\lambda\rho}g_{\mu\nu}+g_{\mu\rho}g_{\lambda\nu}+g_{\nu\rho}g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}(\Pi-\varepsilon)_{3\rho}D_3[\tilde\phi_3]) + \cdots\Big\rangle. \end{aligned} \tag{40}$$

The high-energy part reads

$$\begin{aligned} \Delta E_{\rm high} = -\frac{\alpha}{2\pi}\Big\langle &\frac{\tilde\Pi^2}{m} - \frac{\overline{\tilde\Pi^4}}{6m^3} + \frac{\overline{\tilde\Pi^6}}{45m^5} - \frac{1}{4m^2}\{\gamma_\nu,\{\Pi_\nu,H\}\} + \frac{1}{16m^2}\{\gamma_\nu,[\gamma_\mu,[\gamma_\mu,\{\Pi_\nu,H\}]]\} + \gamma_\nu\frac{\overline{\tilde\Pi^2\Pi_\nu}}{6m^2} \\ &+ \frac{1}{24m^4}\{\gamma_\nu,\overline{\Pi_\nu\tilde\Pi^2 H}\} - \frac{1}{96m^4}\{\gamma_\nu,[\gamma_\mu,[\gamma_\mu,\overline{\Pi_\nu\tilde\Pi^2 H}]]\} + \gamma_\nu\left(-\frac{\overline{\tilde\Pi^4\Pi_\nu}}{60m^4} - \frac{\overline{\tilde\Pi^4\Pi_\nu H}}{90m^6} + \frac{\overline{\tilde\Pi^6\Pi_\nu}}{630m^6}\right) + \cdots\Big\rangle. \end{aligned} \tag{41}$$

Note that in contrast to Refs. [10,12–14] the separation into high- and low-energy parts is done here in Lorentz-invariant fashion and was achieved without breaking of the integration over a virtual photon into separate pieces.

For the state-independent part of the S states the low-energy part, Eq. (40), yields the exact values of coefficients A_{41} and A_{62} and parts of coefficients A_{40}, A_{50}, A_{61}, and A_{60} [21,22]. The terms involving the function $\tilde{\phi}_4$ and its derivations have to be evaluated between Schrödinger wave functions, otherwise they diverge. (The Dirac wave function of the S states has the logarithmic singularity at the origin. Thus evaluation of an operator expression between the Schrödinger wave functions could yield a finite result even when evaluation between the Dirac wave functions leads to a divergent result.) The first two terms of the high-energy part yield the remaining part of the coefficient A_{40}. The second term has to be evaluated between Schrödinger wave functions; otherwise, it diverges. The remaining terms of the high-energy part diverge even when evaluated between Schrödinger wave functions. These divergencies are connected to the separations (30) and (31) and the expansions (32). If these separations and expansions are avoided and the functions ϕ are considered in full the divergencies disappear [21].

For the state-dependent part of the S states and non-S states the low-energy part yields the exact value of the coefficient A_{61}, see Appendix C, and a part of coefficients A_{40} and A_{60}. The high-energy part yields the remaining parts of these coefficients. Some of these terms have to be for the state-dependent part of the S states and P states evaluated between Schrödinger wave functions; otherwise, they diverge.

One can consider further expansion of the functions $\tilde{\phi}$ defined by the separations (30) and (31) in powers of h. This is, however, not at all advantageous. The expansion of the functions $\tilde{\phi}$ yields the terms proportional to $\ln(h)$. Such terms have to be evaluated numerically, in the same way as Eq. (40), so from a practical point of view nothing is gained by such an expansion. On the contrary, one then loses the contribution of the intermediate electron states with large wave numbers contributing at the order $\alpha(Z\alpha)^7$ and further terms of the $Z\alpha$ expansion. This results in significant loss of accuracy for the atoms with higher nuclear charges. Further, the convergence properties of the terms containing only the terms proportional to $\ln(h)$ is significantly worse than those appearing in Eq. (40); see text below Eq. (49) for further discussion of this point. The only thing that is missed by avoiding the expansion of the functions $\tilde{\phi}$ in series in h is that the contribution to the coefficient A_{60} cannot be isolated. We checked [23] that by performing such an expansion the same value of the A_{60} coefficient is obtained from Eqs. (40) and (41) as that found in Ref. [12]. However, the proof is not too illuminating and will not be presented here.

B. Evaluation of low-energy part

Up to this point, the discussion has been valid for an arbitrary time-independent electromagnetic field. From now on, we shall narrow our focus on the case of the Coulomb field (4).

In Eq. (40) the operator H appears with the subscripts. To evaluate Eq. (40) as it stands we have to use the spectral decomposition of the operator H many times. Fortunately, by means of the operator identities derived below, the number of the spectral decompositions of the operator H can be always reduced to one.

It follows from the definition (14) and identity

$$P_j = \frac{i}{2}[X_j, H] \tag{42}$$

that

$$\begin{aligned}(P_j)_1 D_1[\phi(H)] &= \frac{i}{2}(X_j)_1(H_{12} - H_{01}) \\ &\quad \times \left(\frac{\phi(H_{01})}{H_{01} - H_{12}} + \frac{\phi(H_{12})}{H_{12} - H_{01}}\right) \\ &= \frac{i}{2}(X_j)_1[\phi(H_{12}) - \phi(H_{01})] \\ &= \frac{i}{2}[X_j, \phi(H)].\end{aligned} \tag{43}$$

Further, it follows from the definition (15), identities (42),

$$\begin{aligned}[X_j X_k, H] &= (-2i)(P_j X_k + X_j P_k) \\ &= (-4i)P_j X_k + 2\delta_{jk} = (-4i)X_j P_k - 2\delta_{jk},\end{aligned} \tag{44}$$

and an elementary observation

$$\lim_{H_{12}=H_{01}=H} \frac{\phi(H_{12}) - \phi(H_{01})}{H_{12} - H_{01}} = \phi'(H) \tag{45}$$

that

$$\begin{aligned}(P_j)_1(P_k)_2 D_2[\phi(H)] &= \frac{i}{2}\frac{X_{1j}P_{2k}\phi(H_{01}) + P_{1j}X_{2k}\phi(H_{23})}{-H_{01} + H_{23}} \\ &\quad + \frac{1}{4}X_{1j}X_{2k}\phi(H_{12}) \\ &= -\frac{1}{8}[X_j,[X_k,\phi(H)]] + \frac{\delta_{jk}}{4}\phi'(H).\end{aligned} \tag{46}$$

Furthermore, it follows from the definition (14), identity

$$\Pi_0 - m = \frac{H + m^2 - Em}{E} + \frac{i}{2E}[\vec{X}\cdot\vec{P}, H], \tag{47}$$

and Eq. (45) that

$$\begin{aligned}(\Pi_0 - m)_1 D_1[\phi(H)] &= \frac{H + m^2 - Em}{E}\phi'(H) \\ &\quad + \frac{i}{2E}[\vec{X}\cdot\vec{P}, \phi(H)].\end{aligned} \tag{48}$$

These examples show how the subscripts of the operators Π and H can be eliminated. Elimination of the subscripts leads generally to the expressions involving multiple commutators of the operators $\vec{X}$, $\vec{X}\cdot\vec{P}$, and functions $\phi(H)$. For actual evaluation of Eq. (40) to the desired accuracy the only identities necessary to use are Eqs. (43), (46), and (48). There are simplifications resulting from the Dirac equation and neglect of some of the terms that contribute at a higher order than $\alpha(Z\alpha)^6$. These are described in considerable detail in Appendix A. Taking full advantage of these simplifications allows us to bring the expression (40) for the low-energy part into a computationally useful form (recall that the prime denotes

differentiation with respect to H),

$$\Delta E_{\rm low} = -\frac{\alpha}{2\pi}\Bigg\{ -\left\langle P_i\left(\frac{\phi_0}{m}+\frac{m\tilde\phi_2}{H^2}\right)P_i\right\rangle + \left\langle [\sigma_i,\sigma_j][P_i,\Pi_0]m^2\left(-\frac{\tilde\phi_1'}{H^2}+\frac{4\tilde\phi_1}{H^3}-\frac{\phi_0}{2m^3H}\right)[P_j,\Pi_0]\right\rangle_0$$
$$+\left\langle P_j\left[-\frac{1}{8}\left[X_i,\left[X_i,\frac{\tilde\phi_2}{m}+\frac{\tilde\phi_4}{H^2}\right]\right]+\frac{3}{4}\left(\frac{\tilde\phi_2}{m}+\frac{\tilde\phi_4}{H^2}\right)'\right]P_j\right\rangle_0 + 2\left\langle P_i\left[-\frac{1}{8}\left[X_i,\left[X_j,\frac{\tilde\phi_4}{H^2}\right]\right]+\frac{\delta_{ij}}{4}\left(\frac{\tilde\phi_4}{H^2}\right)'\right]P_j\right\rangle_0$$
$$-\left\langle P_j\left(\frac{1}{2E}\left[r\frac{\partial}{\partial r},\tilde\phi_2'+\frac{m^2\tilde\phi_4'}{H^2}\right]+\frac{H+m^2-Em}{E}\left(\tilde\phi_2'+\frac{m^2\tilde\phi_4'}{H^2}\right)'\right)P_j\right\rangle_0$$
$$+\left\langle P_j\left(\frac{H\phi_0}{2m^3}+\frac{\tilde\phi_2'}{2m}-\frac{\tilde\phi_1}{H}-\frac{m^2\tilde\phi_3'}{H^2}\right)P_j\right\rangle_0 - \left\langle (\Pi_0-m)\frac{i}{2}\left[X_i,2\frac{\tilde\phi_2}{H}+2m^2\frac{\tilde\phi_4'}{H^2}\right]P_i\right\rangle_0$$
$$+\left\langle (\Pi_0-m)\left(\frac{\phi_0}{m}+\frac{m\tilde\phi_2}{H^2}+\frac{2m\tilde\phi_2'}{H}+\frac{m^3\tilde\phi_4''}{H^2}\right)(\Pi_0-m)\right\rangle_0\Bigg\}, \tag{49}$$

where

$$\langle O\rangle_0 = \langle\psi_0|O|\psi_0\rangle \tag{50}$$

and ψ_0 stands for the Schrödinger limit of the Dirac wave function ψ. The replacement $\psi\to\psi_0$ in Eq. (49) is accompanied by the replacement of the second-order Hamilton operator H by its nonrelativistic limit,

$$H \simeq 2m(\Pi_0-m)-\vec P\cdot\vec P. \tag{51}$$

Henceforth it is understood that notation (50) implies that the exact Hamilton operator, Eq. (6), is replaced by the approximate one, Eq. (51). The expression (49) is evaluated by calculating the explicit form of the functions $\tilde\phi$ and then using the spectral decomposition of the Hamilton operator H. The method is essentially the same as that described in Ref. [21]. Further extensions and simplifications of that method are described in Appendix A.

The functions $\tilde\phi$ can be brought to the form that involves the calculation of the inverse of the operator $y+wh$, i.e., the Green function of the hydrogen [22]. Thus an alternative way of the evaluation of Eq. (49) is to use a known form of the Green functions [24]. Such an approach was followed in Refs. [12,13] for the calculation of the Bethe logarithm and its relativistic corrections. However, such an approach seems to be limited to the states with principal quantum number n lesser than 9; see the remark in Ref. [14]. The evaluation based on the spectral decomposition of the Hamilton operator H that is followed here does not possess such a restriction.

