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Nonrelativistic QED expansion for the electron self-energy

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The recently proposed relativistic multipole expansion (RME) of the self-energy effect suggests some observations on the nonrelativistic expansion of the effect. First, the nature of the series for the one-loop self-energy of an electron bound by the Coulomb field of the nucleus is clarified. It is shown that the expansion of the energy shift caused by the self-energy effect contains terms of the form $\alpha(Z\alpha)^7\ln(Z\alpha)$, $\alpha(Z\alpha)^8\ln^3(Z\alpha)$, $\alpha(Z\alpha)^9\ln^2(Z\alpha)$, $\alpha(Z\alpha)^{10}\ln^4(Z\alpha)$, and so on. Here Z is the charge of the nucleus. The origin of these terms is traced back to the logarithmic divergence of the Dirac S-wave function at the origin. These terms eventually lead to breakdown of the nonrelativistic quantum electrodynamics approach. Second, at leading order relativistic multipole expansion requires an evaluation of the "extended Bethe logarithm" (EBL). When expanded in series in $Z\alpha$ EBL reduces at leading order to the ordinary Bethe logarithm. However, it is argued that it is both more accurate and easier to calculate the EBL than the ordinary Bethe logarithm. Both variants of the Bethe logarithm can be calculated by means of the pseudostate method. An improvement of this method is suggested. Finally, the contribution of the combined self-energy vacuum polarization contribution to the Lamb shift in muonic hydrogen for the $1s$-$4s$ and $2p$-$4p$ states by means of the EBL is calculated. For cases that had already been calculated the results reported here are more accurate than the previous ones.

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I. INTRODUCTION

Quantum electrodynamical (QED) effects shift the atomic spectral lines by an amount that is smaller only by the factor $\alpha\ln(Z\alpha)^{-2}$ than leading-order relativistic and magnetic effects. Therefore, if accurate determination of the positions of the spectral lines is sought, they have to be taken into account.

Calculation of these effects is far from trivial. The reason is that they belong to a class of problems involving more than one significant scale. On the simplest level, there are at least two distinct regions: highly relativistic and nonrelativistic regions. Both of these regions have to be simultaneously described with sufficient accuracy. A way to deal with this difficulty that has received much attention is nonrelativistic quantum electrodynamics (NRQED). Originally proposed by Caswell and Lepage [1], it flourished in the hands of Pachucki and coworkers (for the latest developments see, e.g., [2]). The method is based on integrating out high-energy degrees of freedom and constructing an effective nonrelativistic Hamiltonian H_0 and corrections to this Hamiltonian:

$$H = m\alpha^2(H_0 + \alpha^2 H^{(4)} + \alpha^3 H^{(5)} + \alpha^4 H^{(6)} + \alpha^5 H^{(7)} + \cdots). \tag{1}$$

Here $H^{(4)}$ contains the most important relativistic and magnetic effects. QED starts to contribute in $H^{(5)}$. Further, $H^{(5)}$, $H^{(7)}$, and so on contain also logarithmic terms. More precisely, part of $H^{(5)}$ is proportional to $\ln\alpha$. Further, $H^{(7)}$ contains a term of the order of unity, a term proportional to $\ln\alpha$, and a term proportional to $\ln^2\alpha$. Not much is known about the logarithmic dependence of additional terms. The above Hamiltonian is then treated by the standard perturbation method of nonrelativistic quantum mechanics.

Recently, relativistic multipole expansion (RME) of the self-energy effect has been proposed [3–5]. This expansion leads to the following two observations about NRQED. First, we clarify the nature of the series for the one-loop self-energy of an electron bound in the Coulomb field of the nucleus. This also clarifies the structure of series (1). Second, evaluation of $H^{(5)}$ involves a rather difficult calculation of the so-called Bethe logarithm [6,7], here called the ordinary Bethe logarithm (OBL). The problem becomes especially severe when considering two- and three-electron atoms [8,9] or higher-order QED effects [10]. We point out that RME enables the calculation of the quantity we call the extended Bethe logarithm (EBL). We show that calculation of this quantity is much less computationally demanding than that of the OBL. Moreover, this quantity provides a much better approximation to the energy shift caused by QED effects than the OBL does. We show the utility of the EBL by calculating the combined self-energy vacuum polarization effect in muonic hydrogen, which is known to be difficult to evaluate by means of the OBL [11].

Both variants of the Bethe logarithm have to be, in general, calculated numerically. The method of pseudostates, the expansion of the exact wave functions into entirely discrete basis sets, is one of the most often used methods in atomic calculation in general. In general, the method has problems evaluating accurately expressions whose significant contribution is given by the upper part of the continuous spectrum. The Bethe logarithm is a prime example of such a situation [7]. We show that this problem can be cured by splitting the pertinent expression into two parts. The first part is evaluated exactly; the second part, by the method of pseudostates. In the first part, one expands about the free-particle solution. In the second part the contribution of the upper part of the continuous spectrum is strongly suppressed. This procedure does not work generally, but a number of important cases are solved by it very efficiently.

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The paper is organized as follows. In Sec. II the role of relativistic corrections in the self-energy effect is elucidated. The following Sec. III, sets the stage for further considerations. The expressions to be evaluated are given and motivated there. Namely, the EBL, OBL, and Uehling potential created by vacuum polarization are introduced. In Sec. IV the method of pseudostates is described and used for evaluation of the EBL for a particle moving in the Coulomb potential and for a particle moving in the Coulomb potential perturbed by the Uehling potential. Section V reports conclusions. The Appendixes are devoted to some technical details needed in Secs. II and IV.

II. ROLE OF RELATIVISTIC CORRECTIONS IN THE SELF-ENERGY EFFECT

It is customary to write the ground-state energy shift caused by the self-energy effect for a hydrogenlike atom in the limit of an infinitely massive nucleus in the form

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

where the dimensionless function $F(Z\alpha)$ can be written in the form of a series in $Z\alpha$,

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

where the series for the remainder function $G(Z\alpha)$ has been supposed to have the form

$$G(Z\alpha) = A_{60} + (Z\alpha)[\ln(Z\alpha)^{-2}A_{71} + A_{70}] + \cdots . \tag{3}$$

The known coefficients A are summarized, e.g., in [12,13]. The form of the coefficient A_{70} is unknown. The form of the series beyond the displayed term is not known.

In this section we show that the RME enables us to determine some of the general properties of the series, Eq. (3). The basic idea of the RME method is to expand the electron propagator in powers of the difference between the four-momentum of the virtual electron and the four-momentum of the electron at rest [3–5]. After integrating out four-momenta of the virtual photon by means of Feynman parameters one is left only with summation and integration over the discrete and continuous part of the hydrogen spectrum and integration over two Feynman parameters. The summation over the discrete part of the hydrogen spectrum does not bring any additional interesting features. After subtracting the terms contributing at the leading order, $m\alpha(Z\alpha)^4$ and $m\alpha(Z\alpha)^4\ln(Z\alpha)^{-2}$, we are left with a generic integral,

$$m\frac{\alpha(Z\alpha)^6}{\pi}C_0\int_0^1 dw f(w)\int_0^1 dy y^u\int_0^\infty dk_e \times\frac{k_e^{-2l_0}}{y+a\left(1+k_e^2\right)}\left(1+\frac{C_1 k_e}{1+k_e^2}+\cdots\right), \tag{4}$$

where $u \geqslant 0$ depends of the order of the RME. The parameters C_0 and C_1 are some complicated functions of quantum numbers of intermediate states, the pertinent order of the RME, and so on. Here a stands for

$$a = w(Z\alpha)^2. \tag{5}$$

Further, k_e are the electron wave numbers of the continuous spectrum and y and w are the Feynman parameters; $f(w)$ is some polynomial function of w. Furthermore, l_0 stands for relativistic angular number of the S-states

$$l_0 = \sqrt{1-(Z\alpha)^2} - 1. \tag{6}$$

This number will be of greatest importance in the following considerations. It enters into Eq. (4) through the overlap integrals between the Dirac ground-state wave function of hydrogen

$$\psi_{1s} \sim \exp\{-r/(l_0+1)\}\, r^{l_0} \tag{7}$$

and the wave functions of the hydrogen intermediate states;see Eqs. (21) and (49) in [5]. In Appendix A we show that the integrals, Eq. (4), can be arrived at by Eqs. (42), (48), (49), (56), (59), and (66) in [5] and further manipulation of the resulting expression. In particular, the denominator $y + a(1 + k_e^2)$ originates from the spectral decomposition of the electron propagator in intermediate states. Further, we explicitly display the first two terms in the asymptotic expansion of the integrand in Eq. (4) for large wave numbers k_e. The expansion has its origin in the expansion of the electron propagator in powers of the interactions of an electron with the Coulomb potential created by the nucleus.

Because of the factor r^{l_0}, the Dirac wave function, (7), diverges logarithmically at the origin. This mild divergence makes it appearance through the factor $k_e^{-2l_0}$ in the integrand of expression (4). Comparing the Dirac wave function with the Schrödinger wave function, $\psi_{1s}^{(0)} \sim \exp\{-r\}$, it is seen that the latter is finite at the origin. The appearance of the factor $k_e^{-2l_0}$ in Eq. (4) is thus a relativistic effect.

