Heavy-particle quantum electrodynamics

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The quantum electrodynamic formalism is presented for the systematic and exact in $Z\alpha$ derivation of nuclear recoil corrections in hydrogenic systems.

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I. INTRODUCTION

The quantum electrodynamics (QED) of atomic systems has so far been formulated for an infinitely heavy nucleus, using the so-called Furry picture, in which the Dirac propagator includes the Coulomb potential [1]. The inclusion of finite nuclear mass effects in the exact relativistic formalism is highly nontrivial. The unperturbative in the $Z\alpha$ formula for the leading recoil correction to the binding energy was originally derived about 40 years ago by Shabaev in Refs. [2,3] and was confirmed by an independent derivation in Ref. [4]. This formula formed the basis of extensive numerical QED calculations of nuclear recoil effects in heavy hydrogenic [5,6] and heavy few-electron ions within the so-called $1/Z$ expansion [7]. This leading recoil correction was later extended to the presence of the homogenous magnetic field [8], and recently to the finite-size nucleus [9], but no other progress has been achieved so far.

Nuclear recoil effects are significant for light hydrogenic systems, where a different QED approach has been developed. These corrections have been calculated over many years using $Z\alpha$ expansion, which led to very accurate results and consequently the accurate determination of fundamental constants and quantum electrodynamics tests. Nevertheless, some important higher-order recoil corrections are not yet known and limit theoretical predictions. For example, the radiative recoil correction $\alpha(Z\alpha)^6\, m/M$ currently limits theoretical predictions for the hydrogen Lamb shift and the muonium hyperfine structure [10]. This is due to the high complexity in calculations of higher order (in α and $Z\alpha$) recoil corrections. Some of them have been calculated only by one group, such as the $(Z\alpha)^2\, m/M$ correction to the hyperfine splitting in hydrogen about 40 years ago by Bodwin and Yennie [11], which has not yet been confirmed. Therefore, the exact in $Z\alpha$ formulas for recoil and radiative recoil corrections of arbitrary order in mass ratio would be very desirable.

Very recently, the method from Refs. [4,9] has been extended to derive the exact, in $Z\alpha$, pure recoil correction to the hyperfine splitting in hydrogenic systems [12]. It was noticed there that the use of the temporal gauge for the photon exchange propagators greatly simplifies the derivation and final formulas, so they can be a basis for direct numerical calculations, but also they can be a basis for the analytic derivation of $Z\alpha$ expansion coefficients, such as that of Bodwin and Yennie [11].

In this paper, we demonstrate that the method from Ref. [12] can be further developed to derive exact, in $Z\alpha$, formulas for corrections of an arbitrary order in the mass ratio and α. As an example, we present them for the leading radiative recoil correction and for the complete nonradiative second order in mass ratio correction. Finally, we perform an exemplary numerical calculation of nuclear recoil with the electron vacuum polarization for muonic atoms. Theoretical units $\hbar = c = 1$ are used throughout this work with $\alpha = e^2/(4\pi)$ and e being an electron charge.

II. EXPANSION IN THE ELECTRON-NUCLEAR MASS RATIO

To begin with the precise formulation of the nuclear recoil correction, let us note that on the basis of QED theory, the binding energy of a two-body system is a function of α, $Z\alpha$, and the mass ratio m/M, namely $E = E(m/M, Z\alpha, \alpha)$. Assuming that one of the particles is much heavier and of extended size, one can perform an expansion in the mass ratio together with the expansion in the fine-structure constant α,

$$E\left(\frac{m}{M}, Z\alpha, \alpha\right) = \sum_{i,j} E^{(i,j)}(Z\alpha), \tag{1}$$

where the dependence on the finite nuclear size, typically $m\, r_C$, is not explicitly shown, and where

$$E^{(i,j)}(Z\alpha) = m\left(\frac{m}{M}\right)^i \alpha^j\, \mathcal{E}^{(i,j)}(Z\alpha). \tag{2}$$

The power of α represents the number of QED loops, namely the number of the lepton self-energy and the vacuum-polarization loops. Here, $E^{(0,0)}(Z\alpha) = E_D$ is the Dirac energy in the infinite nuclear mass limit,

$$H_D\,\phi = E_D\,\phi, \tag{3}$$

where

$$H_D = \vec{\alpha}\cdot\vec{p} + \beta m + V_C, \tag{4}$$

and where V_C is a Coulomb potential including the nuclear charge distribution $\rho_C(r)$,

$$V_C(r) = -\int d^3r' \frac{Z\alpha}{|\vec{r}-\vec{r}\,'|}\rho_C(r'). \tag{5}$$

The next term, $E^{(0,1)}(Z\alpha) = E_{\rm self} + E_{\rm vp}$, is the sum of the one-loop electron self-energy and vacuum-polarization corrections. Namely, the electron self-energy correction is