The dominant contribution to the low-energy part comes from the first term in Eq. (49). If the function $\phi_0/m+m\tilde\phi_2/H^2$ is expanded in the powers of h one obtains at the leading order $mh[13/18-2\ln(h)/3]$, where the second term corresponds to the well-known Bethe logarithm [5]. However, when the first term in Eq. (49) is left unchanged, its calculation is both more accurate and easily done than the calculation of the Bethe logarithm. For to use the spectral decomposition of the scaled Hamilton operator h one has to sum over the quantum numbers n' and integrate over the wave numbers k_e; see Eq. (A33). The eigenvalues of the operator h for the discrete and continuous parts of the spectrum are given in the nonrelativistic limit as $(Z\alpha)^2(1/n^2-1/n'^2)$ and $(Z\alpha)^2(1/n^2+k_e^2)$, respectively. Now, for the S states the operator $P_ih\ln(h)P_i$ has to be evaluated between Schrödinger wave functions, otherwise it diverges. For large wave numbers k_e one integrates an expression that behaves for the S states as $k_e^{-2}\ln k_e$, i.e., is on the very border of convergence. On the other hand, the function $\phi_0/m+m\tilde\phi_2/H^2$ behaves for large h as $\ln(h)$. Therefore, the average of the operator $P_i(\phi_0/m+m\tilde\phi_2/H^2)P_i$ converges even when evaluated between Dirac wave functions. When this average is taken between Schrödinger wave functions it behaves for large k_e for the S states as $k_e^{-4}\ln k_e$. The same kind of argument also applies to further terms in Eq. (49). For example, the expansion of the function $m\tilde\phi_4/H^2$ yields at the leading order $mh^3[47/900-\ln(h)/15]$, where the second term corresponds to the correction to the Bethe logarithm due to quadrupole interaction of the electron with the electromagnetic field [12]. The average of the operator $P_iX_jh^3\ln(h)X_iP_j$ diverges when evaluated for the S states and converges only when normalized difference of the averages of the operators [11,12]

$$\langle\langle O\rangle\rangle = n^3\langle\psi_n|O|\psi_n\rangle - \langle\psi_1|O|\psi_1\rangle \tag{52}$$

between the Schrödinger wave functions is considered. In contrast to it, the function $m\tilde\phi_4/H^2$ behaves for large h as $mh^2/6$. When the average of the operator $P_iX_j(m\tilde\phi_4/H^2)X_iP_j$ is taken between Schrödinger wave functions it behaves for the S states for large k_e as k_e^{-2}.

C. Evaluation of high-energy part

As shown in Appendix B, the expressions in Eq. (41) can be converted to multiple commutators involving the components of Π and H. Taking advantage again of simplifications following from neglect of the terms that contribute to higher order than $\alpha(Z\alpha)^6$, Eq. (41) can be for the case of the external Coulomb field (4) brought to the form

$$\Delta E_{\rm high} = -\frac{\alpha}{2\pi}\Bigg\{\langle\gamma_0\gamma_j[P_j,\Pi_0]\rangle\frac{1}{2m^2}+\langle[P_i,[P_i,\Pi_0]]\gamma_0\rangle \times\frac{5}{12m^3}-\langle[P_i,[P_i,[P_j,\Pi_0]]]\gamma_0\gamma_j\rangle\frac{1}{12m^4}$$
$$-\langle[P_i,\Pi_0][P_i,\Pi_0]\rangle_0\frac{1}{2m^4}$$
$$-\langle[P_i,[P_i,[P_j,[P_j,\Pi_0]]]]\rangle_0\frac{7}{120m^5}\Bigg\}. \tag{53}$$

Reduction of the reference wave function to the upper components yields (see Appendix B for details)

$$\begin{aligned}\langle\gamma_0\vec{\gamma}\cdot[\vec{P},\Pi_0]\rangle &\simeq \frac{1}{2m}\langle -[P_j,[P_j,\Pi_0]]-[\sigma_i,\sigma_j][P_j,\Pi_0]P_i\rangle_{\rm FW}\\ &+\frac{1}{4m^3}\langle([P_j,[P_j,\Pi_0]]+[\sigma_k,\sigma_j][P_j,\Pi_0]P_k)\\ &\times P^2+m[P_j,\Pi_0][P_j,\Pi_0]\rangle_0,\end{aligned}\tag{54}$$

$$\begin{aligned}\langle\gamma_0[P_j,[P_j,\Pi_0]]\rangle &\simeq \langle[P_j,[P_j,\Pi_0]]\rangle_{\rm FW}\\ &-\frac{1}{8m^2}\langle[P_k,[P_k,[P_j,[P_j,\Pi_0]]\\ &+[\sigma_i,\sigma_j][P_j,\Pi_0]P_i]]\rangle_0,\end{aligned}\tag{55}$$

and

$$\begin{aligned}\langle[P_k,[P_k,[P_j,\Pi_0]]]\gamma_0\gamma_j\rangle &\simeq -\frac{1}{2m}\langle[P_k,[P_k,[P_j,[P_j,\Pi_0]]\\ &+[\sigma_i,\sigma_j][P_j,\Pi_0]P_i]]\rangle_0,\end{aligned}\tag{56}$$

where

$$\langle O\rangle_{\rm FW}=\langle\psi_{\rm FW}|O|\psi_{\rm FW}\rangle\tag{57}$$

and $\psi_{\rm FW}$ is the Foldy-Wouthuysen form of the Dirac wave function containing corrections at least of the order $(Z\alpha)^2$ to the Schrödinger limit.

1. Evaluation for the S states

For the S states the expressions in Eqs. (53)–(56) are generally divergent. One has to consider the normalized difference of the averages of the operators, Eq. (52). For nonvanishing terms in Eqs. (53)–(56) one then gets for this difference [12]

$$\begin{aligned}&\frac{1}{m^2}\langle\langle[P_j,[P_j,\Pi_0]]\rangle\rangle_{\rm FW}\\ &=m(Z\alpha)^4\langle\langle 4\pi\delta(\vec{r})\rangle\rangle_{\rm FW}\\ &=m(Z\alpha)^6\left(6+\frac{4}{n}-\frac{10}{n^2}-4[\gamma+\Psi(n)-\ln(n)]\right),\end{aligned}\tag{58}$$

$$\begin{aligned}&\frac{1}{m^3}\langle\langle[P_j,\Pi_0][P_j,\Pi_0]\rangle\rangle_0\\ &=-m(Z\alpha)^6\left\langle\left\langle\frac{1}{r^4}\right\rangle\right\rangle_0\\ &=-8m(Z\alpha)^6\left(-\frac{2}{3}+\frac{1}{2n}+\frac{1}{6n^2}+\gamma+\Psi(n)-\ln(n)\right),\end{aligned}\tag{59}$$

$$\frac{1}{m^4}\langle\langle[P_k,[P_k,[P_j,[P_j,\Pi_0]]]]\rangle\rangle_0=-m(Z\alpha)^6\frac{8(1-n^2)}{n^2},\tag{60}$$

and

$$\frac{1}{m^4}\langle\langle[P_j,[P_j,\Pi_0]]P^2\rangle\rangle_0=-m(Z\alpha)^6\frac{4(1-n^2)}{n^2}.\tag{61}$$

2. Evaluation for the P states

For the P states one gets for nonvanishing terms in Eqs. (53)–(56) [12]

$$\begin{aligned}\frac{1}{m^2}\langle[\sigma_k,\sigma_j][P_j,\Pi_0]P_k\rangle_{\rm FW}&=2m(Z\alpha)^4\left\langle\frac{\vec{\sigma}\cdot\vec{L}}{r^3}\right\rangle_{\rm FW}=\frac{2m(Z\alpha)^4}{n^3}\left\{\frac{\langle\vec{\sigma}\cdot\vec{L}\rangle_0}{3}+(Z\alpha)^2\left[-\frac{\langle\vec{\sigma}\cdot\vec{L}\rangle_0}{4}\left(-\frac{346}{135}-\frac{4}{3n}+\frac{22}{5n^2}\right)\right.\right.\\ &\left.\left.+\frac{2-\langle\vec{\sigma}\cdot\vec{L}\rangle_0}{2}\left(-\frac{227}{540}-\frac{1}{6n}+\frac{1}{5n^2}\right)\right]\right\},\end{aligned}\tag{62}$$

$$\frac{1}{m^4}\langle[\sigma_k,\sigma_j][P_j,\Pi_0]P_kP^2\rangle_0=\frac{m(Z\alpha)^6}{n^3}\langle\vec{\sigma}\cdot\vec{L}\rangle_0\frac{2}{5}\left(4-\frac{13}{3n^2}\right),\tag{63}$$

$$\begin{aligned}&\frac{1}{m^4}\langle[P_m,[P_m,[P_j,\Pi_0]]]P_k[\sigma_k,\sigma_j]\rangle_0\\ &=\frac{m(Z\alpha)^6}{n^3}\langle\vec{\sigma}\cdot\vec{L}\rangle_0\frac{8(n^2-1)}{3n^2},\end{aligned}\tag{64}$$

$$\frac{1}{m^3}\langle[P_j,\Pi_0][P_j,\Pi_0]\rangle_0=-\frac{m(Z\alpha)^6}{n^3}\frac{2(3n^2-2)}{15n^2},\tag{65}$$

and

$$\frac{1}{m^4}\langle[P_k,[P_k,[P_j,[P_j,\Pi_0]]]]\rangle_0=-\frac{m(Z\alpha)^6}{n^3}\frac{8(n^2-1)}{3n^2}.\tag{66}$$

Here, we take

$$\langle\vec{\sigma}\cdot\vec{L}\rangle_0=-2,\quad j=1/2,\quad \langle\vec{\sigma}\cdot\vec{L}\rangle_0=1,\quad j=3/2.\tag{67}$$

3. Evaluation for the states $j > 1/2$

For the states with $j > 1/2$ we have

$$\langle[P_i,[P_i,\Pi_0]]\gamma_0\rangle=0\tag{68}$$

and

$$\langle[P_i,[P_i,[P_j,\Pi_0]]]\gamma_0\gamma_j\rangle=0.\tag{69}$$

Furthermore, for the states with $l > 1$ we have

$$\langle[P_i,[P_i,[P_j,[P_j,\Pi_0]]]]\rangle_0=0.$$

The remaining terms in Eq. (53) are evaluated by means of Eqs. (A44) and (B16).

IV. RESULTS AND DISCUSSION

In Tables I–III the results for the self-energy effect on the states of hydrogenlike atoms with the principal number n ranging from 2 to 10, the orbital quantum number l ranging

TABLE I. Result for the scaled energy function $F(Z\alpha,n,l_j)$ for low-lying S and P states of hydrogenlike atoms obtained by various methods. For the S states the results for the difference $F(\alpha,n,0) - F(\alpha,1,0)$ are given. The numerical results are taken from Ref. [17] for $Z = 1$–5 and from Ref. [16] for $Z = 10$–30. The results obtained by means of Eq. (8) are taken from Ref. [12] for the S states, and from Ref. [13] for the P states.

