QED theory of the nuclear recoil effect in atoms

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The quantum electrodynamic theory of the nuclear recoil effect in atoms to all orders in αZ is formulated. The nuclear recoil corrections for atoms with one and two electrons over closed shells are considered in detail. The problem of the composite nuclear structure in the theory of the nuclear recoil effect is discussed. [S1050-2947(97)07212-0]

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I. INTRODUCTION

The complete αZ-dependence expressions for the nuclear recoil corrections to the energy levels of hydrogenlike atoms were derived in [1]. These expressions consist of three contributions: the Coulomb contribution, the one-transverse-photon contribution, and the two-transverse-photon contribution. For a state a the Coulomb contribution is given by (the relativistic units $\hbar=c=1$ are used in the paper)

$$\Delta E_c=\Delta E_c^{(1)}+\Delta E_c^{(2)},$$

$$\Delta E_c^{(1)}=\left\langle a\left|\frac{\mathbf{p}^2}{2M}\right|a\right\rangle, \tag{1}$$

$$\Delta E_c^{(2)}=\frac{2\pi i}{M}\int_{-\infty}^{\infty}d\omega\ \delta_+^2(\omega)\langle a|[\mathbf{p},V_c]G(\omega+\varepsilon_a)[\mathbf{p},V_c]|a\rangle, \tag{2}$$

where $|a\rangle$ is the unperturbed state of the Dirac electron in the Coulomb field of the nucleus, $V_c=-\alpha Z/r$ is the Coulomb potential of the nucleus, $\mathbf{p}$ is the momentum operator, $\delta_+(\omega)=i/[2\pi(\omega+i0)]$, $G(\omega)=[\omega-H(1-i0)]^{-1}$ is the relativistic Coulomb Green function, and $H=\boldsymbol{\alpha}\cdot\mathbf{p}+\beta m+V_c$. The scalar product is implicit in Eq. (2) and below [Eqs. (4)–(6)]. The one-transverse-photon contribution is

$$\Delta E_{\mathrm{tr}(1)}=\Delta E_{\mathrm{tr}(1)}^{(1)}+\Delta E_{\mathrm{tr}(1)}^{(2)},$$

$$\Delta E_{\mathrm{tr}(1)}^{(1)}=-\frac{1}{2M}\langle a|[\mathbf{D}(0)\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{D}(0)]|a\rangle, \tag{3}$$

$$\Delta E_{\mathrm{tr}(1)}^{(2)}=-\frac{1}{M}\int_{-\infty}^{\infty}d\omega\,\delta_+(\omega)\langle a|\{[\mathbf{p},V_c]G(\omega+\varepsilon_a)\mathbf{D}(\omega)-\mathbf{D}(\omega)G(\omega+\varepsilon_a)[\mathbf{p},V_c]\}|a\rangle, \tag{4}$$

where

$$D_m(\omega)=-4\pi\alpha Z\alpha_l D_{lm}(\omega),$$

α_l $(l=1,2,3)$ are the Dirac matrices, and $D_{lm}(\omega)$ is the transverse part of the photon propagator in the Coulomb gauge. In the coordinate representation it is

$$D_{ik}(\omega,\mathbf{r})=-\frac{1}{4\pi}\left\{\frac{\exp(i|\omega|r)}{r}\,\delta_{ik}+\nabla_i\nabla_k\,\frac{\exp(i|\omega|r)-1}{\omega^2 r}\right\}.$$

The two-transverse-photon contribution is

$$\Delta E_{\mathrm{tr}(2)}=\frac{i}{2\pi M}\int_{-\infty}^{\infty}d\omega\langle a|\mathbf{D}(\omega)G(\omega+\varepsilon_a)\mathbf{D}(\omega)|a\rangle. \tag{5}$$

An attempt to derive the complete αZ-dependence expressions for the nuclear recoil effect was previously undertaken in [2]. Except for the Coulomb contribution, the expressions found in [2] are in disagreement with the ones given above. A dominant part of this disagreement is caused by technical errors made in [2]. If we remove these errors from [2], a discrepancy remains in the one-transverse-photon contribution and, in addition, appears in the Coulomb contribution. This discrepancy was discussed in detail in [1].