$$E_{\rm self} = \langle\bar\phi|\Sigma_{\rm rad}(E_D)|\phi\rangle, \tag{6}$$

where $\bar\phi = \phi^+\gamma^0$, and

$$\Sigma_{\rm rad}(E) = e^2\int \frac{d^4k}{(2\pi)^4 i}\frac{1}{k^2}\gamma^\mu e^{-i\vec{k}\cdot\vec{r}} S_F(E+\omega)\gamma_\mu e^{i\vec{k}\cdot\vec{r}}, \tag{7}$$

with $\omega = k^0$ the Feynman integration contour is assumed, and where

$$S_F(E) = \frac{1}{\not p - \gamma^0 V_C - m} \tag{8}$$

is the Dirac-Coulomb propagator.

In the second contribution $E_{\rm vp}$, the electron vacuum polarization modifies the photon propagator, which is exchanged between the lepton and the nucleus

$$-\frac{g_{\mu\nu}}{k^2} \to -\frac{g_{\mu\nu}}{k^2[1+\bar\omega(k^2)]}. \tag{9}$$

At the one-loop level $\bar\omega$ (in electron mass units) is given by

$$\bar\omega(k^2) = \frac{\alpha}{\pi}k^2\int_4^\infty d(q^2)\frac{1}{q^2\left(m_e^2\,q^2-k^2\right)}u(q^2), \tag{10}$$

where

$$u(q^2) = \frac{1}{3}\sqrt{1-\frac{4}{q^2}}\left(1+\frac{2}{q^2}\right). \tag{11}$$

The resulting vacuum-polarization potential for a point infinitely heavy nucleus is given by

$$V_{\rm vp}(r) = -\frac{Z\alpha}{r}\frac{\alpha}{\pi}\int_4^\infty \frac{d(q^2)}{q^2}e^{-m_e q r}u(q^2), \tag{12}$$

while for the finite-size nucleus it is

$$V_{\rm Cvp}(r) = \int d^3r'\, V_{\rm vp}(|\vec{r}-\vec{r}\,'|)\rho_C(r'), \tag{13}$$

and the corresponding vacuum-polarization correction to the binding energy is

$$E_{\rm vp} = \langle\phi|V_{\rm Cvp}|\phi\rangle. \tag{14}$$

These QED corrections in the infinite nuclear mass limit can be formally extended to an arbitrary number of loops, and calculated numerically (see, for example, the two-loop self-energy calculation of the Lamb shift by one of us [13]).

III. HPQED

Heavy-particle quantum electrodynamics (HPQED) is the formalism that allows to derive nuclear recoil corrections of an arbitrary order in m/M and α. The starting point is the nonrelativistic QED Hamiltonian for the nucleus, namely

$$\begin{aligned}H_{\rm nuc} = {}& \frac{\vec\Pi^2}{2M} + qA^0 - \frac{q}{2M}g\vec{I}\cdot\vec{B} - \frac{q\,\delta_I}{8M^2}\vec\nabla\cdot\vec{E}\\ &- \frac{q}{4M^2}(g-1)\vec{I}\cdot[\vec{E}\times\vec\Pi - \vec\Pi\times\vec{E}] + \cdots,\end{aligned} \tag{15}$$

where $\vec\Pi = \vec{P} - q\vec{A}$, $q = -Z\,e$, I is the nuclear spin, $\delta_0 = 0$, $\delta_{1/2} = 1$, and where we introduced the nuclear g factor, defined as

$$\vec\mu = \frac{q}{2M}g\vec{I}. \tag{16}$$

We will neglect the nuclear quadrupole and all higher electromagnetic moments, because their contribution is usually very small. Moreover, the finite charge and magnetic moment distributions, which are described by electromagnetic form factors $G_E(-k^2)$ and $G_M(-k^2)$ (normalized to 1 at $k^2 = 0$) will be moved to the photon propagator. This can be done, because every photon exchange between the point lepton and the nucleus is associated with the product of the nuclear vertex which contains these form factors and of the photon propagator. Moreover, we will assume at the beginning that all these form factors are the same, namely $G_E(-k^2) = G_M(-k^2) = \rho_C(-k^2)$. This can be generalized at the final stage of derivation. We will also neglect nuclear polarizability, namely all interactions beyond the elastic form factors. Its calculation would require a separate treatment. Moreover, the diagrams involving the photon emission and absorption by the nucleus will also be neglected. Their consideration is very problematic when an elastic approximation is assumed. This is because, even for light elements such as Mg ($Z = 12$), the effective electromagnetic coupling $Z^2\alpha$ is larger than 1 and the QED perturbation theory may not work in such a case, which demonstrates limitations of the elastic form factor approximation.