Consider first the case $u = 0$ in Eq. (4). We investigate the $Z\alpha$ expansion of the integrals

$$I_0 = \int_0^1 dy\int_0^\infty dk_e\frac{k_e^{-2l_0}}{y+a\left(1+k_e^2\right)},$$

$$I_1 = \int_0^1 dy\int_0^\infty dk_e\frac{k_e^{1-2l_0}}{\left(1+k_e^2\right)\left[y+a\left(1+k_e^2\right)\right]}. \tag{8}$$

We first integrate over k_e:

$$\int_0^\infty dk_e\frac{k_e^{-2l_0}}{y+a\left(1+k_e^2\right)} = \frac{\pi}{2}\frac{a^{l_0-1/2}(a+y)^{-1/2-l_0}}{\cos(\pi l_0)} \tag{9}$$

and

$$\int_0^\infty dk_e\frac{k_e^{1-2l_0}}{\left(1+k_e^2\right)\left[y+a\left(1+k_e^2\right)\right]} = -\frac{\pi}{2}\frac{a^{l_0}(a+y)^{-l_0}-1}{\sin(\pi l_0)y}.$$

Next we integrate over y:

$$\int_0^1 dy\left(1+\frac{y}{a}\right)^{-1/2-l_0} = \frac{a}{1/2-l_0}\left[-1+\exp\left\{(1/2-l_0)\ln\left(\frac{1+a}{a}\right)\right\}\right]$$

and

$$\int_0^1 dy\frac{\left(1+\frac{y}{a}\right)^{-l_0}-1}{y} = \ln(a) - \Psi(l_0) - \gamma - \frac{\exp\{l_0\ln(a)\}}{l_0} \times F(l_0,l_0,l_0+1,-a).$$

Here Ψ denotes the logarithmic derivative of the Γ function, $\Psi(z) = d\ln\Gamma(z)/dz$. Expanding these expressions now in powers of $Z\alpha$ we get

$$\begin{aligned}\frac{I_0}{\pi} &= \frac{1}{Z\alpha w^{1/2}} - 1 - \frac{Z\alpha}{2w^{1/2}}\{2 - w + \ln[w(Z\alpha)^2]\}\\ &\quad + (Z\alpha)^2 + \frac{(Z\alpha)^3}{8w^{1/2}}\{\ln^2[w(Z\alpha)^2] + \cdots\}\\ &\quad + \cdots - \frac{(Z\alpha)^5}{48w^{1/2}}\{\ln^3[w(Z\alpha)^2] + \cdots\} + \cdots\end{aligned} \tag{10}$$

and

$$\begin{aligned}I_1 &= \frac{\pi^2}{12} + \frac{\ln^2[w(Z\alpha)^2]}{4}\\ &\quad + (Z\alpha)^2\left\{-\frac{\ln^3[w(Z\alpha)^2]}{24} - \frac{w}{2} + \frac{\zeta(3)}{4}\right\}\\ &\quad + \frac{15(Z\alpha)^4}{2880}\{\ln^4[w(Z\alpha)^2] + \cdots\} + \cdots .\end{aligned} \tag{11}$$

Now, the remainder function $G(Z\alpha)$ is given by a linear combination of the integrals, Eq. (4). Therefore, the structure of the series for the remainder function $G(Z\alpha)$ is determined by the structure of the series for the integrals, Eq. (4). It turns out that the worst nonanalyticies in $Z\alpha$ are present for just the considered case $u = 0$. It is not difficult to convince oneself that the $Z\alpha$ expansion of the integrals, Eq. (4), is less complex for $u > 0$ than for $u = 0$. Therefore, it follows from the foregoing that the remainder function $G(Z\alpha)$ has the form

$$\begin{aligned}G(Z\alpha) &= A_{60} + (Z\alpha)[\ln(Z\alpha)^{-2}A_{71} + A_{70}]\\ &\quad + (Z\alpha)^2[\ln^3(Z\alpha)^{-2}A_{83} + \ln^2(Z\alpha)^{-2}A_{82}\\ &\quad + \ln(Z\alpha)^{-2}A_{81} + A_{80}]\\ &\quad + (Z\alpha)^3[\ln^2(Z\alpha)^{-2}A_{92} + \ln(Z\alpha)^{-2}A_{91}\\ &\quad + A_{90}] + \cdots .\end{aligned} \tag{12}$$

Now comparing Eqs. (4), (10), and (11) with Eq. (12) we see that the particular case $u = 0$ yields the ratios

$$\begin{aligned}&\frac{A_{71}}{A_{50}} = \frac{1}{2}, \quad \frac{A_{92}}{A_{50}} = \frac{1}{8}, \quad \frac{A_{11,3}}{A_{50}} = \frac{1}{48},\\ &\frac{A_{83}}{A_{62}} = \frac{1}{6}, \quad \frac{A_{10,4}}{A_{62}} = \frac{1}{48},\end{aligned} \tag{13}$$

and so on. Here $A_{10,4}$ and $A_{11,3}$ are coefficients in front of terms of the order $\alpha\,(Z\alpha)^{10}\ln^4(Z\alpha)^{-2}$ and $\alpha\,(Z\alpha)^{11}\ln^3(Z\alpha)^{-2}$ in Eq. (3), respectively.

Now these ratios hold not just for the particular case $u = 0$, but for the whole remainder function $G(Z\alpha)$. The point is that *the ratios* A_{71}/A_{50}, A_{83}/A_{62}, *and so on, are determined solely by the presence of the factor* $k_e^{-2I_0}$ *in expression (4)*. It is not difficult to convince oneself that a nonzero contribution to A_{62} is obtained only for $u = 0$ in Eq. (4). The coefficient A_{62} will generally depend on the precise form of C_0, C_1, and the functions $f(w)$, but the ratios in Eq. (13) clearly not. This is seen directly from Eq. (11). Likewise, the coefficient A_{50} will generally depend on C_0, C_1, $f(w)$, and u, but the ratios in Eq. (13) not. To see this, it suffices to expand the right-hand side (r.h.s.) of Eq. (9) directly in powers of $Z\alpha$. One finds that the ratios A_{71}/A_{50}, A_{92}/A_{50}, and $A_{11,3}/A_{50}$ displayed in Eq. (13) are independent of both integrations over the Feynman parameters y and w. Additional terms on the r.h.s. of Eq. (4) do not influence values of the ratios, (13), either. For the case $u > 0$ we can make the expansion $1/[y + a(1 + k_e^2)] = 1/y + a(1 + k_e^2)/y/[y + a(1 + k_e^2)]$. The first term contributes to the coefficient A_{60}, Eq. (3); the contribution of the second term is suppressed with respect to that given by expression (4) by a factor of $(Z\alpha)^2$. For the case $u = 0$ the lower bound of the integration over y contributes to the coefficients A_{61} and A_{60}, Eq. (3). For the upper bound of the integration over y the situation is the same as for the case $u > 0$. Thus, *the ratios in Eq. (13) are the exact ratios for the coefficients of series (12) for the whole remainder function* $G(Z\alpha)$.

The first relation in Eq. (13) has been noted by Karshenboim [14]. The others are not known.

NRQED is based on the successive generation of individual terms in series (1). The above result shows that this program eventually breaks down: for $\alpha\ln^3(\alpha)^{-2} \simeq 6.95 > 1$. Thus it does not appear meaningful to calculate the coefficient A_{70} and neglect A_{83}. Nobody has been able to do so, anyway. With increasing powers of α the power of logarithmic terms increases [see Eq. (12)], but their numerical coefficients decrease [see Eq. (13)]. The influence of the logarithmic terms seems to be slight.

III. EXTENDED BETHE LOGARITHM

A. Energy shift caused by the self-energy effect

The leading order of the RME yields the self-energy effect of the bound particle in the form [4]

$$\Delta E = \Delta E_{\text{low}} + \Delta E_{\text{high}}, \tag{14}$$

$$\begin{aligned}\Delta E_{\text{low}} &= \frac{\alpha}{\pi m}\langle\psi|P_i f\left(-\frac{H}{m^2}\right)P_i|\psi\rangle,\\ f(x) &= \frac{x}{2}\int_0^1 dy\int_0^1 dw\,\frac{1 - 2w(1 - w)}{y + wx},\end{aligned} \tag{15}$$

$$\begin{aligned}\Delta E_{\text{high}} &= -\frac{\alpha}{\pi m^2}\langle\psi|\frac{1}{12}[P_j,[P_j,\Pi_0]]\\ &\quad + \frac{1}{8}[\sigma_i,\sigma_j][P_j,\Pi_0]P_i\ |\psi\rangle.\end{aligned} \tag{16}$$

Here

$$H = 2m(\Pi_0 - m) - \vec{P}\cdot\vec{P}, \quad \Pi_0 = E - V, \tag{17}$$

where, as usual, E and ψ denote the energy and wave function of the reference state, respectively. At the leading order they are determined from the Schrödinger equation

$$H\psi = 0.$$

Furthermore, $\vec{P}$ is the momentum of the particle and V the external potential. Equation (15) is given by the first term in Eq. (49) and Eqs. (25), (27), and (30) in [4]. Equation (16) is given by the first two terms in Eq. (53), the first two terms in Eq. (54), and the first term in Eq. (55) of [4]. Corrections to Eqs. (15) and (16) are at least of the order of $Z\alpha$ [4].