State	Z	This paper	Numerical	Eq. (8)
$2s - 1s$	1	0.23002947	0.23003154	0.23003040
	5	0.23302946	0.233233342	0.23309401
	10	0.23887771	0.24028	0.23917098
	20	0.25130292	0.260392	0.25216758
$2p_{1/2}$	1	−0.1263965908	−0.12639637	−0.12639773
	5	−0.1227963730	−0.12277494	−0.12292993
	10	−0.1149935477	−0.11483	−0.11601084
	20	−0.09335685260	−0.092519	−0.10100723
	30	−0.06613153145	−0.0643302	−0.091200090
$2p_{3/2}$	1	0.1234982498	0.12349856	0.12349766
	5	0.1255937276	0.12562330	0.12552595
	10	0.1301591823	0.13036	0.12965824
	20	0.1426153201	0.143839	0.13905128
	30	0.1571646516	0.160647	0.14614776
$3s - 1s$	1	0.28881828	0.28882057	0.28881946
	5	0.29154791	0.29175898	0.29163760
	10	0.29682921	0.2982	0.29729576
	20	0.30772309	0.3170	0.30974380
$3p_{1/2}$	10	−0.1022064452	−0.1021	−0.10341245
	20	−0.07688197377	−0.0760	−0.085950786
	30	−0.04471096715	−0.0430	−0.074424272
$3p_{3/2}$	10	0.1418508156	0.1421	0.14125930
	20	0.1556877238	0.1572	0.15148550
	30	0.1718101044	0.1761	0.15882288
$4s - 1s$	1	0.31259262	0.31259475	0.31259391
	5	0.31492838	0.31513180	0.31503165
	10	0.31939228	0.3253	0.31996353
	20	0.32820025	0.3371	0.33100244
$4p_{1/2}$	10	−0.09650194613	−0.0963	−0.097772470
	20	−0.06983105648	−0.0690	−0.079374572
	30	−0.03588964739	−0.0344	−0.067119757
$4p_{3/2}$	10	0.1471460730	0.1477	0.14652274
	20	0.1593951831	0.1630	0.15703404
	30	0.1781270585	0.1827	0.16444487
$5s - 1s$	10	0.33036787	0.3316	0.33100744
	20	0.33748936	0.3460	0.34082239
$5p_{1/2}$	10	−0.09340485640	−0.0933	−0.094704519
	20	−0.06609711910	−0.0652	−0.075850139
	30	−0.03133848193	−0.0299	−0.063219658
$5p_{3/2}$	10	0.1500435251	0.1502	0.14940540
	20	0.1645702624	0.1662	0.16003876
	30	0.1814730287	0.1861	0.16746710

from 0 to 3, and nuclear charges Z ranging from 1 to 30 are presented.

As follows from discussion in Sec. I the error of the present calculation is of the order $\alpha(Z\alpha)^7$ for the normalized difference of the S states and for the P states and of the order $\alpha(Z\alpha)^8$ for the states with the angular quantum number l greater than 1. However, some of the terms in Eq. (49) are treated with greater accuracy than $\alpha(Z\alpha)^6$. Therefore, the present method should yield the results that are closer to the accurate numerical results obtained by partial wave expansion [16,17] than the results obtained in Refs. [12,13] by expanding the self-energy in $Z\alpha$, Eq. (8). Looking at Table I one can see that this is indeed true for P states, but not for the normalized difference of the S states, where the present method yields results that are slightly smaller than both the numerical and perturbative results. However, whatever is the cause of the difference, it is not significant. There is no need at this moment and for some time to come to further improve the accuracy of the result achieved either here or in Refs. [12,17] for the atoms with low nuclear charge. The observable difference of the self-energies

TABLE II. Results for the self-energy function $F(Z\alpha,n,l_j)$ for $Z = 1$, $n = 3$–10, $l = 0$–3, and $j = 1/2$–$7/2$. For the S states the results for the difference $F(\alpha,n,0) - F(\alpha,1,0)$ are given. The results obtained by means of Eq. (8) are taken from Ref. [12] for the S states, from Ref. [15] for the $5F$ states, from Ref. [14] for the 9D–10D states, and from Ref. [13] for the other states.

State	Low-energy part	High-energy part	Total	Eq. (8)
$3p_{1/2}$	0.05123609530	−0.1666954947	−0.1154593994	−0.11546075
$3p_{3/2}$	0.051087381807	0.08332663172	0.1344140135	0.13441331
$3d_{3/2}$	0.00698293324	−0.0500012647	−0.0430183315	−0.0430183314
$3d_{5/2}$	0.00698282332	0.0333333531	0.0403161764	0.040315728
$4p_{1/2}$	0.05627005992	−0.1666959457	−0.1104258857	−0.11042730
$4p_{3/2}$	0.05611336273	0.08332639032	0.1394397530	0.13943901
$4d_{3/2}$	0.00899544159	−0.0500014034	−0.0410059618	−0.0410059616
$4d_{5/2}$	0.00899532578	0.0333334209	0.0423287466	0.042328177
$4f_{5/2}$	0.00231274299	−0.0238097629	−0.0214970199	−0.021497015
$4f_{7/2}$	0.00231272472	0.0178571748	0.0201698996	0.020169900
$5s - 1s$	0.32456588	−0.000011833054	0.32455404	0.32455540
$5p_{1/2}$	0.05904972297	−0.1666960022	−0.1076462793	−0.10764773
$5p_{3/2}$	0.05888941069	0.08332624055	0.1422156512	0.14221489
$5d_{3/2}$	0.0101422290	−0.0500014448	−0.0398592158	−0.0398592155
$5d_{5/2}$	0.0101421091	0.0333334421	0.0434755512	0.043474936
$5f_{5/2}$	0.00293755438	−0.0238097949	−0.0208722406	−0.0208722397
$5f_{7/2}$	0.00293753396	0.0178571948	0.0207947288	0.0207947296
$6s - 1s$	0.33142715	−0.000011371781	0.33141578	0.33141718
$6p_{1/2}$	0.06075659360	−0.1666959508	−0.1059393572	−0.10594083
$6p_{3/2}$	0.06059436226	0.08332613865	0.1439205009	0.14391973
$6d_{3/2}$	0.0108710371	−0.0500014549	−0.0391304178	−0.0391304174
$6d_{5/2}$	0.0108709134	0.0333334481	0.0442043616	0.044203727
$6f_{5/2}$	0.00333764381	−0.0238098084	−0.0204721646	
$6f_{7/2}$	0.00333762227	0.0178572035	0.0211948257	
$7s - 1s$	0.33572642	−0.000010994923	0.33571542	0.33571685
$7p_{1/2}$	0.06188266713	−0.1666958704	−0.1048132033	−0.10481469
$7p_{3/2}$	0.06171930504	0.08332606486	0.1450453699	0.14504460
$7d_{3/2}$	0.0113671876	−0.0500014536	−0.0386342660	−0.0386342655
$7d_{5/2}$	0.0113670606	0.0333334485	0.0447005091	0.044699866
$7f_{5/2}$	0.00361357688	−0.0238098142	−0.0201962373	
$7f_{7/2}$	0.00361355458	0.0178572073	0.0214707619	
$8s - 1s$	0.33859759	−0.000010686353	0.33858691	0.33858835
$8p_{1/2}$	0.06266557694	−0.1666957862	−0.1040302093	
$8p_{3/2}$	0.06250149745	0.08332600896	0.1458275064	
$8d_{3/2}$	0.0117216955	−0.0500014480	−0.0382797525	−0.0382797518
$8d_{5/2}$	0.0117215656	0.0333334466	0.0450550122	0.0450543659
$8f_{5/2}$	0.00381363141	−0.0238098164	−0.0199961850	
$8f_{7/2}$	0.00381360854	0.0178572090	0.0216708175	
$9s - 1s$	0.34060985	−0.000010430983	0.34059941	
$9p_{1/2}$	0.06323228165	−0.1666957066	−0.1034634249	
$9p_{3/2}$	0.06306772116	0.08332596516	0.1463936863	
$9d_{3/2}$	0.0119844041	−0.0500014408	−0.0380170367	−0.0380170366
$9d_{5/2}$	0.0119842719	0.0333334438	0.0453177157	0.0453177160
$9f_{5/2}$	0.00396403419	−0.0238098169	−0.0198457827	
$9f_{7/2}$	0.00396401084	0.0178572096	0.0218212204	
$10s - 1s$	0.34207453	−0.000010217001	0.34206431	
$10p_{1/2}$	0.06365584559	−0.1666956339	−0.1030397883	
$10p_{3/2}$	0.06349094851	0.08332592992	0.1468168784	
$10d_{3/2}$	0.0121847643	−0.0500014333	−0.0378166690	−0.0378166678
$10d_{5/2}$	0.0121846301	0.0333334408	0.0455180709	0.0455180723
$10f_{5/2}$	0.00408030566	−0.0238098165	−0.0197295108	
$10f_{7/2}$	0.00408028192	0.0178572095	0.0219374915	

TABLE III. Results for the self-energy function $F(Z\alpha,n,l_j)$ for $Z = 10$–30, $n = 3$–10, $l = 0$–3, and $j = 1/2$–$7/2$.

State	$Z = 10$	$Z = 20$	$Z = 30$
$3d_{3/2}$	−0.0427179723	−0.0420823419	−0.0412544602
$3d_{5/2}$	0.0407323104	0.0417137667	0.0431019645
$4d_{3/2}$	−0.0406712184	−0.0399624855	−0.0390316449
$4d_{5/2}$	0.0427988310	0.0439098686	0.0454864309
$4f_{5/2}$	−0.0214413415	−0.0213183565	−0.0211555427
$4f_{7/2}$	0.0202506194	0.0204496148	0.0207395023
$5d_{3/2}$	−0.0395056287	−0.0387538976	−0.0377592207
$5d_{5/2}$	0.0439701187	0.0451397241	0.0468013236
$5f_{5/2}$	−0.0208109431	−0.0206763255	−0.0204988563
$5f_{7/2}$	0.0208859960	0.0211115123	0.0214407403
$6s - 1s$	0.33646424	0.34228099	
$6p_{1/2}$	−0.09152245608	−0.06386341969	−0.02866483271
$6p_{3/2}$	0.1518120874	0.1664470985	0.1834670953
$6d_{3/2}$	−0.0387650529	−0.0379851595	−0.0369473916
$6d_{5/2}$	0.0447118426	0.0459121250	0.0476181050
$6f_{5/2}$	−0.0204073538	−0.0202650016	−0.0200771519
$6f_{7/2}$	0.0212916826	0.0215311862	0.0218811026
$7s - 1s$	0.34016445	0.34496208	
$7p_{1/2}$	−0.09028882430	−0.06241509348	−0.02695387655
$7p_{3/2}$	0.1529737796	0.1676693504	0.1847521660
$7d_{3/2}$	−0.0382609103	−0.0374612730	−0.0363927129
$7d_{5/2}$	0.0452154962	0.0464334427	0.0481648359
$7f_{5/2}$	−0.0201290318	−0.0199811675	−0.0197856080
$7f_{7/2}$	0.0215708918	0.0218185366	0.0221804457
$8s - 1s$	0.34255769	0.34654410	
$8p_{1/2}$	−0.08943500943	−0.06142008301	−0.02578997709
$8p_{3/2}$	0.1537787026	0.1685102685	0.1856283268
$8d_{3/2}$	−0.0379006583	−0.0370864941	−0.0359949816
$8d_{5/2}$	0.0455746675	0.0468034719	0.0485503713
$8f_{5/2}$	−0.0199272499	−0.0197752692	−0.0195737852
$8f_{7/2}$	0.0217730018	0.0220257196	0.0223950641
$9s - 1s$	0.34418136	0.34750949	
$9p_{1/2}$	−0.08881893254	−0.06070588271	−0.02496088841
$9p_{3/2}$	0.1543597058	0.1691135696	0.1862518076
$9d_{3/2}$	−0.0376336445	−0.0368083944	−0.0356992008
$9d_{5/2}$	0.0458404213	0.0470762214	0.0488330185
$9f_{5/2}$	−0.0197755445	−0.0196203819	−0.0194142218
$9f_{7/2}$	0.0219247615	0.0221808015	0.0225549855
$10s - 1s$	0.34532463	0.34810919	
$10p_{1/2}$	−0.08835949620	−0.06017526145	−0.02434859620
$10p_{3/2}$	0.1547929114	0.1695609671	0.1867106947
$10d_{3/2}$	−0.0374299512	−0.0365959944	−0.0354728156
$10d_{5/2}$	0.0460428455	0.0472833114	0.0490466341
$10f_{5/2}$	−0.0196582588	−0.0195005693	−0.0192906366
$10f_{7/2}$	0.0220419641	0.0223002626	0.0226777126

can be written as

$$\Delta E_n - \Delta E_1 = \frac{n^3 \Delta E_n - \Delta E_1}{n^3} + \left(\frac{1}{n^3} - 1\right)\Delta E_1. \qquad (70)$$