Returning to the nuclear Hamiltonian in Eq. (15) we construct the quantum electrodynamic theory using the Coulomb gauge and the Furry picture. Namely, the Coulomb interaction V_C between the finite-size nucleus and the lepton is accounted for unperturbatively, and all other interactions are treated using the perturbation theory. At the zeroth order, we have the standard QED with the static Coulomb potential, as described in the previous section. The first-order term in the mass ratio is represented as an expectation value

$$E^{(1)} = \langle\Psi|\frac{(\vec{P}-q\vec{A})^2}{2M} - \frac{q}{2M}g\vec{I}\cdot\vec{B}|\Psi\rangle_{\rm QED} \tag{17}$$

on a hydrogenic state $|\Psi\rangle$, which is a second-quantized Fock state centered at the position of nucleus $\vec{R}$. The meaning of the "QED" expectation value needs to be explained and we here follow Refs. [1,12]. The matrix element of an arbitrary operator Q on a state Ψ in a QED theory is

$$\langle\Psi|Q|\Psi\rangle_{\rm QED} = \frac{\langle\Psi|{\rm T}Q\exp[-i\int d^4y\,H_I(y)]|\Psi\rangle}{\langle\Psi|{\rm T}\exp[-i\int d^4y\,H_I(y)]|\Psi\rangle}, \tag{18}$$

where T denotes chronological ordering with an assumption that the time coordinate of Q is $t = 0$, the interaction Hamiltonian is

$$H_I(y) = e\, j_\mu(y) A^\mu(y), \tag{19}$$

and j^μ is the four-vector current.

The second term in Eq. (17) leads to the well-known hyperfine splitting, and its calculation is standard. The crucial point is the interpretation of $\vec{P}$ from the first term in Eq. (17) and its action on $|\Psi\rangle$ and $\hat\psi$. Namely, let us consider the representation of the fermion field $\hat\psi$ in terms of creation and annihilation operators of one-particle hydrogenic states ϕ_s,

$$\hat\psi(x) = \sum_s^{+} a_s \phi_s(\vec x) e^{-i E_s t} + \sum_s^{-} b_s \phi_s(\vec x) e^{-i E_s t},$$
$$\hat\psi^+(x) = \sum_s^{+} a_s^+ \phi_s^+(\vec x) e^{i E_s t} + \sum_s^{-} b_s^+ \phi_s^+(\vec x) e^{i E_s t}. \tag{20}$$

The differentiation $\vec\nabla_R$ acts on functions ϕ_s and operators a_s, b_s, and this can be represented as [12]

$$\vec\nabla_R = \int d^3r\, \hat\psi^+(\vec r) \vec\partial_R\, \hat\psi(\vec r) + \vec\partial_R$$
$$= -\int d^3r\, \hat\psi^+(\vec r) \vec\partial_r\, \hat\psi(\vec r) + \vec\partial_R, \tag{21}$$

where $\hat\psi(\vec r) \equiv \hat\psi(0, \vec r)$, and $\vec\partial_R$ is understood in the following sense. The hydrogenic state ϕ_s is a function of $\phi_s(\vec r - \vec R)$ of the difference in electron and nucleus position vectors; therefore $\vec\partial_R\, \phi_s = -\vec\partial_r\, \phi_s$, and $\hat a_s, \hat b_s$ remain intact. As a test, for $t = 0$,

$$\vec\nabla_R \hat\psi(0, \vec x) = -\int d^3r\, \hat\psi^+(\vec r) \vec\partial_r\, \hat\psi(\vec r)\ \hat\psi(0, \vec x) - \vec\partial_x \hat\psi(0, \vec x)$$
$$= 0, \tag{22}$$

as it should. Moreover, for an arbitrary Fock state $|\Psi\rangle$,

$$\vec\nabla_R |\Psi\rangle = -\int d^3r\, \hat\psi^+(\vec r) \vec\partial_r\, \hat\psi(\vec r) |\Psi\rangle, \tag{23}$$

and this holds in particular for the vacuum state $|0\rangle$.

A crucial observation was made in Ref. [12], that every occurrence of $\vec P - q\vec A$ in the Coulomb gauge can be replaced by $-q\vec A$ in the temporal gauge, where the photon propagator becomes

$$G_T^{ij}(\omega, \vec k) = \frac{\rho_C(-k^2)}{k^2}\left(\delta^{ij} - \frac{k^i k^j}{\omega^2}\right). \tag{24}$$

The temporal gauge is a particular case of the axial gauge and is defined by the condition $G_T^{0\mu} = 0$ for every μ. The singularity at $\omega = 0$ is taken care of, as explained below. This crucial observation leads to a significant simplification of matrix elements for all recoil corrections, because one can use standard perturbation theory, such as a two-time Green's function approach [1], and thus avoid cumbersome $\vec\nabla_R$ differentiation. Below, we present formulas for the leading two terms in the large nuclear mass expansion for hydrogenic atoms.