Equations (15) and (16) were derived in an external field approximation. To include the dominant part of the recoil effects it suffices to note that Eq. (17) can be written as

$$H = -2m(H_{\mathrm{NR}} - E_{\mathrm{NR}}),$$

where H_{NR} is a nonrelativistic Hamilton operator. At the nonrelativistic level, the recoil effects in two-particle atoms are accounted for by substituting the reduced mass for the particle mass:

$$H_{\mathrm{NR}} = \frac{\vec{P}\cdot\vec{P}}{2m_r} + V, \quad m_r = \frac{mM}{m+M}.$$

Here M is the nuclear mass. Inserting this back into the previous equation and going to atomic units,

$$R = \frac{r}{m_r Z\alpha}, \tag{18}$$

we obtain

$$-\frac{H}{m^2} = 2\frac{m_r}{m}(Z\alpha)^2(h - e_N),$$

where h and e_N are the nonrelativistic Hamilton operator and the energy of the reference state in atomic units. Here, N is the principal quantum number of the reference state. For the Coulomb potential $V = -\frac{Z\alpha}{R}$ one has

$$v(r) = -\frac{1}{r}, \quad h = \frac{p^2}{2} + v(r), \quad e_N = -\frac{1}{2N^2}.$$

Equation (14) then can be written as

$$\Delta E = m\frac{\alpha}{\pi N^3}(Z\alpha)^4\left(\frac{m_r}{m}\right)^3 F(Z\alpha), \quad F = F_{\mathrm{low}} + F_{\mathrm{high}}, \tag{19}$$

where

$$F_{\mathrm{low}} = \langle\psi|p_i f(h - e_N) p_i|\psi\rangle,$$
$$f(x) = N^3 x \int_0^1 dy \int_0^1 dw \frac{1 - 2w(1-w)}{y + w2(Z\alpha)^2\frac{m_r}{m}x}, \tag{20}$$

and

$$F_{\mathrm{high}} = N^3\langle\psi|\left[-\frac{1}{12}\nabla^2 v(r) + \frac{1}{2}\frac{\vec{S}\cdot\vec{L}}{r}\left[\frac{d}{dr},v(r)\right] + \frac{m}{2M}\frac{\vec{S}\cdot\vec{L}}{r^3}\right]|\psi\rangle. \tag{21}$$

Here, the last term, the correction to the coupling between the spin of the electron and the nucleus orbit due to the anomalous magnetic moment of the electron, was included. A more careful derivation of such an inclusion of recoil effects will be given elsewhere. The term F_{low}, Eq. (20), is called here the extended Bethe logarithm. Its relation to the ordinary Bethe logarithm is clarified immediately. The expansion of the function $f(x)$ yields

$$f(x) = N^3 x\left(\frac{13}{8} - \frac{2}{3}\ln\left[2(Z\alpha)^2\frac{m_r}{m}x\right] + \cdots\right). \tag{22}$$

When this is inserted back into Eq. (20), the term

$$\frac{N^3}{2}\langle\psi|p_i(h - e_N)\ln(h - e_N)p_i|\psi\rangle \tag{23}$$

is usually called the Bethe logarithm [6,7].

B. Uehling potential

Two-loop corrections to the Lamb shift in light hydrogen-like atoms are difficult and still a far from solved problem (see, e.g., [10]). Here, we are concerned with the calculation of one of the simplest contributions, namely, contribution of the combined self-energy vacuum polarization effect. These are of two types. First, the vacuum polarization adds to the Coulomb potential the Uehling potential, thus modifying the electron propagator. Second, the vacuum polarization modifies the photon propagator. In muonic hydrogen the significance of these contributions among two-loop corrections is next to that of the pure vacuum polarization contribution and they were estimated in [15]. This estimate was later improved in [11]. Modification of the photon propagator by the vacuum polarization gives the photon an effective mass [see Eqs. (24) and (25) bellow]. This makes the calculation of this correction relatively simple. The former effect, the adddition of the Uehling potential, is much more difficult to evaluate. Furthermore, evaluation is much more difficult for muonic, rather than ordinary, hydrogen. In this paper we are concerned with such an evaluation.

Vacuum polarization modifies the photon propagator in momentum space as

$$\frac{1}{k^2} \to \frac{1}{k^2}[1 + \Pi_2(k^2) - \Pi_2(0)], \tag{24}$$

where (see, e.g., Eq. (7.91) in [16]),

$$\begin{aligned}\frac{\Pi_2(k^2) - \Pi_2(0)}{k^2} &= \frac{1}{k^2}\frac{2\alpha}{\pi}\int_0^1 dx\, x(1-x)\ln\left(1 - \frac{k^2}{m_e^2}x(1-x)\right)\\ &= -\frac{\alpha}{\pi}\int_0^1 dx\frac{x\left(1-\frac{2}{3}x\right)(1-2x)}{1-x}\frac{1}{k^2 - \frac{m_e^2}{x(1-x)}}.\end{aligned} \tag{25}$$

In the latter equality we have used an integration by parts.

For time-independent fields $k_0 = 0$; then $k^2 = -\omega^2$. In this case Fourier transform of (24) and transition to atomic units (18) lead to the modification of the Coulomb potential

$$\begin{aligned}-\frac{1}{r} &\to -\frac{1}{r} + v_U,\\ v_U &= \frac{\alpha}{\pi}\int_0^1 dx\frac{x\left(1-\frac{2}{3}x\right)(1-2x)}{1-x}\frac{e^{-\frac{m_e}{m_r(Z\alpha)}\frac{r}{\sqrt{x(1-x)}}}}{r}\\ &= \frac{\alpha}{\pi}\int_0^1 dx\, U(x)\frac{e^{-\mu(x)r}}{r},\end{aligned} \tag{26}$$

where obviously $U(x) = \frac{x(1-\frac{2}{3}x)(1-2x)}{1-x}$ and $\mu(x) = \frac{m_e}{m_r(Z\alpha)}\frac{1}{\sqrt{x(1-x)}}$. The potential v_U is usually called the Uehling potential. In the case of muonic hydrogen

$$\frac{m_e}{m_r(Z\alpha)} = \frac{m_e\left(1 + \frac{m_\mu}{m_p}\right)}{m_\mu\alpha} \simeq 0.737\,384, \tag{27}$$

where we have inserted [13]

$$\alpha = 1/137.035\,999\,1, \quad \frac{m_e}{m_\mu} = 4.836\,331\,7\times10^{-3},$$
$$\frac{m_e}{m_p} = 5.446\,170\,218\times10^{-4}. \tag{28}$$

There is a distinct difference between ordinary and muonic hydrogen in this case. For ordinary hydrogen the ratio, (27), is about 137 and the Uehling potential is close to the δ function.

IV. THE METHOD OF PSEUDOSTATES

A. Description of the method

The radial part of the nonrelativistic Schrödinger equation for the hydrogen atom,

$$\left[\frac{p_r^2}{2}+\frac{l(l+1)}{2r^2}-\frac{1}{r}\right]R_{n,l}(r/n)=E_nR_{n,l}(r/n), \tag{29}$$

where $p_r=-i(\frac{d}{dr}+\frac{1}{r})$ denotes the radial momentum, has negative-energy (discrete spectra) and positive-energy (continuous spectra) solutions. For spectral decomposition of the Hamilton operator one thus has to use expansion in both parts of the spectra. The continuous part cannot be omitted since in many cases it represents the dominant contribution. A prime example of this is the case of the Bethe logarithm.

Writing the energy in the form $E_n=-1/(2n^2)$ and making the energy-dependent scaling $r\to nr$, Eq. (29) is transformed into the equation

$$\left[\frac{p_r^2}{2}+\frac{l(l+1)}{2r^2}-\frac{n}{r}\right]R_{n,l}(r)=-\frac{1}{2}R_{n,l}(r), \tag{30}$$

where the functions $R_{n,l}(r)$ are usually called the Sturmian functions. As can be seen from comparison of Eqs. (29) and (30) the transformation corresponds to a transition from the case of different energies $E=-1/(2n^2)$ for fixed nuclear charge $Z=1$ to the case of a fixed energy $E=-1/2$ for different nuclear charges $Z=n$. Upon multiplying Eq. (30) by r and rearranging terms one can rewrite it in the form [17]

$$T_3R_{n,l}(r)=nR_{n,l}(r), \tag{31}$$

where the operator T_3 is

$$T_3=\frac{r}{2}\left(p_r^2+\frac{l(l+1)}{r^2}\right)+\frac{r}{2}. \tag{32}$$

The spectrum of this operator is purely discrete. This is seen by noting the existence of ladder operators

$$T_\pm=\frac{r}{2}\left(p_r^2+\frac{l(l+1)}{r^2}\right)-\frac{r}{2}\pm irp_r,\quad [T_3,T_\pm]=\pm T_\pm. \tag{33}$$

By the usual procedure, analogous to that used in the angular momentum theory, one easily proves that [17]

$$n=l+1+K,\quad K=0,1,2,\dots,$$

and

$$T_\pm R_{n,l}=\sqrt{(n\pm l\pm 1)(n\mp l)}R_{n\pm1,l}. \tag{34}$$

It follows from Eqs. (32)–(34) that

$$\begin{aligned}2rR_{n,l}(r)&=(2T_3-T_+-T_-)R_{n,l}(r)\\&=2nR_{n,l}(r)-\sqrt{(n+l+1)(n-l)}R_{n+1,l}(r)\\&\quad-\sqrt{(n-l-1)(n+l)}R_{n-1,l}(r).\end{aligned} \tag{35}$$