The difference between the result for the normalized difference obtained here and in Ref. [17] amounts to the difference of 210.5 Hz and 69 Hz for $2S - 1S$ and $3S - 1S$ transitions in hydrogen, respectively. This is much smaller than the difference between the results in Ref. [22] and in Ref. [17] for the ground-state self-energy ΔE_1 that amounts to the difference of 15 kHz for $2S - 1S$ transition in hydrogen. Also this is much smaller than the uncertainty of 82 kHz for $2S - 1S$ transition in hydrogen arising from the uncertainty about the proton radius [25].

Further, it can be seen from Table I that for the normalized difference of the S states the agreement between the present method and the partial wave expansion goes slowly down with the increase of the nuclear charge Z. The decrease of the accuracy of the present method is in this case roughly the same as that of the series (8) truncated after the $\alpha(Z\alpha)^6$ term. On the other hand, for the P states, the decrease of the accuracy of the present method is significantly slower than

that of the series (8). To sum up, the present method yields quantitative results for the self-energy effect up to Z about 20 for the normalized difference of the S states and up to Z about 30 for the P states. This is remarkable, since for Z about 30 we are for the P states clearly out of the perturbative region. The accuracy and reliability of the present method for the atoms with higher nuclear charges can be further improved by avoiding the separations (30) and (31), expansions (32), and nonrelativistic approximation of the reference wave function; see results in Ref. [21]. The calculation is then, however, somewhat more involved.

In Table II the results for the self-energy effect in hydrogen for the excited states are presented. For the states where the effect was calculated earlier by means of the expansion in $Z\alpha$, Eq. (8), the agreement between the present and perturbative method is for all practical purposes more than sufficient. We note that we achieved calculating the effect for the excited states whose radial wave functions have more than seven nodes.

In Table III the results for the self-energy effect for hydrogenlike atoms with nuclear charge between $Z = 10$ and $Z = 30$ on the excited states are presented. For S and P states their accuracy can be judged from the comparison between the results of the present method and accurate numerical evaluations [16] in Table I for low-lying states. One can see from Table III that for D and F states the results change only slowly with the increase of the nuclear charge. Clearly, for these states for $Z = 30$ we are still at the perturbative region. Therefore, the accuracy of the results for D and F states will be even higher than that for S and P states.

V. CONCLUSIONS

In this paper we suggested the method for evaluation of the self-energy of the bound electron for the excited states. The method was applied to the states with $n = 2$–10, $l = 0$–3, and $Z = 1$–30. In the cases that were already considered in the literature a very good agreement with previous calculations was found, especially for the atoms with lower nuclear charges. These results can be used for the determination of nuclear masses and for the improvement of the accuracy of the Rydberg constant by high-precision spectroscopy in the way proposed in Ref. [15].

In comparison with the calculation based on the expansion in powers of $Z\alpha$ [12–14] the decline of the accuracy and reliability of the present method with the increase of the nuclear charge Z is much slower. Further, the numerical part of the calculation is easier to do since for the S states the behavior of the integrals encountered here is much better than the behavior of the integrals encountered in Ref. [12]. Also, the spectral decomposition of the Hamilton operator used here for the evaluation of the low-energy term is somewhat simpler than the approach followed in Refs. [12–14].

In comparison with the calculation based on the partial wave expansion [15–20] the performance of the method improves with the increase of the principal quantum number n and decrease of the nuclear charge Z. The difficulty of the present calculation, as with any other calculation, grows with the increase of the number of nodes of the reference wave function ψ. However, the difficulty of the calculation does not increase with the increase of the angular quantum number l. In either case there are no problems associated with the numerical stability of the method; compare this with discussion in Ref. [15]. The present method involves just a few one-dimensional integrals over the continuous part of the hydrogen atom spectrum. The same holds for the approach based on the expansion in $Z\alpha$ followed in Refs. [12–14]. This should be contrasted with the partial wave expansion that involves three-dimensional numerical integration that has to be done, especially for the atoms with low nuclear charges, for a huge number of partial waves [17].

In comparison with both of the approaches followed in Refs. [12–20] the present method avoids the explicit separation of the integration over four-momentum of virtual photon. Further, this integration is done in the way that preserves manifest Lorentz invariance.

Bearing in mind the foregoing arguments we believe that the method presented in this paper is of some interest and its extension to higher loops [26] and many-electron atoms [27] will lead to further progress in bound-state QED.

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APPENDIX A: EVALUATION OF LOW-ENERGY PART

The first two parts of this appendix show how to get from Eqs. (40) to (49). The remaining parts are devoted to the practical evaluation of Eq. (49).

1. Simplifications due to the Dirac equation

Multiplicating the first-order Dirac equation (3) by $(\gamma \cdot \Pi + m)$ yields the second-order Dirac equation

$$H\psi = 0. \tag{A1}$$

It follows from the definition (15) and the last equation that if $\phi(H = 0) = 0$, then

$$D_1[\phi]_{H_{01}=0} = \frac{\phi(H_{12})}{H_{12}} \tag{A2}$$

and generally

$$D_n[\phi]_{H_{01}=0} = D_{n-1}\left[\frac{\phi(H)}{H}\right]. \tag{A3}$$

If further also $[\phi(H)/H]_{H=0} = 0$, then

$$D_2[\phi]_{H_{01}=H_{23}=0} = \frac{\phi(H_{12})}{H_{12}^2}, \tag{A4}$$

and generally

$$D_n[\phi]_{H_{01}=H_{n,n+1}=0} = D_{n-2}\left[\frac{\phi(H)}{H^2}\right]. \tag{A5}$$

If $[\phi(H)/H^2]_{H=0} = 0$, then

$$D_1[\phi]_{H_{01}=H_{12}=0} = 0. \tag{A6}$$

These identities lead to certain simplifications when evaluating Eq. (40) and will be used in the following part.

2. Nonrelativistic approximation

Further, we will discard in Eq. (40) some of the contributions of higher order than $\alpha(Z\alpha)^6$. There are several simplifications resulting from this.

By means of the identity

$$\phi(H) = (\gamma\cdot\Pi - m)\frac{\phi(H)}{H}(\gamma\cdot\Pi + m) \tag{A7}$$

and the Dirac equation (3) the first term in Eq. (40) can be rewritten into the form

$$\langle\gamma_\mu\phi_0\Pi_\mu\rangle = \frac{1}{m}\left\langle\Pi_\mu\phi_0\Pi_\mu + \gamma_\rho[\Pi_\mu,\Pi_\rho]\frac{\phi_0}{H}\gamma_\nu[\Pi_\mu,\Pi_\nu]\right\rangle. \tag{A8}$$

Now, the second term on the right member of the last equation can be evaluated with sought accuracy between the Schrödinger wave function ψ_0 instead of the Dirac wave function ψ and the exact operator H can be replaced by the approximation (51),

$$\begin{aligned}&\frac{1}{m}\left\langle\gamma_\rho[\Pi_\mu,\Pi_\rho]\frac{\phi_0}{H}\gamma_\nu[\Pi_\mu,\Pi_\nu]\right\rangle\\ &\quad\simeq \frac{1}{2m^3}\langle P_i H\phi_0 P_i\rangle_0 - \frac{1}{2m}\left\langle[\sigma_i,\sigma_j][P_i,\Pi_0]\frac{\phi_0}{H}[P_j,\Pi_0]\right\rangle_0.\end{aligned} \tag{A9}$$

The second term on the right member of Eq. (A9) corresponds to the interaction of the electron spin with the electromagnetic field [12]. Such interaction also arises from the term

$$\begin{aligned}&-\frac{1}{8}\langle\{\gamma_\nu,[\gamma_\mu,[\gamma_\mu,\varepsilon_\nu\tilde\phi_1' + (\Pi-\varepsilon)_{1\nu}D_1[\tilde\phi_1]]]\}\rangle\\ &\quad= -\frac{1}{8}\left\langle\{\gamma_0,[\gamma_\mu,[\gamma_\mu,m\tilde\phi_1']]\} - \frac{i}{2}\{\gamma_j,[X_j,[\gamma_\mu,[\gamma_\mu,\tilde\phi_1]]]\}\right\rangle\\ &\quad\simeq -\frac{1}{4}\left\langle 2m[\gamma_0\gamma_j,H]\frac{\tilde\phi_1'}{H^2}[\gamma_j,H] - \{\gamma_j,[\gamma_\mu,[\gamma_\mu,H]]\}\frac{\tilde\phi_1}{H^2}P_j\right\rangle\\ &\quad\simeq m\left\langle[\sigma_i,\sigma_j][P_i,\Pi_0]\left(-\frac{\tilde\phi_1'}{H^2} + 4\frac{\tilde\phi_1}{H^3}\right)[P_j,\Pi_0]\right\rangle_0,\end{aligned} \tag{A10}$$

where the identities (43),

$$[\gamma_i,H] = 2[P_i,\Pi_0]\gamma_0,\quad [\gamma_0\gamma_i,H] = [\Sigma_i,\Sigma_j][P_j,\Pi_0], \tag{A11}$$

and

$$\{\gamma_j,[\gamma_\mu,[\gamma_\mu,H]]\} = -8\gamma_0[\Sigma_i,\Sigma_j][P_i,\Pi_0] \tag{A12}$$

were used.

The second and third terms in Eq. (40) can be rewritten into the form

$$\begin{aligned}&\langle\gamma_\mu((\Pi-\varepsilon)_{1\lambda}\varepsilon_\lambda D_1[\tilde\phi_2'] + (\Pi-\varepsilon)_{1\lambda}(\Pi-\varepsilon)_{2\lambda}D_2[\tilde\phi_2])\Pi_\mu\rangle\\ &\quad= m\left\langle\Pi_\mu\frac{\tilde\phi_2}{H^2}\Pi_\mu\right\rangle + \langle[\gamma_\mu,(\Pi-\varepsilon)_{1\lambda}\varepsilon_\lambda D_1[\tilde\phi_2']\\ &\qquad+(\Pi-\varepsilon)_{1\lambda}(\Pi-\varepsilon)_{2\lambda}D_2[\tilde\phi_2]]\Pi_\mu\rangle,\end{aligned} \tag{A13}$$

where in the first term on the right member we used the Dirac equations (3) and (A4).