IV. PURE RECOIL CORRECTION

The leading pure recoil correction is $E_{\rm rec} = E^{(1,0)}(Z\alpha)$. It is given by the first term in Eq. (17). As we have already mentioned, for the point nucleus it was first derived by Shabaev in Refs. [2,3], and the generalization for the finite-size nucleus was achieved recently in Refs. [9,12], namely

$$E_{\rm rec} = \langle\bar\phi|\Sigma_{\rm rec}(E_D)|\phi\rangle \tag{25}$$

$$\Sigma_{\rm rec}(E) = \frac{i}{M}\int_s \frac{d\omega}{2\pi} D_T^j(\omega) S_F(E+\omega) D_T^j(\omega), \tag{26}$$

where

$$D_T^j(\omega, \vec r) = -4\pi Z\alpha\, \gamma^i\, G_T^{ij}(\omega, \vec r). \tag{27}$$

The subscript s in the integration denotes a symmetric integration path. Namely, we perform Wick rotation and symmetrically integrate around the pole at $\omega = 0$. The apparent singularity at $\omega = 0$ is a spurious one, as can be seen by changing to the Coulomb gauge propagators

$$D_C^j(\omega) = D_T^j(\omega) + \frac{1}{\omega^2}[\omega + E_D - H_D, p^j(V_C)]. \tag{28}$$

Moreover, the temporal gauge propagator for a point nucleus with $w = \sqrt{-\omega^2 + i\,\varepsilon}$,

$$G_T^{ij}(\omega, \vec r) = -\left(\delta^{ij} + \frac{\nabla^i\nabla^j}{\omega^2}\right)\frac{e^{-w\, r}}{4\pi\, r}, \tag{29}$$

contains the Dirac δ function; therefore, the Coulomb gauge propagators are more convenient for numerical calculations.

V. RADIATIVE RECOIL CORRECTION

The exact, in $Z\alpha$, radiative recoil correction $E_{\rm radrec} = E^{(1,1)}$ has not yet been published in the literature. We split it into self-energy and vacuum-polarization parts,

$$E_{\rm radrec} = E_{\rm selfrec} + E_{\rm vprec}. \tag{30}$$

The vacuum-polarization part can be implemented by the effective charge density $\rho_{\rm vp}(-k^2)$, namely using Eqs. (9) and (10),

$$\rho_{C\rm vp}(-k^2) = -\bar\omega(k^2)\rho_C(-k^2), \tag{31}$$

and thus takes the form analogous to Eq. (26),

$$E_{\rm vprec} = \delta_{\rm vp}\frac{i}{M}\int_s \frac{d\omega}{2\pi}\langle\bar\phi|D_T^j(\omega) S_F(E_D+\omega) D_T^j(\omega)|\phi\rangle, \tag{32}$$

where $\delta_{\rm vp}$ perturbs ϕ, H_D, E_D, and D_T^j, whenever ρ_C is present, namely

$$E_{\rm vprec} = \frac{i}{M}\int_s \frac{d\omega}{2\pi}\big[2\langle\bar\phi|D_{T\rm vp}^j(\omega) S_F(E_D+\omega) D_T^j(\omega)|\phi\rangle$$
$$+ 2\langle\bar\phi|\gamma^0\, V_{C\rm vp}\, S_F'(E_D) D_T^j(\omega) S_F(E_D+\omega) D_T^j(\omega)|\phi\rangle$$
$$+ \langle\bar\phi|D_T^j(\omega) S_F(E_D+\omega)\gamma^0(V_{C\rm vp} - \langle V_{C\rm vp}\rangle)$$
$$\times\ S_F(E_D+\omega) D_T^j(\omega)|\phi\rangle\big], \tag{33}$$

and where $S_F'(E_D)$ is the reduced Dirac propagator (the reference state with the energy E_D is subtracted out).

The self-energy part is obtained as follows. The fermion propagator

$$\frac{1}{\not{p} - m - \Sigma(E)} \tag{34}$$

has corrections due to the self-energy and the recoil

$$\Sigma(E) = \Sigma_{\rm rad}(E) + \Sigma_{\rm rec}(E) + \Sigma_{\rm radrec}(E) + \cdots, \tag{35}$$

where $\Sigma_{\rm rad}$ is defined in Eq. (7), $\Sigma_{\rm rec}$ in Eq. (26), and