The operator T_3 is Hermitian with respect to the inner product with weight r, not r^2,

$$\int_0^\infty dr\,r\,R_{n_1,l}(r)T_3R_{n_2,l}(r)=\int_0^\infty dr\,r\,R_{n_2,l}(r)T_3R_{n_1,l}(r).$$

Thus its eigenfunctions are orthonormal with respect to this inner product,

$$\int_0^\infty dr\,r\,R_{n_1,l}(r)R_{n_2,l}(r)=\delta_{n_1,n_2}. \tag{36}$$

Returning now to Eq. (29) where we multiply the potential by the nuclear charge Z, this time we perform the energy-independent scaling

$$r\to r/\xi$$

and multiply this equation by r/ξ^2. This brings it to the form

$$\left(T_3-\frac{Z}{\xi}\right)\psi_{N,L}=\tilde{E}_Nr\psi_N,\quad \tilde{E}_N=\left(\frac{E_N}{\xi^2}+\frac{1}{2}\right). \tag{37}$$

Inserting the expansion

$$\psi_{N,L}(r)=\sum_{n=L+1}^{L+\nu}c_n^NR_{n,L}(\xi r) \tag{38}$$

into Eq. (37), multiplying the equation by $R_{m,l}(\xi r)$, and taking the inner product between the Sturmian functions, one obtains the generalized eigenvalue problem for the energies $\tilde{E}_N$ and the coefficients c_n^N:

$$\begin{aligned}\left(m-\frac{Z}{\xi}\right)c_m^N&=\tilde{E}_N\sum_nS_{m,n}c_n^N,\\ S_{m,n}&=\int_0^\infty dr\,r^2R_{m,L}(\xi r)R_{n,L}(\xi r).\end{aligned} \tag{39}$$

The overlap integrals $S_{m,n}$ are calculated by means of Eqs. (35) and (36) [see Eq. (C6)]. The eigenstates $\psi_{N,L}$ determined via Eqs. (38) and (39) are called pseudostates.

The spectral decomposition of a function f of the Hamiltonian h is then

$$\langle r|f(h)|r'\rangle=\sum_{N,L}\psi_{N,L}(r)\psi_{N,L}(r')f\left[\left(\tilde{E}_N-\frac{1}{2}\right)\xi^{-2}\right],$$

where the pseudostates $\psi_{N,L}$ are assumed to be normalized as

$$\int_0^\infty dr\,r^2|\psi_{N,L}|^2=1\,.$$

In actual calculations described in Secs. IV D and IV E we set $\xi=1$ in Eq. (37).

B. First-order correction to a function of the Hamilton operator

For a general function of the Hamilton operator one can write the spectral decomposition

$$f(-z+h)=\sum_nP_nf(-z+e_n),$$

where

$$P_n=|\psi_n\rangle\langle\psi_n|. \tag{40}$$

Apparently, e_n and ψ_n are eigenvalues and eigenstates of the Hamiltonian h. Splitting the Hamiltonian into "large" and "small" parts, h_0 and λh_1, respectively,

$$h = h_0 + \lambda h_1, \tag{41}$$

the expansion of the function f in the first order of λ reads

$$\sum_n P^0_n f\left(-z+e^0_n\right) + \lambda\left(P^1_n f\left(-z+e^0_n\right) + P^0_n e^1_n \frac{df\left(-z+e^0_n\right)}{de^0_n}\right) + \cdots . \tag{42}$$

Here

$$P^0_n = |\psi^0_n\rangle\langle\psi^0_n|, \quad P^1_n = |\psi^1_n\rangle\langle\psi^0_n| + |\psi^0_n\rangle\langle\psi^1_n|, \tag{43}$$

and the perturbation energies and wave functions are determined by the well-known formulas

$$\left(h_0 - e^0_n\right)|\psi^0_n\rangle = 0$$

and

$$\left(h_0 - e^0_n\right)|\psi^1_n\rangle = \left(e^1_n - h_1\right)|\psi^0_n\rangle.$$

From the latter equation we have

$$e^1_n = \langle\psi^0_n|h_1|\psi^0_n\rangle \tag{44}$$

and

$$|\psi^1_n\rangle = -\sum_{m\neq n}\frac{|\psi^0_m\rangle\langle\psi^0_m|h_1|\psi^0_n\rangle}{e^0_m - e^0_n}. \tag{45}$$

By inserting Eqs. (43) and (45) into Eq. (42) we obtain that the first correction to the propagator due to the first correction to the wave function reads

$$\begin{aligned}\sum_n P^1_n f\left(-z+e^0_n\right) &= -\sum_{n,m,m\neq n}\Big(|\psi^0_n\rangle\langle\psi^0_n|h_1|\psi^0_m\rangle\langle\psi^0_m| \\ &\quad + |\psi^0_m\rangle\langle\psi^0_m|h_1|\psi^0_n\rangle\langle\psi^0_n|\Big)\frac{1}{\left(e^0_m - e^0_n\right)} f\left(-z+e^0_n\right) \\ &= \sum_{n,m,m\neq n} |\psi^0_m\rangle\langle\psi^0_m|h_1|\psi^0_n\rangle\langle\psi^0_n| \\ &\quad \times \frac{f\left(-z+e^0_m\right) - f\left(-z+e^0_n\right)}{e^0_m - e^0_n}.\end{aligned} \tag{46}$$

C. First-order correction to the EBL

Using the above formulas and assuming that h_1 is spherically symmetric we can write the EBL, Eq. (20), as

$$F_{\text{low}} = F^0_{\text{low}} + \lambda F^1_{\text{low}} + \cdots ,$$

where the unperturbed EBL is given by

$$F^0_{\text{low}} = \sum_{q=l+1}^{Q} \langle\psi^0_{N,L}|p_i|\psi^0_{q,l}\rangle\langle\psi^0_{q,l}|p_i|\psi^0_{N,L}\rangle f\left(e^0_q - e^0_N\right)$$

and the first perturbation to EBL is given by the sum

$$F^1_{\text{low}} = \left(F^1_{\text{low}}\right)_{\text{wf}} + \left(F^1_{\text{low}}\right)_{\text{ver}} + \left(F^1_{\text{low}}\right)_{\text{en}}, \tag{47}$$

where

$$\left(F^1_{\text{low}}\right)_{\text{wf}} = -2\sum_{m=L+1\neq N}^{L+M}\sum_{q=l+1}^{l+Q}\langle\psi^0_{N,L}|h_1|\psi^0_{m,L}\rangle\langle\psi^0_{m,L}|p_i|\psi^0_{q,l}\rangle\langle\psi^0_{q,l}|p_i|\psi^0_{N,L}\rangle\frac{f\left(e^0_q - e^0_N\right)}{e^0_m - e^0_N} \tag{48}$$

comes from the correction to the wave function of the reference state,

$$\begin{aligned}\left(F^1_{\text{low}}\right)_{\text{ver}} = \sum_{q=l+1}^{l+Q}\Bigg\{&\sum_{m=l+1\neq n}^{l+Q}\langle\psi^0_{N,L}|p_i|\psi^0_{m,l}\rangle\langle\psi^0_{m,l}|h_1|\psi^0_{q,l}\rangle\langle\psi^0_{q,l}|p_i|\psi^0_{N,L}\rangle\frac{f\left(e^0_m - e^0_N\right) - f\left(e^0_q - e^0_N\right)}{e^0_m - e^0_q} \\ &+ \langle\psi^0_{N,L}|p_i|\psi^0_{q,l}\rangle\langle\psi^0_{q,l}|h_1|\psi^0_{q,l}\rangle\langle\psi^0_{q,l}|p_i|\psi^0_{N,L}\rangle\frac{df\left(e^0_q - e^0_N\right)}{de^0_q}\Bigg\}\end{aligned} \tag{49}$$

is the vertex correction derived in the previous section [see Eqs. (42), (44), and (46)], and

$$\left(F^1_{\text{low}}\right)_{\text{en}} = \sum_{q=l+1}^{l+Q}\langle\psi^0_{N,L}|p_i|\psi^0_{q,l}\rangle\langle\psi^0_{q,l}|p_i|\psi^0_{N,L}\rangle\frac{df\left(e^0_q - e^0_N\right)}{de^0_q}\langle\psi^0_{N,L}|h_1|\psi^0_{N,L}\rangle \tag{50}$$

comes from the correction to the energy of the reference state.

These formulas are used in the following two sections: first for a free particle perturbed by the Coulomb potential, then for a particle moving in the Coulomb potential perturbed by the Uehling potential.

D. The case of the Coulomb potential

Let us now turn to the calculation of Eq. (20) for the case of a hydrogen atom in the infinite nucleus mass limit. The symmetries of the hydrogen atom allow us to convert expression (20) into a slightly more advantageous form. For the ground state one can write (for the derivation see Appendix D)

$$\begin{aligned}&\langle 1,0,0|p_i f(h-e_1)p_i|1,0,0\rangle\\&\quad=2\langle 1,0,0|\frac{1}{r}\frac{f(h-e_1)}{h-e_1}\frac{1}{r}|1,0,0\rangle.\end{aligned}\tag{51}$$

For the matrix elements of $1/r$ between the ground state and a state $|p,0,0\rangle$ of the continuous part of the spectrum,

$$h|p,0,0\rangle=\frac{p^2}{2}|p,0,0\rangle,\quad h=\frac{p^2}{2}-\frac{Z}{r},\tag{52}$$

one has (see, e.g., [18])

$$\begin{aligned}&2\left|\langle 1,0,0|\frac{1}{r}|p,0,0\rangle\right|^2\\&\quad=\frac{16}{\pi}\frac{p^2}{(p^2+1)^2}\left[1+Z\frac{\pi-4\arctan(p)}{p}+O(1/p^2)\right].\end{aligned}\tag{53}$$

The first term on the r.h.s. corresponds to the case where the exact wave function is replaced by the free-particle function, i.e., setting $Z=0$ in Eq. (52).