Recently, Eqs. (1)–(5) were rederived in [3,4]. In Ref. [3], it was noted that the sum of these expressions can be written in the following compact form:

$$\Delta E_{\mathrm{tot}}=\frac{i}{2\pi M}\int_{-\infty}^{\infty}d\omega\langle a|[\mathbf{p}-\mathbf{D}(\omega)]G(\omega+\varepsilon_a)\times[\mathbf{p}-\mathbf{D}(\omega)]|a\rangle. \tag{6}$$

The terms $\Delta E_c^{(1)}$ and $\Delta E_{\mathrm{tr}(1)}^{(1)}$ can easily be calculated by using the virial relations for the Dirac equation [5]. Such a calculation gives [1]

$$\Delta E^{(1)}\equiv\Delta E_c^{(1)}+\Delta E_{\mathrm{tr}(1)}^{(1)}=\frac{m^2-\varepsilon_a^2}{2M}. \tag{7}$$

This simple formula contains all the nuclear recoil corrections within the $(\alpha Z)^4 m^2/M$ approximation. The remaining terms [Eqs. (2), (4), and (5)] taken to the lowest order in αZ give the Salpeter corrections [6]. Evaluation of these terms to all orders in αZ in the range $Z=1-100$ was done in [7]. In particular, it was found in [7] that the complete (in αZ) nuclear recoil correction, in addition to the Salpeter one, to the Lamb shift $(n=2)$ in hydrogen constitutes $-1.32(6)$ kHz. This value almost coincides with the value of the $(\alpha Z)^6 m^2/M$ correction found in [4,8–10].

The complete αZ-dependence expressions for the nuclear recoil corrections for high-Z few-electron atoms were de-

rived in [11]. These formulas were used in [7] to calculate the nuclear recoil corrections to all orders in αZ for high-Z lithiumlike atoms. As follows from these formulas, within the $(\alpha Z)^4 m^2/M$ approximation the nuclear recoil corrections can be obtained by averaging the operator

$$H_M=\frac{1}{2M}\sum_{s,s'}\left[\mathbf{p}_s\cdot\mathbf{p}_{s'}-\frac{\alpha Z}{r_s}\left(\boldsymbol{\alpha}_s+\frac{(\boldsymbol{\alpha}_s\cdot\mathbf{r}_s)\mathbf{r}_s}{r_s^2}\right)\cdot\mathbf{p}_{s'}\right] \quad (8)$$

with the Dirac wave functions. An independent derivation of this operator was done in [12]. The operator (8) was employed in [13] to calculate the $(\alpha Z)^4 m^2/M$ corrections to the energy levels of two- and three-electron multicharged ions.

In the present paper we generalize the theory of the nuclear recoil effect to an arbitrary case of a many-electron atom. In particular, this generalization allows one to use as the zero approximation a potential that is different from the pure Coulomb field. In addition, it allows one to use the formalism in which the closed shells are referred to the vacuum state. In Sec. II we formulate the basic equations of the method. In Sec. III we apply this method to an atom with one electron over closed shells. In Sec. IV the case of an atom with two electrons over closed shells is considered. In Sec. V the problem of the composite nuclear structure is discussed.

II. BASIC FORMALISM

As in Refs. [3, 4], we will consider the nucleus as a nonrelativistic particle. In the Schrödinger representation and the Coulomb gauge, the Hamiltonian of the whole system is

$$\begin{aligned}H=&\int d\mathbf{x}\ \psi^\dagger(\mathbf{x})\{\boldsymbol{\alpha}\cdot[-i\nabla_{\mathbf{x}}-e\mathbf{A}(\mathbf{x})]+\beta m\}\psi(\mathbf{x})\\&+\frac{e^2}{8\pi}\int d\mathbf{x}\,d\mathbf{y}\,\frac{\rho_e(\mathbf{x})\rho_e(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}+\frac{1}{2}\int d\mathbf{x}[\mathcal{E}_t^2(\mathbf{x})+\boldsymbol{\mathcal{H}}^2(\mathbf{x})]\\&+\frac{e|e|Z}{4\pi}\int d\mathbf{x}\,\frac{\rho_e(\mathbf{x})}{|\mathbf{x}-\mathbf{X}_n|}+\frac{1}{2M}[\mathbf{P}_n-|e|Z\mathbf{A}(\mathbf{X}_n)]^2\\&-\boldsymbol{\mu}\cdot\boldsymbol{\mathcal{H}}(\mathbf{X}_n),\end{aligned} \quad (9)$$

where m is the electron mass, M is the nucleus mass, e is the electron charge ($e<0$), $\mathbf{X}_n$ is the radius vector of the nucleus, $\mathbf{P}_n=-i\nabla_{\mathbf{X}_n}$, and $\boldsymbol{\mu}$ is the magnetic moment of the nucleus. The term $-\boldsymbol{\mu}\cdot\boldsymbol{\mathcal{H}}$ causes the hyperfine splitting structure of atomic levels and will not be discussed here. The total momentum of the system is given by