$$\begin{aligned}\Sigma_{\rm radrec}(E) = \frac{i}{M}\int_s \frac{d\omega'}{2\pi} e^2 \int \frac{d^4k}{(2\pi)^4\, i}\frac{1}{k^2}\big[&\gamma^\mu\, e^{-i\vec{k}\cdot\vec{r}}\, S_F(E+\omega) D_T^j(\omega') S_F(E+\omega+\omega') D_T^j(\omega') S_F(E+\omega)\gamma_\mu\, e^{i\vec{k}\cdot\vec{r}}\\
&+ D_T^j(\omega') S_F(E+\omega')\gamma^\mu\, e^{-i\vec{k}\cdot\vec{r}}\, S_F(E+\omega+\omega')\gamma_\mu\, e^{i\vec{k}\cdot\vec{r}}\, S_F(E+\omega') D_T^j(\omega')\\
&+ \gamma^\mu\, e^{-i\vec{k}\cdot\vec{r}}\, S_F(E+\omega) D_T^j(\omega') S_F(E+\omega+\omega')\gamma_\mu\, e^{i\vec{k}\cdot\vec{r}}\, S_F(E+\omega') D_T^j(\omega')\\
&+ D_T^j(\omega') S_F(E+\omega')\gamma^\mu\, e^{-i\vec{k}\cdot\vec{r}}\, S_F(E+\omega+\omega') D_T^j(\omega') S_F(E+\omega)\gamma_\mu\, e^{i\vec{k}\cdot\vec{r}}\big]\end{aligned} \tag{36}$$

is a sum of all one-particle irreducible diagrams (in the temporal gauge). The change in the position of the pole of the fermion propagator in Eq. (34) due to the presence of $\Sigma(E)$ is

$$\begin{aligned}E_{\rm selfrec} = {}&\langle\bar{\phi}|\Sigma_{\rm radrec}(E_D)|\phi\rangle\\
&+ 2\langle\bar{\phi}|\Sigma_{\rm rad}(E_D) S'_F(E_D)\Sigma_{\rm rec}(E_D)|\phi\rangle\\
&+ \langle\bar{\phi}|\Sigma'_{\rm rad}(E_D)|\phi\rangle\langle\bar{\phi}|\Sigma_{\rm rec}(E_D)|\phi\rangle\\
&+ \langle\bar{\phi}|\Sigma'_{\rm rec}(E_D)|\phi\rangle\langle\bar{\phi}|\Sigma_{\rm rad}(E_D)|\phi\rangle.\end{aligned} \tag{37}$$

This radiative recoil correction has been calculated only up to $\alpha\,(Z\alpha)^5$ order, and the higher-order terms are unknown, which limits the accuracy of the hydrogen Lamb shift [10]. Moreover, we expect this correction to be significant for light muonic atoms, where the electron vacuum polarization is combined with a relatively large muon-nucleus mass ratio. Therefore, we perform exemplary calculation of this correction for several hydrogenic ions in Sec. VIII.

VI. RECOIL CORRECTION TO THE HYPERFINE SPLITTING

The nonperturbative formula for the recoil correction to the hyperfine splitting in hydrogenlike ions has recently been derived in Ref. [12]. It comes from the NRQED Hamiltonian of the nucleus in Eq. (15) (including the relevant terms only),

$$\begin{aligned}H_{\rm nuc} = {}&\frac{\vec{\Pi}^2}{2M} - \frac{q}{2M} g\,\vec{I}\cdot\vec{B}\\
&- \frac{q}{4M^2}(g-1)\vec{I}\cdot[\vec{E}\times\vec{\Pi} - \vec{\Pi}\times\vec{E}],\end{aligned} \tag{38}$$

and takes the form

$$E_{\rm hfsrec} = E_{\rm kin} + E_{\rm so} + E_{\rm sec}, \tag{39}$$

where

$$\begin{aligned}E_{\rm kin} = {}&\frac{1}{M}\int_s \frac{d\omega}{2\pi}\frac{1}{\omega}\big[\langle\bar{\phi}|D_T^j(\omega) S_F(E_D+\omega)\partial^j(V_{\rm hfs}(\omega))|\phi\rangle\\
&-\langle\bar{\phi}|\partial^j(V_{\rm hfs}(\omega)) S_F(E_D+\omega) D_T^j(\omega)|\phi\rangle\big]\\
&+ \delta_{\rm hfs}\frac{i}{M}\int_s \frac{d\omega}{2\pi}\langle\bar{\phi}|D_T^j(\omega) S_F(E_D+\omega) D_T^j(\omega)|\phi\rangle,\end{aligned} \tag{40}$$

$$\begin{aligned}E_{\rm so} = {}&-\frac{(g-1)}{M^2}\epsilon^{ijk} I^i\int_s \frac{d\omega}{2\pi}\omega\\
&\times\langle\bar{\phi}|D_T^j(\omega) S_F(E_D+\omega) D_T^k(\omega)|\phi\rangle,\end{aligned} \tag{41}$$

$$\begin{aligned}E_{\rm sec} = {}&\left(\frac{4\pi Z\alpha}{2M} g\right)^2 \epsilon^{ijk} I^k\int_s \frac{d\omega}{2\pi}\frac{1}{\omega}\\
&\times\langle\bar{\phi}|(\vec{\gamma}\times\vec{\nabla})^i D(\omega) S_F(E_D+\omega)(\vec{\gamma}\times\vec{\nabla})^j D(\omega)|\phi\rangle,\end{aligned} \tag{42}$$

where

$$D(\omega, r) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}}\frac{\rho(\vec{k}^2-\omega^2)}{\omega^2-\vec{k}^2} \tag{43}$$

and

$$V_{\rm hfs}(\omega,\vec{r}) = e\,\vec{\mu}\cdot\vec{\gamma}\times\vec{\nabla}D(\omega, r), \tag{44}$$

such that $V_{\rm hfs}(0,r) = V_{\rm hfs}(r)$, where

$$V_{\rm hfs}(r) = \frac{e}{4\pi}\vec{\mu}\cdot\vec{\gamma}\times\left[\frac{\vec{r}}{r^3}\right]_{\rm fs}. \tag{45}$$