Equation (53) clearly shows the problem with numerical evaluation of the Bethe logarithm, Eq. (23). When integrating over the continuous part of the spectrum, the integrand behaves for large p as $\ln(p^2)/p^2$. The integral over the continuous part of the spectrum is convergent, but is on the very border of convergence. In contrast to this, when evaluating the EBL, Eq. (20), the integrand behaves for large p as $\ln(p)/p^4$. This holds for s states. For p states the integrand behaves for large p as $\ln(p)/p^6$. When considering the normalized difference of the s states, $[\Delta E(N)-\Delta E(1)]/N^3$ [14,19], the integrand behaves for large p as $\ln(p)/p^6$. Knowledge of the normalized difference reduces the calculation of the EBL for the general s state to the calculation of the EBL for the ground state.

For the ground state, we can improve the situation further by identifying in Eq. (41)

$$h_0=\frac{p^2}{2},\quad h_1=-\frac{1}{r},\quad \lambda=Z$$

and writing

$$F_{\rm low}=\left[F^0_{\rm low}+Z\left(F^1_{\rm low}\right)_{\rm ver}\right]+\left[F_{\rm low}-F^0_{\rm low}-Z\left(F^1_{\rm low}\right)_{\rm ver}\right].\tag{54}$$

The trick is to calculate the first term on the r.h.s. exactly and the second term numerically, by the method of pseudostates.

The first term on the r.h.s. of Eq. (54) is calculated by inserting Eqs. (51) and (53) into Eq. (20),

$$\begin{aligned}&\left[F^0_{\rm low}+Z\left(F^1_{\rm low}\right)_{\rm ver}\right]\\&\quad=\int_0^1 dw\frac{1-2w(1-w)}{aw}\int_0^1 dy\,\phi\left(z=\frac{y}{wa}\right),\end{aligned}\tag{55}$$

where

$$a=(Z\alpha)^2$$

and

$$\begin{aligned}\phi(z)&=\frac{16}{\pi}\int_0^\infty dp\frac{p^2}{(p^2+1)^2(z+p^2+1)}\\&\quad\times\left[1+Z\frac{\pi-4\arctan(p)}{p}\right]\\&=\frac{4}{[\sqrt{1+z}+1]^2}+Z\frac{8}{z^3}\ln\left(\frac{[1+\sqrt{1+z}]^4}{2^4(1+z)}\right).\end{aligned}$$

The following integrals over y and w can be performed exactly, though the resulting expression is rather complex.

TABLE I. Calculation of the EBL for the ground state of the ordinary hydrogen atom in the infinite nucleus mass limit. $F^0_{\rm low}$ and $(F^1_{\rm low})_{\rm ver}$ are calculated from Eq. (55). $F_{\rm low}-F^0_{\rm low}-(F^1_{\rm low})_{\rm ver}$ is obtained by using the expansion, Eq. (38), for $\nu=20$–30 and extrapolating the results by means of the Thiele-Padé method.

$F^0_{\rm low}$	22.817 746 017
$(F^1_{\rm low})_{\rm ver}$	2.059 023 576
$F_{\rm low}-F^0_{\rm low}-(F^1_{\rm low})_{\rm ver}$	−14.240 719 010
$F_{\rm low}$	10.636 050 583(9)

The second term on the r.h.s. of Eq. (54), the expression $[F_{\rm low}-F^0_{\rm low}-Z(F^1_{\rm low})_{\rm ver}]$ is calculated as follows. $F_{\rm low}$ and $F^0_{\rm low}$ are calculated from Eq. (37) for $Z=1$ and $Z=0$, respectively. The quantity $Z(F^1_{\rm low})_{\rm ver}$ is calculated from Eq. (49). As follows from Eq. (53) the contribution of the upper part of the continuous spectrum goes, for $[F_{\rm low}-F^0_{\rm low}-Z(F^1_{\rm low})_{\rm ver}]$, as $\ln(k)/k^6$ so the expansion, Eq. (38), converges very rapidly. In fact, it is sufficient to consider ν in Eq. (38) to be between 20 and 30 and then extrapolate the result. In Table I the calculation of the EBL by the described procedure for infinite nuclear mass $m/m_r=1$ is reported. This should be compared with the previous attempts to calculate the OBL by the method of pseudostates [7]. As is clear from Table I, replacement of the exact wave function with the free-particle wave function for intermediate states is not a good approximation for calculation of the EBL. But that is not the point. What is the point is that for the expression $[F_{\rm low}-F^0_{\rm low}-Z(F^1_{\rm low})_{\rm ver}]$ the contribution of the upper part of the continuous spectrum is strongly suppressed and the method of pseudostates converges rapidly.

For the ground state we obtain, for the function F in Eq. (19) in the infinite nucleus mass limit,

$$F(\alpha)=10.636\,051-1/3=10.302\,717.$$

If the r.h.s. of Eq. (22) is used instead, i.e., if one uses the OBL instead of the EBL, one gets

$$F(\alpha)=10.252\,922.$$

This should be contrasted with the exact result [5,12],

$$F(\alpha)=10.316\,794.$$

It is clear that use of the EBL leads to a significantly better estimate of the self-energy effect than the OBL does. To understand why this is so, let us expand Eq. (55) in powers of a:

$$\begin{aligned}&\left[F_{\rm low}^0 + Z\left(F_{\rm low}^1\right)_{\rm ver}\right]\\ &\simeq -\frac{16}{3}\ln(2a^{1/2}) + \frac{2}{9} + \frac{736}{105}a^{1/2}\\ &\quad + \cdots + Z\left[\frac{32}{3}\ln(2) - \frac{16}{3} + \frac{32}{3}a\ln(a) + \cdots\right].\end{aligned}$$

The most interesting is the term proportional to $a^{1/2} = Z\alpha$ because it does not receive any correction from the neglected terms in Eq. (53). The function F has the expansion in $Z\alpha$ given by Eq. (2). The exact form of A_{50} coefficient reads

$$A_{50} = 4\pi\left(\frac{139}{128} - \frac{\ln 2}{2}\right) \simeq 9.2911.$$

$F_{\rm low}$ contains complete coefficients A_{41} and A_{40}. These are obtained from the expansion, Eq. (22). Now $\frac{736}{105} \simeq 7.0095$, that is, $F_{\rm low}$ contains also 75% of coefficient A_{50}. This explains why the EBL is more accurate than the OBL.

E. The case of the Coulomb potential perturbed by the Uehling potential

When considering the effect of the Uehling potential, we substitute into Eq. (41)

$$h_0 = \frac{p^2}{2} - \frac{1}{r}, \quad h_1 = \int_0^1 dx\, U(x)\frac{e^{-\mu(x)r}}{r}, \quad \lambda = \frac{\alpha}{\pi}, \tag{56}$$

where $U(x)$ and $\mu(x)$ are given by Eq. (26). The matrix elements of the Yukawa-like potential $\frac{e^{-\mu(x)r}}{r}$ and momentum operator between the Sturmian functions are given in Appendixes B and C.

Evaluating now Eqs. (48)–(50), the most difficult part is calculation of the correction to the wave function of the reference S states, Eq. (48). The crucial observation here is that the number of pseudostates M used to approximate the reference wave function has to be greater than the number of pseudostates Q used to approximate the spectral decomposition of the Hamilton operator [see Eq. (48)]. We found that for fixed Q and M greater than about $Q + 10$, the result is independent of M. In the actual calculation we extrapolated the results from the interval $Q \in (260,290)$ and $M = 300$. For vertex and energy corrections we took $Q \in (200,220)$ and $Q \in (100,120)$ in Eqs. (49) and (50), respectively. For P states the convergence is, not surprisingly, much faster than for S states.

Further, we consider the high-energy part, (21). The first-order perturbation due to the Uehling potential, Eq. (26), is the sum of two contributions,

$$F_{\rm high}^1 = \left(F_{\rm high}^1\right)_{\rm wf} + \left(F_{\rm high}^1\right)_{\rm pot}, \tag{57}$$

where the former is due to the correction to the wave function,

$$\begin{aligned}&\left(F_{\rm high}^1\right)_{\rm wf}\\ &= -2N^3\sum_{m=L+1\neq N}^{L+M}\langle\psi_{N,L}^0|\left[-\frac{\pi}{3}\delta^3(\vec{r}) + \frac{m_\mu + M}{2M}\frac{\vec{S}\cdot\vec{L}}{r^3}\right]\\ &\quad\times|\psi_{m,L}^0\rangle\int_0^1 dx\, U(x)\langle\psi_{m,L}^0|\frac{e^{-\mu(x)r}}{r}|\psi_{N,L}^0\rangle\frac{1}{e_m^0 - e_N^0},\end{aligned} \tag{58}$$

and the latter is caused by modification of the Coulomb potential by the Uehling potential,

$$\begin{aligned}\left(F_{\rm high}^1\right)_{\rm pot} = N^3\int_0^1 dx\, U(x)\langle\psi_{N,L}^0|e^{-\mu(x)r}\Bigg[\frac{\pi}{3}\delta^3(\vec{r}) - \frac{\mu(x)^2}{12r}\\ - \frac{1}{2}\frac{\vec{S}\cdot\vec{L}}{r^3}[1+\mu(x)r]\Bigg]|\psi_{N,L}^0\rangle.\end{aligned} \tag{59}$$

TABLE II. Calculation of the EBL for muonic hydrogen and the Coulomb potential perturbed by the Uehling potential. The second column, $F_{\rm low}^1$, was obtained from Eqs. (47)–(50). The third column, $F_{\rm high}^1$, was obtained from Eqs. (57)–(59). Further, $F^1 = F_{\rm low}^1 + F_{\rm high}^1$. See Sec. IV E for further details.