The second term on the right member of Eq. (A13) can again be evaluated with sought accuracy between the Schrödinger wave function ψ_0 instead of the Dirac wave function ψ and with the approximation (51),

$$\begin{aligned}&\langle[\gamma_\mu,(\Pi-\varepsilon)_{1\lambda}\varepsilon_\lambda D_1[\tilde\phi_2'] + (\Pi-\varepsilon)_{1\lambda}(\Pi-\varepsilon)_{2\lambda}D_2[\tilde\phi_2]]\Pi_\mu\rangle\\ &\quad\simeq\left\langle\left[\gamma_\mu,m\left(\frac{H+m^2-Em}{E}\tilde\phi_2'' + \frac{i}{2E}[\vec X\cdot\vec P,\tilde\phi_2']\right)\right.\right.\\ &\qquad\left.\left.+\frac{1}{8}[X_i,[X_i,\tilde\phi_2]] - \frac{3}{4}\tilde\phi_2'\right]\Pi_\mu\right\rangle\\ &\quad\simeq -\frac{1}{m}\left\langle\left[P_j,m(\Pi_0-m)_1D_1[\tilde\phi_2']\right.\right.\\ &\qquad\left.\left.-\frac{1}{2}\tilde\phi_2' - (P_i)_1(P_i)_2D_2[\tilde\phi_2]\right]P_j\right\rangle_0\\ &\quad= -\frac{1}{m}\left\langle P_j\left(m(\Pi_0-m)_1D_1[\tilde\phi_2'] - \frac{1}{2}\tilde\phi_2'\right.\right.\\ &\qquad\left.\left.+\frac{1}{8}[X_i,[X_i,\tilde\phi_2]] - \frac{3}{4}\tilde\phi_2'\right)P_j\right\rangle_0\\ &\qquad+2\left\langle(\Pi_0-m)\left(m\frac{\tilde\phi_2'}{H}(\Pi_0-m) - \frac{i}{2}\left[X_i,\frac{\tilde\phi_2}{H}\right]P_i\right)\right\rangle_0,\end{aligned} \tag{A14}$$

where in the first equality the identities (46) and (48) were used. In the second equality we used the approximation

$$\left[\gamma_j,\int_0^1\frac{dy}{m^2y-H}\right] \simeq \frac{\gamma_0}{m}\left[P_j,\int_0^1\frac{dy}{m^2y-H}\right] \tag{A15}$$

following from the approximation

$$[\gamma_j,H] \simeq \frac{\gamma_0}{m}[P_j,H]. \tag{A16}$$

The last approximation follows from the identity

$$[\gamma_\mu,H] = 2[\Pi_\mu,\Pi_\lambda]\gamma_\lambda \tag{A17}$$

for $\mu = j$ and approximation (51). When pushing P_j to the left, we used the identitities

$$[X_j,[X_j,[P_k,O]]] = [P_k,[X_j,[X_j,O]]], \tag{A18}$$

$$[\vec X\cdot\vec P,[P_k,O]] = [P_k,[\vec X\cdot\vec P,O] + iO] \tag{A19}$$

valid for any operator O. In the third equality in Eq. (A14) the Schrödinger limit

$$H\psi_0 \simeq ((2m(\Pi_0-m) - \vec P\cdot\vec P)\psi_0 = 0 \tag{A20}$$

of the iterated Dirac equation (A1) and the identities (A2) and (A3) following from it were used.

Furthermore, using Eqs. (A4), (A5), (43), and (46) we get for the sum of the fourth, fifth, and sixth terms in Eq. (40)

$$
\begin{aligned}
&m\langle\varepsilon_\mu\varepsilon_\nu(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\nu}D_2[\tilde\phi_4'']+(\varepsilon_\lambda g_{\mu\nu}+\varepsilon_\mu g_{\lambda\nu}+\varepsilon_\nu g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}(\Pi-\varepsilon)_{3\nu}D_3[\tilde\phi_4']\\
&\quad+(g_{\lambda\rho}g_{\mu\nu}+g_{\mu\rho}g_{\lambda\nu}+g_{\nu\rho}g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}(\Pi-\varepsilon)_{3\rho}(\Pi-\varepsilon)_{4\nu}D_4[\tilde\phi_4]\rangle\\
&=m\Bigg\langle\varepsilon_\mu\varepsilon_\nu(\Pi-\varepsilon)_\mu\frac{\tilde\phi_4''}{H^2}(\Pi-\varepsilon)_\nu+(\varepsilon_\lambda g_{\mu\nu}+\varepsilon_\mu g_{\lambda\nu}+\varepsilon_\nu g_{\mu\lambda})(\Pi-\varepsilon)_\mu(\Pi-\varepsilon)_{1\lambda}D_1\left[\frac{\tilde\phi_4'}{H^2}\right](\Pi-\varepsilon)_\nu\\
&\quad+(g_{\lambda\rho}g_{\mu\nu}+g_{\mu\rho}g_{\lambda\nu}+g_{\nu\rho}g_{\mu\lambda})(\Pi-\varepsilon)_\mu(\Pi-\varepsilon)_{1\lambda}(\Pi-\varepsilon)_{2\rho}D_2\left[\frac{\tilde\phi_4}{H^2}\right](\Pi-\varepsilon)_\nu\Bigg\rangle\\
&\simeq m\Bigg\langle m^2(\Pi_0-m)\frac{\tilde\phi_4''}{H^2}(\Pi_0-m)-2m(\Pi_0-m)\frac{i}{2}\left[X_i,\frac{\tilde\phi_4'}{H^2}\right]P_i-P_i(\Pi_0-m)_1D_1\left[\frac{\tilde\phi_4'}{H^2}\right]P_i\\
&\quad+(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})P_i\left[-\frac{1}{8}\left[X_k,\left[X_l,\frac{\tilde\phi_4}{H^2}\right]\right]+\frac{\delta_{kl}}{4}\left(\frac{\tilde\phi_4}{H^2}\right)'\right]P_j\Bigg\rangle_0.
\end{aligned}
\tag{A21}
$$

Finally, using Eqs. (A4) and (A6) we get for the last displayed terms in Eq. (40) with the sought accuracy

$$
\begin{aligned}
&\langle\gamma_\nu(\varepsilon_\nu\tilde\phi_1'+(\Pi-\varepsilon)_{1\nu}D_1[\tilde\phi_1]+\varepsilon_\mu\varepsilon_\nu(\Pi-\varepsilon)_{1\mu}D_1[\tilde\phi_3'']+(\varepsilon_\lambda g_{\mu\nu}+\varepsilon_\mu g_{\lambda\nu}+\varepsilon_\nu g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}D_2[\tilde\phi_3']\\
&\quad+(g_{\lambda\rho}g_{\mu\nu}+g_{\mu\rho}g_{\lambda\nu}+g_{\nu\rho}g_{\mu\lambda})(\Pi-\varepsilon)_{1\mu}(\Pi-\varepsilon)_{2\lambda}(\Pi-\varepsilon)_{3\rho}D_3[\tilde\phi_3])\rangle\simeq-m\left\langle P_i\left(\frac{\tilde\phi_1}{m^2H}+\frac{\tilde\phi_3{}'}{H^2}\right)P_i\right\rangle_0.
\end{aligned}
\tag{A22}
$$

Insertion of Eqs. (A8)–(A10), (A13), (A14), (A21), and (A22) into Eq. (40) yields Eq. (49).

3. Spectral decomposition of the second-order Hamilton operator H

In the case of Coulomb potential (4), there is a complete set of mutually commuting operators $\{H,J^2,J_z,K,\Gamma\}$ [21,28]. Here J^2 and J_z are the operators of the square and the third component of the total angular momentum with eigenvalues $j(j+1)$ and m, respectively. K and Γ are the relativistic parity and the relativistic angular momentum operators [21,28] with eigenvalues

$$K=p(j+1/2),\quad p=\pm1, \tag{A23}$$

and

$$\Gamma=\pm\sqrt{(j+1/2)^2-(Z\alpha)^2}, \tag{A24}$$

respectively.

The Hamilton operator (6) can be after scaling

$$R=\frac{r}{EZ\alpha}, \tag{A25}$$

put into the form that is, up to additive and multiplicative constants, the same as the Hamilton operator for the nonrelativistic hydrogen atom [21,28]

$$H=E^2-m^2-2(EZ\alpha)^2\left[\frac{1}{2}\left(p_r^2+\frac{\Gamma(\Gamma-1)}{r^2}\right)-\frac{1}{r}\right]. \tag{A26}$$

Here p_r designates the radial momentum $p_r=-i(\frac{\partial}{\partial r}+\frac{1}{r})$. The eigenstates of the operator (A26) are products of the radial functions and the eigenstates of the operator Γ,

$$R_{n,l_\Gamma}(r)|\Gamma,K,j,m\rangle. \tag{A27}$$

The radial functions R_{n,l_Γ} are the same as nonrelativistic hydrogen wave functions except for the fact that l_Γ is not an integer but equal to

$$l_\Gamma=\Gamma-1,\quad \Gamma>0, \tag{A28}$$

and

$$l_\Gamma=-\Gamma,\quad \Gamma<0. \tag{A29}$$

The explicit form of the eigenstates of the operator Γ reads [21,28]

$$|\Gamma,K,j,m\rangle=\begin{pmatrix}c^\Gamma_{1,K}|j,m\rangle^p\\ c^\Gamma_{2,K}|j,m\rangle^p\end{pmatrix}, \tag{A30}$$

where $|j,m\rangle^p$ stands for spherical spinors. The coefficients c satisfy the relation

$$c^\Gamma_{2,K}=\frac{i}{Z\alpha}(\Gamma-K)c^\Gamma_{1,K} \tag{A31}$$

and are normalized to unity

$$\left|c^\Gamma_{1,K}\right|^2+\left|c^\Gamma_{2,K}\right|^2=1. \tag{A32}$$

Further, the eigenvalues of the Hamilton operator are $E^2-m^2+\frac{(EZ\alpha)^2}{n^2}$ where $n=n_r+l_\Gamma+1, n_r=0,1,2,\ldots$ for a discrete part of the spectrum. The continuous part is obtained by the substitution $n\to-i/k_e$.

Thus the spectral decomposition of the second-order Hamilton operator H reads

$$
\begin{aligned}
H=&\sum_{n'=l_\Gamma+1}^{\infty}\left(E^2-m^2+\frac{(EZ\alpha)^2}{n'^2}\right)P_{n'}\\
&+\int_0^\infty dk_e\left[E^2-m^2-(EZ\alpha)^2k_e^2\right]P_{k_e},
\end{aligned}
\tag{A33}
$$

where the projector operator on the nth eigenstate reads

$$P_{n'} = \sum_{\Gamma,K,j,m} P_{n',l_\Gamma} \frac{|\Gamma,K,j,m\rangle\langle\Gamma,K,j,m|\gamma_0}{\langle\Gamma,K,j,m|\gamma_0|\Gamma,K,j,m\rangle}. \quad \text{(A34)}$$

Here, the radial part of the projector is equal to

$$\langle r|P_{n',l_\Gamma}|r'\rangle = R_{n',l_\Gamma}(r)R^*_{n',l_\Gamma}(r'). \quad \text{(A35)}$$

The projector operators on the eigenstates of the continuous part are obtained by the substitution $n' \to k_e$ in the last two equations.