This recoil correction has not yet been numerically calculated. Expansion terms up to $(Z\alpha)^2 E_F$ are presently known [11], but the higher-order recoil terms have not yet been studied.

VII. SECOND-ORDER RECOIL CORRECTION

The second-order recoil correction $E_{\rm quadrec} = E^{(2,0)}$ has also not yet been considered in the literature. It comes from the NRQED Hamiltonian for the nucleus in Eq. (15) (including relevant terms only),

$$H_{\rm nuc} = \frac{\vec{\Pi}^2}{2M} - \frac{q}{2M} g\,\vec{I}\cdot\vec{B} - \frac{q\,\delta_I}{8M^2}\vec{\nabla}\cdot\vec{E}, \tag{46}$$

and is split into three parts,

$$E_{\rm quadrec} = E_{\rm kin} + E_{\rm mag} + E_{\rm zit}, \tag{47}$$

which are obtained as follows.

The kinetic energy part $E_{\rm kin}$ is the second-order correction due to the nonrelativistic kinetic energy of the nucleus,

$$E_{\rm kin} = \langle\bar\phi|\Sigma_{\rm quadrec}(E_D)|\phi\rangle + \langle\bar\phi|\Sigma_{\rm rec}(E_D)S'(E_D)\Sigma_{\rm rec}(E_D)|\phi\rangle + \langle\bar\phi|\Sigma'_{\rm rec}(E_D)|\phi\rangle\langle\bar\phi|\Sigma_{\rm rec}(E_D)|\phi\rangle, \tag{48}$$

where $\Sigma_{\rm rec}(E)$ is defined in Eq. (26), and $\Sigma_{\rm quadrec}(E)$ is a sum of all one-particle irreducible diagrams, namely

$$\begin{aligned}\Sigma_{\rm quadrec}(E) = {}& \left(\frac{i}{M}\int_s\frac{d\omega_1}{2\pi}\right)\left(\frac{i}{M}\int_s\frac{d\omega_2}{2\pi}\right)\\ &\times\big[D_T^j(\omega_1)S_F(E_D+\omega_1)D_T^j(\omega_2)S_F(E_D+\omega_1+\omega_2)D_T^j(\omega_1)S_F(E_D+\omega_2)D_T^j(\omega_2)\\ &+D_T^j(\omega_1)S_F(E_D+\omega_1)D_T^j(\omega_2)S_F(E_D+\omega_1+\omega_2)D_T^j(\omega_2)S_F(E_D+\omega_1)D_T^j(\omega_1)\big].\end{aligned} \tag{49}$$

The magnetic contribution $E_{\rm mag}$ is the second-order correction due to $-\vec\mu\cdot\vec B$ in Eq. (46),

$$E_{\rm mag} = \langle\bar\phi|V_{\rm hfs}\,S'_F(E_D)V_{\rm hfs}|\phi\rangle, \tag{50}$$

and the product of the nuclear magnetic moments in the above is to be replaced by $\mu^a\,\mu^b \to \delta^{ab}\,\vec\mu^{\,2}/3$. We note that the antisymmetric part would contribute to the hyperfine splitting, but it would be incorrect. The correct formula was presented in the previous section in Eq. (42).

Finally, the *zitterbewegung* term $E_{\rm zit}$ depends on the nuclear spin. It vanishes for scalar particles (nuclei), while for spin 1/2 it is $\delta_{1/2}=1$, and

$$E_{\rm zit} = \frac{\delta_I}{8\,M^2}\langle\vec\nabla^2(V_C)\rangle. \tag{51}$$

The numerical calculation of this second-order correction is not trivial, but what is important is that all such formulas can be written down.