State	$F_{\rm low}^1$	$F_{\rm high}^1$	F^1
$1s$	20.330	−0.871	19.459
$2s$	18.900	−0.772	18.129
$3s$	18.33	−0.745	17.585
$4s$	18.02	−0.731	17.289
$2p_{\frac{1}{2}}$	−0.274	−0.039	−0.313
$2p_{\frac{3}{2}}$		0.028	−0.246
$3p_{\frac{1}{2}}$	−0.286	−0.043	−0.329
$3p_{\frac{3}{2}}$		0.031	−0.255
$4p_{\frac{1}{2}}$	−0.288	−0.044	−0.332
$4p_{\frac{3}{2}}$		0.032	−0.256

The former contribution is calculated by using the expansion, (58), for $M = 40$–50 and extrapolating the results. Regarding the latter contribution, after analytic integration over r, one integrates numerically over x.

The complete results for both low- and high-energy contributions are listed in Table II. In particular, for the $2s$ and $2p_{\frac{1}{2}}$ states we obtain

$$\begin{aligned}\Delta E(2s) &\simeq m_\mu\left(\frac{1}{1+\frac{m_\mu}{m_p}}\right)^3\left(\frac{\alpha}{\pi}\right)^2\frac{(Z\alpha)^4}{2^3}F^1(2s)\\ &\simeq 2.6597\times 10^{-6}\ \text{eV},\end{aligned}$$

and

$$\begin{aligned}\Delta E(2p_{\frac{1}{2}}) &\simeq m_\mu\left(\frac{1}{1+\frac{m_\mu}{m_p}}\right)^3\left(\frac{\alpha}{\pi}\right)^2\frac{(Z\alpha)^4}{2^3}F^1(2p_{\frac{1}{2}})\\ &\simeq -4.59\times 10^{-8}\ \text{eV},\end{aligned}$$

where $F^1(2s)$ and $F^1(2p_{\frac{1}{2}})$ are taken from the corresponding cells in Table II.

For the contribution of the effect considered here to the Lamb shift in muonic hydrogen we thus obtain

$$\Delta E(2p_{\frac{1}{2}}) - \Delta E(2s) \simeq -2.706\times 10^{-6}\ \text{eV},$$

which differs by 8% from the result, -2.5×10^{-6} eV, given in [11].

V. CONCLUSIONS

In this paper two observations about NRQED have been made. First, the general pattern of appearance of logarithmic terms is clarified. We derive the actual form of the coefficients of leading logarithmic terms at a given order of $Z\alpha$. We argue that these coefficients come entirely from the divergent behavior of the Dirac S-wave function at the origin. Second, we suggest a way to circumvent the calculation of the Bethe logarithm. The trick is to calculate expression (15), here called the extended Bethe logarithm (EBL). This expression simultaneously is easier to calculate and yields a better estimate of the QED effect than the ordinary Bethe logarithm (OBL). To show nontrivial application of the EBL, we calculated the combined self-energy vacuum polarization effect in muonic hydrogen. Further extension of this method to the calculation of QED effects in many-electron atoms and QED effects beyond the one-loop level thus seems promising. However, it must be pointed out that only part of the problem associated with calculation of the Bethe logarithm in many-electron atoms is solved by the present suggestion. In many-electron atoms the Bethe logarithm appears when considering the self-energy effect and one-photon exchange [20]. The OBL can be replaced by the EBL only when considering the self-energy effect. When calculating one-photon exchange in the usual way [20], one still has to calculate the OBL. Nevertheless, the present suggestion still simplifies the most difficult part of the calculation. For instance, for non-S states of two-electron atoms, the dominant electron configuration is one electron in the s orbital and the other in the non-s orbital. The OBL necessary for evaluation of the electron self-energy in the s orbitals is more difficult to calculate than the OBL necessary for evaluation of one-photon exchange between the electrons.

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APPENDIX A: DERIVATION OF EQ. (4)

In this Appendix we show where Eq. (4) comes from. We start by inserting Eq. (59) from [5] into Eq. (42) from [5]:

$$\sum_{v=0}^{\infty}\sum_{L=0}^{v}\sum_{\rho=\pm1}\sum_{j-\frac{1}{2}=0}^{\infty}\sum_{p=0}^{v-L}\sum_{\pi=\pm1}\Theta_{O_1,O_2}(L,j,\rho,\pi)(EZ\alpha)^{-2(p+L)}\left(-\frac{1}{2}\right)^{p}$$
$$\times\sum_{q=0}^{p}\frac{1}{q!(2L+2q+1)!!}\,\frac{1}{(p-q)!(2L+2(p-q)+1)!!}\,\frac{1}{(v-p-L)!}(-1)^{v}\frac{(2v+1)!!}{2^{2v}}m^{2v}$$
$$\times\sum_{t=0}^{\infty}\left(\frac{m}{E}\right)^{t}\frac{1}{2^{t}t!}\frac{\partial^{t}}{\partial\xi^{t}}\left[\left[\int_{0}^{\infty}dk_{e}P_{l_\Gamma}^{L+2q,L+2(p-q)+c}(k_e,\xi)\,\frac{\partial^{v-p-L}}{\partial\sigma^{v-p-L}}\Phi_{4,0}^{2v,t}(\Delta+\sigma)\Big|_{\sigma=0}+\cdots\right]\right]\Big|_{\xi=1}. \tag{A1}$$

Here, Δ is given by Eqs. (47) and (66) in [5]:

$$-\frac{\Delta}{m^{2}}=(Z\alpha)^{2}\left\{k_{e}^{2}+1+(\xi-1)\frac{2(l_0+1)}{2+l_0}\right\}. \tag{A2}$$

Further, $\Theta_{O_1,O_2}(L,j,\rho,\pi)$ denotes the result of the pertinent spinor-angular integrations (see Eqs. (34) and (35) of [5]). The only thing we need to know now is that it can be converted to series in powers of $(Z\alpha)^2$. The v and t in Eq. (A1) count the number of powers of the space and time components of $\Pi-\varepsilon$, respectively. Here $\Pi=(E+\frac{Z\alpha}{r},\vec{P})$ is the electron's physical four-momentum and $\varepsilon=(m,\vec{0})$ is the four-momentum of the electron at rest. Furthermore, $P_{l_\Gamma}^{L+2q,L+2(p-q)+c}$ are overlap integrals between the ground and the intermediate states (see Eqs. (48) and (66) of [5]):

$$P_{l_\Gamma}^{L+2q,L+2(p-q)+c}=\langle l_0+1,l_0|r^{L+2q}|k_e,l_\Gamma\rangle_{\xi}(\langle l_0+1,l_0|r^{L+2(p-q)+c}|k_e,l_\Gamma\rangle_{\xi})^{*}. \tag{A3}$$

Here, l_Γ is the relativistic orbital quantum number of the intermediate states (see Eqs. (15) and (20) of [5]):

$$l_\Gamma=|\Gamma|-\delta_{\rho,1}\qquad|\Gamma|=\sqrt{(j+1/2)^{2}-(Z\alpha)^{2}}. \tag{A4}$$

Further, $\langle r|l_0+1,l_0\rangle$ and $\langle r|k_e,l_\Gamma\rangle$ are radial parts of the wave functions of the ground and intermediate states, respectively.