As mentioned above, except for the first term in Eq. (49) it suffices to replace the projector (A34) by its nonrelativistic limit

$$P_{n'} \simeq \sum_{l,m} P_{n',l}|l,m\rangle\langle l,m|, \quad \text{(A36)}$$

where the states $|l,m\rangle$ are eigenstates of the operators of the square and the third component of the orbital momentum with eigenvalues $l(l+1)$ and m, respectively.

4. Energy and wave function of the reference state

The energy E of the reference state is obtained by setting the eigenvalue of the Hamilton operator H equal to zero; see Eq. (A1):

$$E = \frac{m}{\sqrt{1+\left(\frac{Z\alpha}{n}\right)^2}}. \quad \text{(A37)}$$

The wave function ψ of the reference state is a linear combination of the functions (A27); while every solution of the first-order Dirac equation is also a solution of the second-order Dirac equation, the opposite is not true. The operator Γ commutes with the second-order Dirac Hamiltonian, but not with the first-order Dirac Hamiltonian. Consequently, the first-order Dirac Hamiltonian mixes the states with different values of Γ. The solution of Dirac equation (3) in the case of Coulomb field (4) thus acquires the form Ref. [28]

$$\psi_\pm = N_\pm(A_\pm R_{n,|\Gamma|-(1\pm1)/2}|\pm|\Gamma|,K,j,m\rangle + B_\pm R_{n,|\Gamma|-(1\mp1)/2}|\mp|\Gamma|,K,j,m\rangle), \quad \text{(A38)}$$

where the coefficients $A_\pm$ and $B_\pm$ read

$$A_\pm = \left(\pm\frac{KE}{|\Gamma|}+m\right), \quad \text{(A39)}$$

$$B_\pm = \pm EZ\alpha\frac{\sqrt{n^2-|\Gamma|^2}}{n|\Gamma|} \quad \text{(A40)}$$

and the normalization coefficient is equal to

$$N_\pm = \left(A_\pm^2 + B_\pm^2 + 2A_\pm B_\pm \frac{Z\alpha}{K}\int dr\, r^2 R_{n,|\Gamma|}R_{n,|\Gamma|-1}\right)^{-1/2}. \quad \text{(A41)}$$

Either of the possibilities displayed in Eq. (A38) can be taken as the solution of Dirac equation (3).

5. Radial functions and radial integrals

The radial functions $R_{n,l}(r)$ appearing in Eq. (A27) satisfy recurrence relations [see, e.g., Eqs. (22) and (23) of Ref. [29]]

$$\left(\frac{d}{dr}+\frac{l+1}{r}\right)R_{n,l}(r) = \frac{1}{l}R_{n,l}(r) + \frac{\sqrt{n^2-l^2}}{ln}R_{n,l-1}(r) \quad \text{(A42)}$$

and

$$\left(\frac{d}{dr}-\frac{l}{r}\right)R_{n,l}(r) = -\frac{1}{l+1}R_{n,l}(r) - \frac{\sqrt{n^2-(l+1)^2}}{(l+1)n} \times R_{n,l+1}(r). \quad \text{(A43)}$$

By subtracting the last two equations, we obtain

$$\frac{\sqrt{n^2-l^2}}{nl}R_{n,l-1} + \frac{\sqrt{n^2-(l+1)^2}}{n(l+1)}R_{n,l+1} + (2l+1) \times \left(\frac{1}{l(l+1)}-\frac{1}{r}\right)R_{n,l} = 0. \quad \text{(A44)}$$

For example, in case $n = l+1$ one gets

$$R_{l+1,l-1}(r) = -\sqrt{2l+1}\left(1-\frac{l(l+1)}{r}\right)R_{l+1,l}(r). \quad \text{(A45)}$$

By means of the recursive relation (A44) the radial integrals $\int_0^\infty dr\, r^{2+p} R_{n,l}R_{n',l'}$ needed for evaluation of Eq. (49) are reduced to the integrals of the form $\int_0^\infty dr\, r^{2+p}R_{l+1,l}R_{n',l'}$. The explicit formula for these integrals is (see, e.g., [30])

$$\int_0^\infty dr\, r^{2+p}R_{l+1,l}(r)R_{n',l'}(r) = C_{l+1,l}C_{n',l'}\Gamma(l'+l+p+3)\left(\frac{1}{l+1}+\frac{1}{n'}\right)^{-(l'+l+p+3)} \times F\left(-n'+l'+1, l+l'+p+3, 2l' + 2, \frac{2/n'}{1/(l+1)+1/n'}\right), \quad \text{(A46)}$$

where $F(a,b,c,z)$ stands for the hypergeometric function. The integrals with the functions of the continuous spectrum are obtained from the above formula by the replacement of $n' \to -i/k_e$ and $C_{n',l'}$ by $C_{k_e,l'}$. The normalization constants for discrete and continuous parts of the spectrum are

$$C_{n,l} = \frac{2}{n^2}\sqrt{\frac{(n+l)!}{(n-l-1)!}}\frac{(2/n)^l}{(2l+1)!} \quad \text{(A47)}$$

and

$$C_{k_e,l} = \sqrt{\frac{2}{\pi}}k_e e^{\pi/(2k_e)}|\Gamma(l+1-i/k_e)|\frac{(2k_e)^l}{(2l+1)!}, \quad \text{(A48)}$$

respectively.

6. Angular-spinor integration

The only angular-spinor integration that is needed to perform for the evaluation of expressions in Eq. (49) are the

integrals

$$\sum_{m'} {}^{\pm}\langle j,m|n_i|j',m'\rangle^{\pm\pm}\langle j',m'|n_i|j,m\rangle^{\pm} = \frac{2j+3}{4(j+1)}\delta_{j,j'-1} + \frac{2j-1}{4j}\delta_{j,j'+1}, \tag{A49}$$

$$\sum_{m'} {}^{\mp}\langle j,m|n_i|j',m'\rangle^{\pm\pm}\langle j',m'|n_i|j,m\rangle^{\mp} = \frac{1}{4j(j+1)}\delta_{j,j'}, \tag{A50}$$

$$\sum_{m'}\langle l,m|n_i|l',m'\rangle\langle l',m'|n_i|l,m\rangle = \frac{l}{2l+1}\delta_{l',l-1} + \frac{l+1}{2l+1}\delta_{l',l+1}, \tag{A51}$$

and

$$\sum_{m'}\langle l,m|n_i n_j|l',m'\rangle\langle l',m'|n_i n_j|l,m\rangle = \delta_{l',l}\frac{2l^2+2l-1}{(2l-1)(2l+3)} + \delta_{l',l-2}\frac{l(l-1)}{(2l-1)(2l+1)} + \delta_{l',l+2}\frac{(l+1)(l+2)}{(2l+3)(2l+1)}. \tag{A52}$$

7. Action of the momentum operator on the reference states

For the evaluation of the first term in Eq. (49) it is advantageous to use the identity

$$\langle P_i f(H) P_i\rangle = \tfrac{1}{4}\langle X_i H^2 f(H) X_i\rangle \tag{A53}$$

following from Eqs. (42) and (A1) and then use Eqs. (A49) and (A50).

For the evaluation of the sixth term and parts of the third, fourth, and seventh terms in Eq. (49) we need to determine the action of the momentum operator on the Schrödinger wave functions:

$$\langle l+1,m'|P_i|\psi\rangle = (-imZ\alpha)\langle l+1,m'|n_i|l,m\rangle\left(\frac{d}{dr} - \frac{l}{r}\right)R_{n,l} = (imZ\alpha)\langle l+1,m'|n_i|l,m\rangle \times\left(\frac{1}{l+1}R_{n,l} + \frac{\sqrt{n^2-(l+1)^2}}{(l+1)n}R_{n,l+1}\right) \tag{A54}$$

and

$$\langle l-1,m'|P_i|\psi\rangle = (-imZ\alpha)\langle l-1,m'|n_i|l,m\rangle\left(\frac{d}{dr} + \frac{l+1}{r}\right)R_{n,l} = (-imZ\alpha)\langle l-1,m'|n_i|l,m\rangle \times\left(\frac{1}{l}R_{n,l} + \frac{\sqrt{n^2-l^2}}{ln}R_{n,l-1}\right). \tag{A55}$$

Here we used Eqs. (5) and (20) of Ref. [29] and recurrence relations for radial functions, Eqs. (A42) and (A43). Using further orthogonality of the radial functions with the same orbital number l and Eq. (A51) we obtain

$$\langle P_i f(H) P_i\rangle_0 = \frac{(mZ\alpha)^2}{2l+1}\left\{\frac{1}{l+1}\langle f(H_{l+1})\rangle_0 + \frac{1}{l}\langle f(H_{l-1})\rangle_0\right\}, \tag{A56}$$

where the radial Hamiltonians read

$$H_l = 2m(\Pi_0 - m) - P_R^2 + \frac{l(l+1)}{R^2}. \tag{A57}$$

For the S states only the first term in curly brackets on the right member of Eq. (A56) is to be taken.

When evaluating the effect of the interaction of the spin with electromagnetic field, the second term in Eq. (49), we write

$$\langle[\sigma_i,\sigma_j][P_i,\Pi_0]g(H)[P_j,\Pi_0]\rangle_0 = -\frac{1}{4m^2}\langle[\sigma_i,\sigma_j]P_i g(H)H^2 P_j\rangle_0 \tag{A58}$$

and

$$\langle[\sigma_i,\sigma_j]P_i f(H)P_j\rangle_0 = 2\langle\vec\sigma\cdot\vec P f(H)\vec\sigma\cdot\vec P - P_i f(H)P_i\rangle_0 = \frac{-2(mZ\alpha)^2}{2l+1} \times\left\{\left(\frac{1}{l+1}\langle f(H_{l+1})\rangle_0 - \frac{l+1}{l^2}\langle f(H_{l-1})\rangle_0\right)\delta_{p,-1} + \left(\frac{1}{l}\langle f(H_{l-1})\rangle_0 - \frac{l}{(l+1)^2}\langle f(H_{l+1})\rangle_0\right)\delta_{p,1}\right\}, \tag{A59}$$

where

$$l = j - \frac{p}{2}. \tag{A60}$$

For the S states the result is zero. Here the identity

$$\vec\sigma\cdot\vec P = -i(mZ\alpha)\vec\sigma\cdot\vec n\left(\frac{\partial}{\partial r} - \frac{\vec\sigma\cdot\vec L}{r}\right) \tag{A61}$$

and equations for spherical spinors

$$\vec\sigma\cdot\vec n|j,m\rangle^p = -|j,m\rangle^{-p} \tag{A62}$$

and

$$\vec\sigma\cdot\vec L|j,m\rangle^p = \left[p\left(j+\tfrac{1}{2}\right) - 1\right]|j,m\rangle^p \tag{A63}$$

have been used.