VIII. NUMERICAL CALCULATION OF THE NUCLEAR RECOIL ELECTRON VACUUM-POLARIZATION CORRECTION IN MUONIC ATOMS

This is an exemplary numerical calculation of the nuclear recoil electron vacuum-polarization (EVP) correction for several muonic (hydrogenlike) atoms. This correction, given by Eq. (32), we transform to the Coulomb gauge

$$\begin{aligned}E_{\rm vprec} = {}& \frac{m_\mu^2}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\,\delta_{\rm vp}\langle\phi|\big[p^j - D_C^j(\omega)\big]\\ &\times[E_D-H_D]^{-1}\big[p^j-D_C^j(\omega)\big]|\phi\rangle,\end{aligned} \tag{52}$$

where m_μ is the muon mass, $\delta_{\rm vp}$ denotes perturbation by the electron vacuum polarization, $D_C^j(\omega) = -4\pi Z\alpha\,\alpha^i\,G_C^{ij}(\omega,\vec r)$ and G_C^{ij} is the transverse part of the photon propagator in the Coulomb gauge given by

$$G_C^{ij}(\omega,\vec r) = \delta^{ij}\,D(\omega,r) + \frac{\nabla^i\nabla^j}{\omega^2}[D(\omega,r)-D(0,r)], \tag{53}$$

and

$$D(\omega,r) = \int\frac{d^3k}{(2\pi)^3}\,e^{i\vec k\cdot\vec r}\frac{\rho(\vec k^2-\omega^2)}{\omega^2-\vec k^2}. \tag{54}$$

See Ref. [9] for details.

We divide $E_{\rm vprec}$ into two parts,

$$E_{\rm vprec} = E_{\rm vprec,ph} + E_{\rm vprec,el}, \tag{55}$$

where $E_{\rm vprec,ph}$ is due to perturbation of $D_C(\omega)$ by vacuum polarization, whereas $E_{\rm vprec,el}$ is the remainder. The calculation of $E_{\rm vprec,el}$ is relatively straightforward. We include the vacuum-polarization potential $V_{\rm Cvp}(r)$ into the Dirac Hamiltonian, calculate the recoil correction using the procedure developed in Ref. [9], and then linearize with respect to $V_{\rm Cvp}$ by taking the numerical derivative.

The computation of $E_{\rm vprec,ph}$ is more complicated. We write it in the Coulomb gauge as follows,

$$\begin{aligned}E_{\rm vprec,ph} = {}& \frac{m_\mu^2}{M}\frac{i}{\pi}\int_{-\infty}^{\infty}d\omega\sum_n\frac{1}{E_D+\omega-E_n(1-i0)}\\ &\times[-\langle\phi|\vec p|n\rangle\langle n|\delta_{\rm vp}\vec D_C(\omega)|\phi\rangle,\\ &+\langle\phi|\vec D_C(\omega)|n\rangle\langle n|\delta_{\rm vp}\vec D_C(\omega)|\phi\rangle].\end{aligned} \tag{56}$$

The function $\delta_{\rm vp}D_C^j(\omega)$ is obtained from $D_C^j(\omega)$ by modifying the photon propagator with vacuum polarization. This modification leads to the replacement

$$D(\omega,r)\to D_{\rm vp}(\omega,r), \tag{57}$$

where

$$D_{\rm vp}(\omega,r) = \int\frac{d^3k}{(2\pi)^3}e^{i\vec k\cdot\vec r}\frac{\rho(\vec k^2-\omega^2)}{\omega^2-\vec k^2}[-\bar\omega(\omega^2-\vec k^2)], \tag{58}$$

and $\bar\omega(k^2)$ is defined in Eq. (10). Let us now obtain $D_{\rm vp}$ for the exponential model of the nuclear charge distribution

$$\rho(\vec k^2) = \frac{\lambda^4}{(\lambda^2+\vec k^2)^2}. \tag{59}$$

We first consider the case of pure imaginary ω. For $w^2 = -\omega^2$, we get

$$D_{\rm vp}(i\,w,r) = -\frac{\alpha}{\pi}\int_4^{\infty}d(q^2)\frac{u(q^2)}{q^2}\int\frac{d^3k}{(2\pi)^3}\,e^{i\vec k\cdot\vec r}X, \tag{60}$$

where

$$\begin{aligned}X &= \frac{1}{\left(m_e^2\,q^2+w^2+\vec k^2\right)}\frac{\lambda^4}{(\lambda^2+w^2+\vec k^2)^2}\\ &= \frac{\lambda^4}{\left(\lambda^2-m_e^2\,q^2\right)^2}\left[\frac{1}{m_e^2\,q^2+w^2+\vec k^2}\right.\\ &\quad\left.-\frac{1}{\lambda^2+w^2+\vec k^2}-\frac{\lambda^2-m_e^2\,q^2}{(\lambda^2+w^2+\vec k^2)^2}\right].\end{aligned} \tag{61}$$

TABLE I. Nuclear-recoil–vacuum-polarization correction to the $2P_{1/2}-2S$ transition energy of H-like muonic ions, in meV.