Equation (A1) is a general form of the contributions to the self-energy in the relativistic multipole expansion (RME). The ellipsis in Eq. (A1) represents the contribution of the discrete part of the spectrum, which is of no interest here. The parameter c acquires just two values, $c=0,-1$. We take the case $c=0$; for $c=-1$ the derivation would be similar. In expression (A1) two cases are considered at once: the scalar part of the electron propagator, denoted 4, and the time component of the vector part of the electron propagator, denoted 0, (see Eq. (7) in [5]). There is also a contribution from the space components of the vector part of the propagator (Eq. (43) in [5]), but again the treatment is very similar to the case considered here. The functions $\Phi_{4,0}^{2v,t}(\Delta+\sigma)$ are determined up to an arbitrary polynomial of the $(2v+t-1)$th order in $\Delta+\sigma$. In the following, we call this the “property of functions Φ”. The functions are given by Eq. (56) in [5],

$$\Phi_{4,0}^{2v,t}(\Delta+\sigma)=2^{v}(-1)^{t}\frac{\partial^{t}}{\partial(\varepsilon_0)^{t}}\int_0^1 dyy^{v}(1,y\varepsilon_0)\int_0^{-\frac{\Delta+\sigma}{m^2}}d^{v+t}w\ln\left(\frac{\varepsilon_0^2y+w}{y}\right)\Bigg|_{\varepsilon_0=1},\tag{A5}$$

where the symbol $d^n w$ stands for iterated integration

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

We can use the property of functions Φ and rewrite Eq. (A5) as

$$\Phi_{4,0}^{2v,t}(\Delta+\sigma)=2^{v}(-1)^{t}\frac{\partial^{t}}{\partial(\varepsilon_0)^{t}}\int_0^1 dyy^{v}(1,y\varepsilon_0)\int_0^{-\frac{\Delta+\sigma}{m^2}}d^{v+t+1}w\frac{1}{\varepsilon_0^2y+w}\Bigg|_{\varepsilon_0=1};\tag{A6}$$

then

$$\frac{\partial^{v-p-L}}{\partial\sigma^{v-p-L}}\Phi_{4,0}^{2v,t}(\Delta+\sigma)\Bigg|_{\sigma=0}=2^{v}(-1)^{t}\frac{\partial^{t}}{\partial(\varepsilon_0)^{t}}\int_0^1 dyy^{v}(1,y\varepsilon_0)\left(-\frac{1}{m^2}\right)^{v-p-L}\int_0^{-\frac{\Delta}{m^2}}d^{t+p+L+1}w\frac{1}{\varepsilon_0^2y+w}\Bigg|_{\varepsilon_0=1}.\tag{A7}$$

For the terms with $v=0$ and $t>0$, some additional terms have to be added to Eq. (A6) in order for it to be equivalent to Eq. (A5). These terms are irrelevant for the following considerations. In the last integration we perform the substitution $w\to w(-\frac{\Delta}{m^2})$.

For exact determination of the coefficients A_{40}, A_{41}, A_{61}, and A_{60} in Eqs. (2) and (3), we need exact evaluation of the overlap integrals, Eq. (A3), given by Eqs. (49) and (66) in [5]. However, for exact determination of the coefficients A_{50} and A_{62} in Eq. (2) and also the ratios, Eq. (13), it suffices to consider the overlap integrals, (A3), in the limit $k_e\to\infty$,

$$P_{l_\Gamma}^{L+2q,L+2(p-q)}(k_e,\xi)\to\frac{B_0}{\left(1+k_e^2\right)^{l_0+2+L+p}}\left[1+\frac{B_1\,k_e}{k_e^2+1}+\frac{B_2\,k_e^2}{\left(k_e^2+1\right)^2}+\cdots\right],\tag{A8}$$

where

$$B_0=B_0(l_\Gamma,l_0,p,q,L),\quad B_1=B_1^0+B_1^1\,\xi,\quad B_2=B_2^0+B_2^1\,\xi+B_2^2\,\xi^2.$$

The corrections B_1^0, B_1^1, and so on are also functions of the parameters $l_\Gamma,\ l_0,\ p,\ q,\ L$.

Consider first the case $t=0$. Combining Eqs. (A1), (A2), (A7), and (A8) we get (omitting all the sums and factors which are not of interest now)

$$\int_0^\infty dk_e\int_0^1 dyy^{v}(1,\varepsilon_0 y)\int_0^1 d^{p+L+1}w\frac{1}{y+w(Z\alpha)^2\left(k_e^2+1\right)}\frac{\left[(Z\alpha)^2\left(k_e^2+1\right)\right]^{p+L+1}}{(Z\alpha)^{2(p+L)}}\frac{B_0}{\left(k_e^2+1\right)^{l_0+2+L+p}}\left[1+\frac{B_1\,k_e}{k_e^2+1}+\cdots\right].\tag{A9}$$

For $v>0$ we use the identity

$$\frac{1}{y+w(Z\alpha)^2\left(k_e^2+1\right)}=\frac{1}{y}\left(1-\frac{w(Z\alpha)^2\left(k_e^2+1\right)}{y+w(Z\alpha)^2\left(k_e^2+1\right)}\right).\tag{A10}$$

For $v=1$ the $1/y$ term yields the contribution to coefficient A_{40}, Eq. (2). For $v>1$ this term does not contribute because of the property of functions Φ. For $v=0$ this term leads to the divergent integral over y. For $v=0$ the lower bound of the integration over the parameter y in expression (A9) yields the contribution to the coefficients A_{41} and A_{40}, Eq. (2). For the upper bound of the integration over y the situation is the same as for the case $v>0$.

After leaving out the first term in Eq. (A10), expression (A9) reduces to

$$(Z\alpha)^4\int_0^\infty dk_e\int_0^1 dyy^{v-1}(1,\varepsilon_0 y)\int_0^1 d^{p+L+1}w\frac{w\,k_e^{-2l_0}}{y+w(Z\alpha)^2\left(k_e^2+1\right)}\,B_0\left[1+B_1\frac{k_e}{k_e^2+1}+B_2\left(\frac{k_e}{k_e^2+1}\right)^2+\cdots\right].\tag{A11}$$

As pointed out above, the coefficients B depend on the relativistic orbital quantum numbers of the ground and virtual states, l_0 and l_Γ, respectively. These numbers depend on $Z\alpha$ [see Eqs. (6) and (A4)]. Now we have to distinguish two cases. First, in the limit $Z\alpha\to 0$ the coefficient B_0 goes to 1. The last equation is then multiplied by the additional factor of $Z\alpha^2$ (see Eqs. (26) and (35) in [5]). Thus we can make the replacement $B_0\to(Z\alpha)^2C_0$. The latter equation then leads to Eq. (4). Second, in the limit $Z\alpha\to 0$ the coefficient B_0 goes to $(Z\alpha)^4$, the product B_0B_1 goes to $(Z\alpha)^2$, and the product B_0B_2 goes to 1. This follows from Eq. (49) in [5]. The first two terms in the last equation are of the form of Eq. (4), albeit the contribution of the first term is suppressed by the additional power of $(Z\alpha)^2$. After leaving out these first two terms, expression (A11) reduces to

$$(Z\alpha)^4 \int_0^\infty dk_e \int_0^1 dy y^{v-1}(1,\varepsilon_0 y) \int_0^1 d^{p+L+1}w \frac{w\, k_e^{-2l_0}}{y + w(Z\alpha)^2\left(k_e^2+1\right)}\, B_0\left[B_2\left(\frac{k_e}{k_e^2+1}\right)^2 + \cdots\right]. \tag{A12}$$

Here we have a situation analogous to that encountered with expression (A9). For $v > 1$ we use identity (A10). The first term yields, for $v = 2$, the contribution to the coefficient A_{40}, Eq. (2), and for $v > 2$ it is cancelled because of the property of functions Φ. After leaving out the first term in Eq. (A10), expression (A12) reduces to

$$(Z\alpha)^6 \int_0^\infty dk_e \int_0^1 dy y^{v-2}(1,\varepsilon_0 y) \int_0^1 d^{p+L+1}w \frac{w^2\, k_e^{-2l_0}}{y + w(Z\alpha)^2\left(k_e^2+1\right)}\, B_0 B_2[1 + \cdots].$$

This is again of the form of Eq. (4). For $v = 1$ the lower bound of the integration in expression (A12) contributes to the coefficients A_{41} and A_{40}, Eq. (2).

Next consider the case $t > 0$. In this case we arrive, instead of Eq. (A9), at the expression

$$\frac{1}{t!}\frac{\partial^t}{\partial \xi^t}\frac{\partial^t}{\partial \varepsilon_0^t}\int_0^\infty dk_e \int_0^1 dy y^{v}(1,\varepsilon_0 y) \int_0^1 d^{t+p+L+1}w \frac{\left[(Z\alpha)^2\left(k_e^2+1+(\xi-1)\frac{2(l_0+1)}{2+l_0}\right)\right]^{t+p+L+1}}{\varepsilon_0^2\, y + w(Z\alpha)^2\left(k_e^2+1+(\xi-1)\frac{2(l_0+1)}{2+l_0}\right)}\Bigg|_{\varepsilon_0=1}$$

$$\times \frac{B_0}{\left(k_e^2+1\right)^{l_0+2+L+p}}\left[1 + \frac{\left(B_1^0 + B_1^1\,\xi\right)k_e}{k_e^2+1} + \frac{\left(B_2^0 + B_2^1\,\xi + B_2^2\,\xi^2\right)k_e^2}{\left(k_e^2+1\right)^2} + \cdots\right]\Bigg|_{\xi=1}.$$

In the limit of $k_e \to \infty$ differentiation of the expression in the last bracket with respect to ξ is more important than differentiation of the fraction; thus the last equation in this limit becomes

$$(Z\alpha)^{2(1+t)}\frac{\partial^t}{\partial \varepsilon_0^t}\int_0^\infty dk_e \int_0^1 dy y^{v}(1,\varepsilon_0 y) \int_0^1 d^{t+p+L+1}w \frac{\left(k_e^2+1\right)^{t-1}k_e^{-2l_0}}{\varepsilon_0^2 y + w(Z\alpha)^2\left(k_e^2+1\right)}\Bigg|_{\varepsilon_0=1} B_0 B_t^t\left(\frac{k_e}{k_e^2+1}\right)^t[1 + \cdots]. \tag{A13}$$