To evaluate the expression $\langle P_i X_j f(H) X_j P_i\rangle_0$ that arises in the third and fourth term in Eq. (49) we use an identity

$$iX_i P_j = n_j n_i r\frac{\partial}{\partial r} - \frac{1}{4}[L^2,n_i n_j] + \frac{3n_i n_j - \delta_{ij}}{2} + \frac{i}{2}\epsilon_{ijk}L_k, \tag{A64}$$

Schrödinger limit of Dirac equation $H_l\psi_0 = 0$, and Eq. (A52). One then gets

$$\begin{aligned}\langle P_i X_j f(H) X_j P_i\rangle_0 &= \frac{2l^2+2l-1}{(2l-1)(2l+3)}\left\langle \frac{d}{dr} r f(H_l) r \frac{d}{dr}\right\rangle_0 \\ &+ \frac{(l+1)(l+2)}{(2l+3)(2l+1)}\left\langle \left(\frac{d}{dr}r - l\right) f(H_{l+2}) \left(r\frac{d}{dr} - l\right)\right\rangle_0 \\ &+ \frac{l(l-1)}{(2l-1)(2l+1)}\left\langle \left(\frac{d}{dr}r + l + 1\right)\right. \\ &\left.\times f(H_{l-2})\left(r\frac{d}{dr} + l + 1\right)\right\rangle_0 . \end{aligned} \tag{A65}$$

It follows from the last two equations that

$$\langle P_i X_j f(H) X_j P_i\rangle_0 = \langle P_j X_i f(H) X_j P_i\rangle_0 . \tag{A66}$$

The action of the operator $f(H_l) r \frac{d}{dr}$ on the reference wave function ψ, that arises in the first term on the right member of Eq. (A65) and the fourth and seventh terms in Eq. (49), can be most easily evaluated by means of Eq. (47):

$$f(H_l) r \frac{d}{dr}\psi = -2\frac{f(H_l)}{H_l} E \frac{Z\alpha}{R}\psi, \tag{A67}$$

provided $\frac{f(H_l)}{H_l}|_{H_l=0} = 0$. In the second and third terms of Eq. (A65) we use Eqs. (A43) and (A42), respectively. Finally, the fifth term in Eq. (49) is evaluated by means of Eqs. (A54), (A55), and (A51), and either Eq. (A67) or equation

$$\begin{aligned}\frac{d}{dr}R_{n,l} = \frac{1}{(2l+1)n}&(\sqrt{n^2-l^2}R_{n,l-1} \\ &- \sqrt{n^2-(l+1)^2}R_{n,l+1}).\end{aligned} \tag{A68}$$

The last equation follows from adding Eq. (A42) multiplied by l and Eq. (A43) multiplied by $l+1$.

In this way all the terms in Eq. (49) involving action of the momentum or radial momentum operators on the reference wave function can be reduced to the integrals of the form $\int_0^\infty dr\, r^{2+p} R_{n,l} R_{n',l'}$. As described above these are evaluated by means of Eqs. (A44) and (A46).

APPENDIX B: EVALUATION OF HIGH-ENERGY PART

In the first part of this Appendix it is shown how to get from Eqs. (41) to (53). The second part deals with the reduction of the reference wave function to the upper components.

1. Evaluation of averages

Equation (41) is evaluated by means of repeated use of the Dirac equations (3) and (A1) and an operator identity

$$ACB + BCA = ABC + CBA - [A,[B,C]]. \tag{B1}$$

For the special case $A = B$ we get from Eq. (B1)

$$ACA = \tfrac{1}{2}(\{A^2,C\} - [A,[A,C]]). \tag{B2}$$

When evaluating the averages of the operators in Eq. (41) we first derive the covariant result and only then apply it to the case of Coulomb field (4).

In the following we shall need the identity following from Eq. (6):

$$\begin{aligned}\langle[\Pi_\nu,[\Pi_\nu,H]]\rangle &= 2\langle m[\Pi_\nu,[\Pi_\nu,\Pi_\lambda]]\gamma_\lambda + [\Pi_\lambda,\Pi_\nu][\Pi_\lambda,\Pi_\nu]\rangle \\ &= -2\langle m[P_i,[P_i,\Pi_0]]\gamma_0 + 2[P_i,\Pi_0][P_i,\Pi_0]\rangle .\end{aligned} \tag{B3}$$

The individual terms in Eq. (41) can then be evaluated as follows:

$$\frac{1}{m^2}\langle\tilde{\Pi}^2\rangle = -\frac{1}{4m^2}\langle[\gamma_\mu,\gamma_\nu][\Pi_\mu,\Pi_\nu]\rangle = -\frac{1}{m^2}\langle\gamma_0\gamma_j[P_j,\Pi_0]\rangle, \tag{B4}$$

$$\begin{aligned}\frac{1}{6m^3}\langle\overline{\tilde{\Pi}^2\Pi_\nu}\gamma_\nu\rangle &= \frac{1}{6m^3}\left\langle\left(\frac{3}{2}\{\tilde{\Pi}^2,\Pi_\nu\} - \frac{1}{2}[\Pi_\mu,[\Pi_\mu,\Pi_\nu]]\right)\gamma_\nu\right\rangle \\ &= -\frac{1}{8m^2}\langle[\gamma_\mu,\gamma_\nu][\Pi_\mu,\Pi_\nu]\rangle - \frac{1}{12m^3}\langle[\Pi_\mu,[\Pi_\mu,\Pi_\nu]]\gamma_\nu\rangle \\ &= -\frac{1}{2m^2}\langle\gamma_0\gamma_i[P_i,\Pi_0]\rangle + \frac{1}{12m^3}\langle[P_i,[P_i,\Pi_0]]\gamma_0\rangle,\end{aligned} \tag{B5}$$

$$\begin{aligned}-\frac{1}{4m^3}\langle\{\gamma_\mu,\{\Pi_\mu,H\}\}\rangle &= \frac{1}{4m^3}\langle[\Pi_\mu,[\gamma_\mu,H]]\rangle \\ &= \frac{1}{2m^3}\langle[\Pi_\mu,[\Pi_\mu,\Pi_\lambda]]\gamma_\lambda\rangle \\ &= -\frac{1}{2m^3}\langle[P_i,[P_i,\Pi_0]]\gamma_0\rangle,\end{aligned} \tag{B6}$$

$$\begin{aligned}\frac{1}{16m^3}&\langle\{\gamma_\nu,[\gamma_\mu,\{[\gamma_\mu,H],\Pi_\nu\}]\}\rangle \\ &= \frac{1}{8m^3}\langle\{\gamma_\nu,[\gamma_\mu,\gamma_\lambda]\}\{[\Pi_\mu,\Pi_\lambda],\Pi_\nu\}\rangle \\ &= \frac{1}{8m^3}\langle[\gamma_\nu,[\gamma_\mu,\gamma_\lambda]][\Pi_\mu,\Pi_\lambda]\Pi_\nu \\ &\quad + [[\gamma_\mu,\gamma_\lambda],\gamma_\nu]\Pi_\nu[\Pi_\mu,\Pi_\lambda] + 4m[\gamma_\mu,\gamma_\lambda][\Pi_\mu,\Pi_\lambda]\rangle \\ &= -\frac{1}{m^3}\langle[\Pi_\nu,[\Pi_\nu,\Pi_\lambda]]\gamma_\lambda\rangle + \frac{1}{2m^2}\langle[\gamma_\mu,\gamma_\nu][\Pi_\mu,\Pi_\nu]\rangle \\ &= \frac{1}{m^3}\langle[P_i,[P_i,\Pi_0]]\gamma_0\rangle + \frac{2}{m^2}\langle\gamma_0\gamma_i[P_i,\Pi_0]\rangle,\end{aligned} \tag{B7}$$

$$\begin{aligned}-\frac{1}{6m^4}\langle\overline{\tilde{\Pi}^4}\rangle &= -\frac{1}{6m^4}\left\langle 3\tilde{\Pi}^2\tilde{\Pi}^2 + \frac{1}{2}[\Pi_\mu,\Pi_\nu][\Pi_\mu,\Pi_\nu]\right. \\ &\quad \left. - [\Pi_\mu,[\Pi_\mu,\tilde{\Pi}_\nu\tilde{\Pi}_\nu]]\right\rangle \\ &= -\frac{1}{6m^4}\left\langle\frac{3}{16}[\gamma_\lambda,\gamma_\mu][\Pi_\lambda,\Pi_\mu][\gamma_\rho,\gamma_\nu][\Pi_\rho,\Pi_\nu]\right. \\ &\quad + \frac{1}{2}[\Pi_\lambda,\Pi_\mu][\Pi_\lambda,\Pi_\mu] \\ &\quad \left. - \left[\Pi_\lambda,\left[\Pi_\lambda,H - \frac{1}{4}[\gamma_\rho,\gamma_\nu][\Pi_\rho,\Pi_\nu]\right]\right]\right\rangle \\ &= -\frac{1}{6m^4}\langle 2m[P_i,[P_i,\Pi_0]]\gamma_0 + 6[P_i,\Pi_0][P_i,\Pi_0] \\ &\quad - \gamma_0\gamma_i[P_j,[P_j,[P_i,\Pi_0]]]\rangle,\end{aligned} \tag{B8}$$

$$\frac{1}{24m^5}\langle\{\gamma_\nu,\overline{\tilde\Pi^2\Pi_\nu H}\}\rangle$$
$$=\frac{1}{24m^5}\langle\{\gamma_\nu,2(H\tilde\Pi^2\Pi_\nu+\Pi_\nu\tilde\Pi^2H+\{\tilde\Pi^2,\{\Pi_\nu,H\}\})$$
$$-\{\Pi_\nu,[\Pi_\lambda,[\Pi_\lambda,H]]\}-\{H,[\Pi_\lambda,[\Pi_\lambda,\Pi_\nu]]\}$$
$$-\{[\Pi_\lambda,H],[\Pi_\lambda,\Pi_\nu]\}\}\rangle$$
$$\simeq\frac{1}{12m^5}\langle-8[\Pi_\mu,\Pi_\nu][\Pi_\mu,\Pi_\rho]\gamma_\rho\Pi_\nu-2m[\Pi_\mu,[\Pi_\mu,H]]$$
$$+[\Pi_\mu,[\Pi_\mu,[\Pi_\nu,[\Pi_\nu,\Pi_\rho]]]]\gamma_\rho\rangle$$
$$\simeq\frac{1}{12m^5}\langle4m^2[P_i,[P_i,\Pi_0]]\gamma_0+16m[P_i,\Pi_0][P_i,\Pi_0]$$
$$+[P_i,[P_i,[P_j,[P_j,\Pi_0]]]]\gamma_0\rangle, \tag{B9}$$

$$-\frac{1}{60m^5}\langle\overline{\tilde\Pi^4\Pi_\nu}\gamma_\nu\rangle$$
$$\simeq-\frac{1}{60m^5}\left\langle5m\overline{\tilde\Pi^4}+\frac{1}{2}[\Pi_\mu,[\Pi_\mu,[\Pi_\lambda,[\Pi_\lambda,\Pi_\nu]]]]\gamma_\nu\right\rangle$$
$$=-\frac{1}{60m^5}\langle5m\overline{\tilde\Pi^4}+\frac{1}{2}[P_i,[P_i,[P_j,[P_j,\Pi_0]]]]\gamma_0\rangle, \tag{B10}$$
$$-\frac{1}{96m^5}\langle\{\gamma_\nu,[\gamma_\mu,[\gamma_\mu,\overline{\tilde\Pi^2\Pi_\nu H}]]\}\rangle$$
$$\simeq\frac{1}{12m^5}\langle m[\Pi_\mu,[\Pi_\mu,[\Pi_\nu,\Pi_\rho]]][\gamma_\nu,\gamma_\rho]$$
$$-2[\Pi_\mu,[\Pi_\mu,[\Pi_\nu,[\Pi_\nu,\Pi_\rho]]]]\gamma_\rho\rangle$$
$$=-\frac{1}{6m^5}\langle2m[P_i,[P_i,[P_j,\Pi_0]]]\gamma_0\gamma_j$$
$$+[P_i,[P_i,[P_j,[P_j,\Pi_0]]]]\gamma_0\rangle, \tag{B11}$$