	^{1}H	^{4}He	^{7}Li	^{12}C	^{132}Xe	^{208}Pb
M/m_μ	8.880243	35.27765	61.83924	105.7641	1162.618	1833.145
r_C (fm)	0.84060	1.67860	2.4440	2.4702	4.7859	5.5012
$E_{\rm vprec,el}$	−56.36324	−78.41878	−107.1656	−241.863	5407.20	6895.5
$E_{\rm vprec,ph}$	0.00555	0.03214	0.1068	1.191	−293.61	−971.2
$E_{\rm vprec}$	−56.35769	−78.38664	−107.0588	−240.672	5113.59	5924.3
$E_{\rm vprec}$(l.o.)	−56.36185	−78.60251	−108.66	−258.91	−1825	−2666

Performing integration over $\vec{k}$, we obtain

$$D_{\rm vp}(i\,w,r) = -\frac{1}{4\pi}\int_2^\infty dq\,A_{\rm vp}(q)\left[\frac{e^{-\sqrt{w^2+m_e^2q^2}\,r}}{r} - \frac{e^{-\sqrt{w^2+\lambda^2}\,r}}{r} - \frac{\lambda^2-m_e^2q^2}{2\sqrt{\omega^2+\lambda^2}}\,e^{-\sqrt{w^2+\lambda^2}\,r}\right], \tag{62}$$

where

$$A_{\rm vp}(q) = \frac{\alpha}{\pi}\frac{2}{3}\frac{\sqrt{q^2-4}(2+q^2)}{q^4}\frac{1}{\left(1-m_e^2q^2/\lambda^2\right)^2}. \tag{63}$$

For the general complex ω, we analytically continue the above formulas and obtain

$$D_{\rm vp}(\omega,r) = -\frac{1}{4\pi}\int_2^\infty dq\,A_{\rm vp}(q)\left[\frac{e^{i\sqrt{\omega^2-m_e^2q^2}\,r}}{r} - \frac{e^{i\sqrt{\omega^2-\lambda^2}\,r}}{r} - \frac{i\left(\lambda^2-m_e^2q^2\right)}{2\sqrt{\omega^2-\lambda^2}}\,e^{i\sqrt{\omega^2-\lambda^2}\,r}\right]. \tag{64}$$

We note that for $\omega=0$, the function $D_{\rm vp}$ becomes proportional to the vacuum-polarization potential $V_{\rm Cvp}$,

$$V_{\rm Cvp}(r) = 4\pi Z\alpha\,D_{\rm vp}(0,r). \tag{65}$$

Results of our numerical calculations of the recoil–vacuum-polarization correction are presented in Table I for the $2P_{1/2}-2S$ transition energy of several muonic H-like ions, together with the contribution of the leading order of the $Z\alpha$ expansion of this correction,

$$E_{\rm vprec}(\text{l.o.}) = -\frac{2}{3\pi}\frac{m_\mu^2c^2}{M}\,\alpha(Z\alpha)^2 \times\int_1^\infty du\frac{\beta^2(-1+6\beta u)\sqrt{u^2-1}(1+2u^2)}{u^2(1+2\beta u)^5}, \tag{66}$$

where $\beta = m_e/(Z\alpha\,m_\mu)$.

It can be seen that the deviation of the all-order result from the lowest-order term is quite small for hydrogen and helium (as expected), but grows fast with the increase of the nuclear charge. For heavy ions, the lowest-order formula does not reproduce even the overall sign of the total correction. Moreover, we note that for light ions the nuclear recoil electron vacuum-polarization correction is larger than the pure nuclear recoil for this particular transition. So, for muonic hydrogen, the first order in m/M nuclear recoil contributes 1.63 meV to the $2P_{1/2}-2S$ energy difference, whereas the nuclear recoil with vacuum-polarization contributes −56.4 meV.

IX. SUMMARY

HPQED enables the systematic inclusion of finite nuclear mass corrections using exact formulas in terms of $Z\alpha$. By recognizing that the nuclear momentum $\vec{P}-q\vec{A}$ can be represented as $-q\vec{A}$ in the temporal gauge, the derivation falls within the realm of standard bound state perturbative QED and can thus be performed straightforwardly. The obtained formulas can be extended to many-electron systems using the $1/Z$ expansion [1], similarly to the leading recoil correction [7]. Numerical calculations would likely require transforming to the Coulomb gauge, resulting in much longer formulas. For electronic atoms, most of higher-order recoil corrections derived here are probably insignificant, except for the radiative recoil, which is required for the improved description of the hydrogen Lamb shift. However, for muonic atoms, these corrections could lead to substantial effects since muons are 206 times heavier than electrons. In fact, there is an ongoing QUARTET project [14] to determine nuclear charge radii from the spectra of $3\leqslant Z\leqslant 10$ muonic atoms. An additional benefit of the obtained formulas is the complete inclusion of finite nuclear size (but not the nuclear polarizability, which needs to be accounted for separately). Finally, the derived formulas can be used to obtain higher-order recoil corrections in the $Z\alpha$ expansion, such as $\alpha(Z\alpha)^6 m/M$, which have yet to be addressed in the literature.

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