For $t = 1$ there are three cases to consider. First, $B_0 B_1^1$ is of the order $(Z\alpha)^2$. Second, the last expression is further multiplied by $(Z\alpha)^2$. In both these cases the last equation leads to Eq. (4). Third, when $B_0 B_2^2$ is of the order of 1. In this case the term with $v = 0$ does not appear. This follows from Eq. (131) in [3]. After leaving out the first term in expression (A13) we get

$$(Z\alpha)^4\frac{\partial}{\partial \varepsilon_0}\int_0^\infty dk_e \int_0^1 dy y^{v}(1,\varepsilon_0 y) \int_0^1 d^{p+L+2}w \frac{k_e^{-2l_0}}{\varepsilon_0^2\, y + w(Z\alpha)^2\left(k_e^2+1\right)}\Bigg|_{\varepsilon_0=1}\frac{B_0 B_2^2}{k_e^2+1}[1 + \ldots].$$

Next, we use the identity, Eq. (A10). Again, we face the same situation as earlier: the first term contributes to the coefficient A_{40}, Eq. (2), for $v = 1$; for $v > 1$ it is cancelled because of the property of functions Φ. After leaving out the first term in Eq. (A10), the last equation reduces to Eq. (4). For $t = 2$ expression (A13) reduces to Eq. (4) only in the case where $B_0 B_2^2$ is of the order of 1; all remaining cases for $t = 2$ are suppressed by the additional power of $(Z\alpha)^2$. For $t > 2$, with some additional effort expression (A13) can also be reduced to the form of Eq. (4), but this time multiplied by the additional power of $(Z\alpha)^2$. So the terms for $t > 2$ do not contribute to the logarithmic terms considered in Sec. II.

APPENDIX B: MATRIX ELEMENTS OF THE YUKAWA POTENTIAL

In this Appendix matrix elements of the Yukawa potential between Sturmian functions are given. They are needed for calculation of Eqs. (48)–(50) and (58) with the Hamiltonian given by Eq. (56).

The explicit form of the Sturmians reads

$$R_{n,l}(\xi,r) = C_{n,l} r^l e^{-\xi r} F(-n+l+1, 2l+2, 2\xi r),$$

where

$$C_{n,l} = \frac{(2\xi)^{l+1}}{\Gamma(2l+2)}\left(\frac{\Gamma(n+l+1)}{\Gamma(n-l)}\right)^{1/2}.$$

Setting $\xi = 1$ and $\xi = 1/n$, the eigenstates of the T_3 operator, Eq. (31), and hydrogen functions are obtained, respectively. For the usual normalization of hydrogen functions (with respect to weight r^2) the normalization coefficient $C_{n,l}$ has to be multiplied by $1/n$.

The matrix element $I_{n_1,n_2,l}(\lambda,\xi_1,\xi_2)$ of the general Yukawa potential $\frac{e^{-\lambda r}}{r}$ between Sturmian or hydrogen functions is given by the formula (see, e.g., [18])

$$I_{n_1,n_2,l}(\lambda,\xi_1,\xi_2) = \int_0^\infty r R_{n_1,l}(\xi_1,r) R_{n_2,l}(\xi_2,r) e^{-\lambda r} dr$$
$$= C_{n_1,l} C_{n_2,l} \frac{\Gamma(2l+2)(\lambda-\xi_1+\xi_2)^{n_1}(\lambda+\xi_1-\xi_2)^{n_2}}{(\lambda+\xi_1+\xi_2)^{n_1+n_2}[\lambda^2-(\xi_1-\xi_2)^2]^{l+1}} F\left(-n_1+l+1,-n_2+l+1,2l+2,\frac{4\xi_1\xi_2}{\lambda^2-(\xi_1-\xi_2)^2}\right).$$

APPENDIX C: MATRIX ELEMENTS OF THE MOMENTUM OPERATOR

In this Appendix matrix elements of the momentum operator between Sturmian functions are given. They are needed for calculation of Eqs. (48)–(50).

From Eqs. (A54) and (A55) in [4] we have, for the matrix elements of the momentum operator relations,

$$\langle n',l+1,m'|p_i|n,l,m\rangle = -i\langle l+1,m'|n_i|l,m\rangle \int_0^\infty r^2 R_{n',l+1}\left(\frac{d}{dr}-\frac{l}{r}\right)R_{n,l} \tag{C1}$$

and

$$\langle n',l-1,m'|p_i|n,l,m\rangle = -i\langle l-1,m'|n_i|l,m\rangle \int_0^\infty r^2 R_{n',l-1}\left(\frac{d}{dr}+\frac{l+1}{r}\right)R_{n,l}. \tag{C2}$$

To calculate the radial integrals on the right-hand sides of the last two equations we again use Eqs. (A54) and (A55) in [4] and we get

$$\left(\frac{d}{dr}-\frac{l}{r}\right)R_{n,l} = -\frac{\sqrt{n^2-(l+1)^2}}{l+1}R_{n,l+1} - \frac{n}{l+1}R_{n,l} \tag{C3}$$

and

$$\left(\frac{d}{dr}+\frac{l+1}{r}\right)R_{n,l} = \frac{\sqrt{n^2-l^2}}{l}R_{n,l-1} + \frac{n}{l}R_{n,l}. \tag{C4}$$

From Eq. (35) in [21] supplemented with orthonormality of the Sturmian functions, Eq. (36), we get

$$\int_0^\infty drr^2 R_{n',l+1}R_{n,l} = \delta_{n',n+1}\frac{\sqrt{(n+l+1)(n+l+2)}}{2} + \delta_{n',n-1}\frac{\sqrt{(n-l-1)(n-l-2)}}{2} - \delta_{n',n}\sqrt{n^2-(l+1)^2}, \tag{C5}$$

and combining Eqs. (35) and (36) we get

$$\int_0^\infty drr^2 R_{n',l}R_{n,l} = -\delta_{n',n+1}\frac{\sqrt{(n-l)(n+l+1)}}{2} - \delta_{n',n-1}\frac{\sqrt{(n+l)(n-l-1)}}{2} + \delta_{n',n}n. \tag{C6}$$

Using Eqs. (C3), (C5), and (C6) we get the final expression for the radial integral on the r.h.s. of (C1):

$$\int_0^\infty drr^2 R_{n',l+1}\left(\frac{d}{dr}-\frac{l}{r}\right)R_{n,l} = -\delta_{n',n+1}\frac{\sqrt{(n+l+1)(n+l+2)}}{2} + \delta_{n',n-1}\frac{\sqrt{(n-l-1)(n-l-2)}}{2}. \tag{C7}$$

From Eq. (36) of [21] and (36) we have

$$\int_0^\infty drr^2 R_{n',l-1}R_{n,l} = \delta_{n',n+1}\frac{\sqrt{(n-l)(n+1-l)}}{2} + \delta_{n',n-1}\frac{\sqrt{(n+l)(n+l-1)}}{2} - \delta_{n',n}\sqrt{n^2-l^2}. \tag{C8}$$

Similarly to the previous case, using Eqs. (C4), (C6), and (C8) we get the expression for the radial integral on the r.h.s. of (C2):

$$\int_0^\infty drr^2 R_{n',l-1}\left(\frac{d}{dr}+\frac{l+1}{r}\right)R_{n,l} = -\delta_{n',n+1}\frac{\sqrt{(n-l)(n-l+1)}}{2} + \delta_{n',n-1}\frac{\sqrt{(n+l)(n+l-1)}}{2}. \tag{C9}$$

APPENDIX D: FROM VIRTUAL *p* STATES TO VIRTUAL *s* STATES

In this Appendix we show how integrals involving radial functions of virtual p states can be converted to the integrals involving radial functions of virtual s states. This includes the derivation of Eq. (51). Further, this can be used when evaluating Eq. (48).

From Eq. (C3) for $l = 0$ we get

$$R_{n,1}\left(\frac{r}{n}\right) = -\frac{n}{\sqrt{n^2-1}}\left(\frac{d}{dr}+1\right)R_{n,0}\left(\frac{r}{n}\right).$$

For energies $e_n = -1/2/n^2$ and $e_1 = -1/2$ the identity

$$-\frac{2n}{\sqrt{n^2-1}} = -\sqrt{\frac{2}{e_n - e_1}}$$

holds. Using the last two relations and integration by parts we get, for the general function $\varphi(r)$,

$$\int_0^\infty drr^2 R_{n,1}\left(\frac{r}{n}\right)\frac{d}{dr}\varphi(r) = \frac{1}{\sqrt{2(e_n-e_1)}}\int_0^\infty drr^2 R_{n,0}\left(\frac{r}{n}\right)\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{d}{dr}\right)\varphi(r).$$

If we insert $\varphi(r) = R_{1,0}(r)$, we get Eq. (51). If $R_{n,0}(\frac{r}{n})$ and $\varphi(r)$ are replaced by the Sturmians $R_{n,0}(r)$ and $R_{m,0}(n)$, respectively, then, by virtue of Eqs. (32), (33), (34), and (36), one gets

$$\begin{aligned}\int_0^\infty drr^2 R_{n,0}(r)\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{d}{dr}\right)R_{m,0}(r) &= -\int_0^\infty drr R_{n,0}(r)(T_3 - 1 + T_+)R_{m,0}(r)\\ &= -\delta_{n,m}(2m-1) - \delta_{n,m+1}\sqrt{m(m+1)}.\end{aligned}$$

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