$$-\frac{1}{180m^7}\langle\{\overline{\tilde\Pi^4\Pi_\nu H},\gamma_\nu\}\rangle\simeq-\frac{1}{15m^6}\langle\overline{\tilde\Pi^4H}\rangle, \tag{B12}$$

$$\langle\overline{\tilde\Pi^4H}\rangle$$
$$\simeq\langle-5[\Pi_\mu,H][\Pi_\mu,H]+\Pi_\rho[\Pi_\mu,[\Pi_\mu,[\Pi_\nu,[\Pi_\nu,\Pi_\rho]]]]\rangle$$
$$\simeq\langle20m^2[P_i,\Pi_0][P_i,\Pi_0]+m[P_i,[P_i,[P_j,[P_j,\Pi_0]]]]\rangle, \tag{B13}$$

$$\frac{1}{45m^6}\langle\overline{\tilde\Pi^6}\rangle\simeq\frac{1}{45m^6}\left\langle-\frac{15}{2}[\Pi_\mu,H][\Pi_\mu,H]\right.$$
$$\left.+3\Pi_\rho[\Pi_\mu,[\Pi_\mu,[\Pi_\nu,[\Pi_\nu,\Pi_\rho]]]]\right\rangle$$
$$\simeq\frac{1}{45m^6}\langle30m^2[P_i,\Pi_0][P_i,\Pi_0]$$
$$+3m[P_i,[P_i,[P_j,[P_j,\Pi_0]]]]\rangle, \tag{B14}$$

and

$$\frac{1}{630m^7}\langle\overline{\tilde\Pi^6\Pi_\nu}\gamma_\nu\rangle\simeq\frac{1}{90m^6}\langle\overline{\tilde\Pi^6}\rangle. \tag{B15}$$

By inserting Eqs. (B4)–(B15) into Eq. (41) we get Eq. (53).

2. Reduction of the reference wave function to the upper components

Using the solution of the Dirac equation (A38), the first term in Eq. (53) can be evaluated exactly:

$$\langle\gamma_0\gamma_i[P_i,\Pi_0]\rangle$$
$$=-(EZ\alpha)^2N_\pm^2\left[\frac{(Z\alpha)^2}{K}\left(A_\pm^2\int_0^\infty dr\,R^2_{n,|\Gamma|-\frac{1}{2}(1\pm1)}+B_\pm\int_0^\infty dr\,R^2_{n,|\Gamma|-\frac{1}{2}(1\mp1)}\right)+2A_\pm B_\pm Z\alpha\int_0^\infty dr\,R_{n,|\Gamma|-1}R_{n,|\Gamma|}\right]. \tag{B16}$$

Except for this first term, the expressions in Eq. (53) are for the states with $j=1/2$ divergent. However, when the Dirac wave function is reduced to the upper components with the accuracy up to the order $(Z\alpha)^3$ then Eq. (53) yields a finite result for the normalized difference of the S states and for the P states.

To reduce the wave function to the upper components we write

$$\psi=e^{-S}\psi_{\rm FW}, \tag{B17}$$

where $\psi_{\rm FW}$ contains the upper components only. The operator S is given as (see, e.g., [12])

$$S\simeq\frac{\vec\gamma\cdot\vec P}{2m}-\frac{\gamma_0\vec\gamma\cdot[\vec P,\Pi_0]}{4m^2}-\frac{\vec\gamma\cdot\vec PP^2}{6m^3}. \tag{B18}$$

Let O be an operator at least of the order $(Z\alpha)^3$. With accuracy up to the order $(Z\alpha)^6$ we get [recall Eq. (57) for notation used]

$$\langle O\rangle=\langle e^S\gamma_0Oe^{-S}\rangle_{\rm FW}\simeq\left\langle O+[S,\gamma_0O]+\frac{1}{2!}[S,[S,\gamma_0O]]+\frac{1}{3!}[S,[S,[S,\gamma_0O]]]\right\rangle_{\rm FW}. \tag{B19}$$

To reduce the wave function to the upper components with needed accuracy, we note that the terms $\langle\gamma_0\vec\gamma\cdot[\vec P,\Pi_0]\rangle$, $\langle\gamma_0[P_j,[P_j,\Pi_0]]\rangle$, and $\langle[P_k,[P_k,[P_j,\Pi_0]]]\gamma_0\gamma_j\rangle$ in Eq. (53) are at least of the order $(Z\alpha)^3$, $(Z\alpha)^4$, and $(Z\alpha)^5$, respectively.

Using Eqs. (B18) and (B19) we get with the accuracy at least of the order $(Z\alpha)^6$ Eqs. (55), (56), and

$$\langle\gamma_0\vec\gamma\cdot[\vec P,\Pi_0]\rangle\simeq\left\langle\frac{1}{2m}[\vec\gamma\cdot\vec P,[\vec\gamma\cdot\vec P,\Pi_0]]\right\rangle_{\rm FW}+\left\langle\frac{1}{3!(2m)^3}[\vec\gamma\cdot\vec P,[\vec\gamma\cdot\vec P,[\vec\gamma\cdot\vec P,[\vec\gamma\cdot\vec P,\Pi_0]]]]\right.$$
$$\left.-\frac{1}{6m^3}[\vec\gamma\cdot\vec PP^2,[\vec\gamma\cdot\vec P,\Pi_0]]-\frac{1}{4m^2}[\gamma_0\vec\gamma\cdot\vec P,[\vec\gamma\cdot\vec P,\Pi_0]]\right\rangle_0. \tag{B20}$$

Inserting

$$\langle[\vec{\gamma}\cdot\vec{P},[\vec{\gamma}\cdot\vec{P},[\vec{\gamma}\cdot\vec{P},[\vec{\gamma}\cdot\vec{P},\Pi_0]]]]\rangle_0 = 4\langle[P_j,[P_j,\Pi_0]]P^2 + m[P_j,\Pi_0][P_j,\Pi_0] + [\sigma_k,\sigma_j][P_j,\Pi_0]P_kP^2\rangle_0, \tag{B21}$$

$$\langle[\vec{\gamma}\cdot\vec{P}P^2,[\vec{\gamma}\cdot\vec{P},\Pi_0]]\rangle_0 = \langle-[P_j,[P_j,\Pi_0]]P^2 + 2m[P_j,\Pi_0][P_j,\Pi_0] - [\sigma_k,\sigma_j][P_j,\Pi_0]P_kP^2\rangle_0, \tag{B22}$$

and

$$\langle[\gamma_0\vec{\gamma}\cdot\vec{P},[\vec{\gamma}\cdot\vec{P},\Pi_0]]\rangle_0 = -2\langle[P_j,\Pi_0][P_j,\Pi_0]\rangle_0 \tag{B23}$$

into Eq. (B20) yields Eq. (54).

APPENDIX C: LOGARITHMIC TERMS

Since h is proportional to $(Z\alpha)^2$, the terms contained in the functions ϕ that are proportional to $\ln h$ yield for the state-dependent part of the S states and non-S states the $A_{61}(Z\alpha)^2\ln(Z\alpha)^{-2}$ term in the expansion (8) and for the state-independent part of the S states the $A_{41}\ln(Z\alpha)^{-2}$ term. For example, when ϕ_0 is expanded in series in h the first term is $-h\ln(h)$. When we are interested only in the terms proportional to $\ln(Z\alpha)^2$ we can replace ϕ_0 in Eq. (40) by $-h\ln(Z\alpha)^2$. Similarly, $\tilde{\phi}_2$ can be replaced in Eq. (40) by $h^3m^23^{-1}\ln(Z\alpha)^2$, and so on. That means that the terms in Eq. (40) proportional to $\ln(Z\alpha)^2$ contain just powers of h and by virtue of Eq. (34) their evaluation can be performed in the same way as evaluation of the terms in the high-energy part. Taking advantage again of Eqs. (37) and (A1) and using the explicit form of the functions ϕ, Eqs. (25) and (26), one can determine the logarithmic terms contained in Eq. (40):

$$\ln(Z\alpha)^2\left\langle -\frac{1}{2m^3}[\Pi_\mu,[\gamma_\mu,H]] - \frac{1}{3m^4}\overline{\tilde{\Pi}^2H} + \frac{1}{6m^5}[\Pi_\mu,[\gamma_\mu,\overline{\tilde{\Pi}^2H}]] + \frac{1}{15m^6}\overline{\tilde{\Pi}^4H} - \frac{1}{48m^4}\{\gamma_\nu,[\gamma_\mu,[\gamma_\mu,\overline{\Pi_\nu H^2}]]\}\right\rangle. \tag{C1}$$

To evaluate this expression we use in the first term Eq. (A17) and in the second term Eqs. (A1), (B2), and (B3). Further, we use Eqs. (B13),

$$\begin{aligned}\langle[\Pi_\mu,[\gamma_\mu,\overline{\tilde{\Pi}^2H}]]\rangle &\simeq \langle 12[\Pi_\mu,\Pi_\nu][\Pi_\mu,\Pi_\rho]\gamma_\rho\Pi_\nu - [\Pi_\mu,[\Pi_\mu,[\Pi_\nu,[\Pi_\nu,\Pi_\rho]]]]\gamma_\rho\rangle\\ &\simeq -\langle 12m[P_i,\Pi_0][P_i,\Pi_0] + [P_i,[P_i,[P_j,[P_j,\Pi_0]]]]\gamma_0\rangle\end{aligned} \tag{C2}$$

and

$$\langle\{\gamma_\nu,[\gamma_\mu,[\gamma_\mu,\overline{\Pi_\nu H^2}]]\}\rangle \simeq 0. \tag{C3}$$

By inserting these equations into Eq. (C1) we get

$$\ln(Z\alpha)^2\left\{\frac{2}{3m^3}\langle[P_j,[P_j,\Pi_0]]\gamma_0\rangle - \left\langle\frac{4}{3m^4}[P_j,\Pi_0][P_j,\Pi_0] + \frac{1}{10m^5}[P_k,[P_k,[P_j,[P_j,\Pi_0]]]]\right\rangle_0\right\}. \tag{C4}$$

Further, by reducing the reference wave function to the upper components, Eq. (55), we obtain

$$\begin{aligned}\ln(Z\alpha)^2\Bigg\{&\frac{2}{3m^3}\langle[P_j,[P_j,\Pi_0]]\rangle_{\rm FW} - \Bigg\langle\frac{4}{3m^4}[P_j,\Pi_0][P_j,\Pi_0] + \frac{11}{60m^5}[P_k,[P_k,[P_j,[P_j,\Pi_0]]]]\\ &+ \frac{1}{12m^5}[\sigma_k,\sigma_j][P_m,[P_m,[P_j,\Pi_0]]]P_k\Bigg\rangle_0\Bigg\}.\end{aligned} \tag{C5}$$

This expression for the logarithmic terms is the same as the one in Ref. [12], Eq. (3.36).

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[1] 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 $A\cdot B = A_\nu B_\nu = A_0B_0 - \vec{A}\cdot\vec{B}$. 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. When integrating over k_0 in Eq. (2) 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 1/137.035 999 11 given in Ref. [4].

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