$$\mathbf{P}=\mathbf{P}_n+\mathbf{P}_e+\mathbf{P}_f, \quad (10)$$

where $\mathbf{P}_e=\int d\mathbf{x}\ \psi^\dagger(\mathbf{x})(-i\nabla_{\mathbf{x}})\psi(\mathbf{x})$ is the electron-positron field momentum and $\mathbf{P}_f=\int d\mathbf{x}[\mathcal{E}_t(\mathbf{x})\times\boldsymbol{\mathcal{H}}(\mathbf{x})]$ is the electromagnetic field momentum. Since the total momentum is an integral of the motion, we can restrict our consideration to the center-of-mass system ($\mathbf{P}=0$) and so can express the nuclear momentum in terms of the electron-positron and electromagnetic-field momenta,

$$\begin{aligned}\mathbf{P}_n=-\mathbf{P}_e-\mathbf{P}_f=&-\int d\mathbf{x}\ \psi^\dagger(\mathbf{x})(-i\nabla_{\mathbf{x}})\psi(\mathbf{x})\\&-\int d\mathbf{x}[\mathcal{E}_t(\mathbf{x})\times\boldsymbol{\mathcal{H}}(\mathbf{x})].\end{aligned} \quad (11)$$

Using this equation and the translation invariance, we find

$$\begin{aligned}H=&\int d\mathbf{x}\ \psi^\dagger(\mathbf{x})\{\boldsymbol{\alpha}\cdot[-i\nabla_{\mathbf{x}}-e\mathbf{A}(\mathbf{x})]+\beta m\}\psi(\mathbf{x})\\&+\frac{e^2}{8\pi}\int d\mathbf{x}\,d\mathbf{y}\,\frac{\rho_e(\mathbf{x})\rho_e(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}+\frac{1}{2}\int d\mathbf{x}[\mathcal{E}_t^2(\mathbf{x})+\boldsymbol{\mathcal{H}}^2(\mathbf{x})]\\&+\frac{e|e|Z}{4\pi}\int d\mathbf{x}\,\frac{\rho_e(\mathbf{x})}{|\mathbf{x}|}+\frac{1}{2M}\left[-\int d\mathbf{x}\ \psi^\dagger(\mathbf{x})\right.\\&\left.\times(-i\nabla_{\mathbf{x}})\psi(\mathbf{x})-\int d\mathbf{x}[\mathcal{E}_t(\mathbf{x})\times\boldsymbol{\mathcal{H}}(\mathbf{x})]-|e|Z\mathbf{A}(0)\right]^2.\end{aligned} \quad (12)$$

Here we have omitted the hyperfine interaction term. The sum of the first four terms in Eq. (12) is the standard Hamiltonian of the electron-positron field interacting with the quantized electromagnetic field and with the classical Coulomb field of the nucleus $V_c=-\alpha Z/r$ [a finite nuclear charge distribution can be taken into account by replacing V_c with the potential of an extended nucleus (see Sec. V)]. The last term in Eq. (12) defines the nuclear recoil corrections of the first order in m/M. The part of this term containing the electromagnetic-field momentum ($\mathbf{P}_f=\int d\mathbf{x}[\mathcal{E}_t(\mathbf{x})\times\boldsymbol{\mathcal{H}}(\mathbf{x})]$) will contribute only in the first and higher orders in α and, so will not be discussed here. It follows, to the zeroth order in α, that the nuclear recoil corrections can be calculated by adding to the standard Hamiltonian the following term:

$$\begin{aligned}H_M=&\frac{1}{2M}\int d\mathbf{x}\ \psi^\dagger(\mathbf{x})(-i\nabla_{\mathbf{x}})\psi(\mathbf{x})\int d\mathbf{y}\ \psi^\dagger(-i\nabla_{\mathbf{y}})\psi(\mathbf{y})\\&-\frac{eZ}{M}\int d\mathbf{x}\ \psi^\dagger(\mathbf{x})(-i\nabla_{\mathbf{x}})\psi(\mathbf{x})\mathbf{A}(0)+\frac{e^2Z^2}{2M}\mathbf{A}^2(0).\end{aligned} \quad (13)$$

As is known, for a description of a many-electron atom within QED it is convenient to use the interaction representation in the Furry picture. In such a theory the normal ordered form of H_M taken in the interaction representation must be added to the interaction Hamiltonian. To derive the formal expressions for the energy-level shifts we will use the method developed in [14,15]. It is based on the application of the Sz-Nagy and Kato technique [16] to the two-time Green function. This method is briefly formulated below (the most detailed description of the method is given in [15]).

We consider that in the zero approximation the electrons interact only with the nuclear Coulomb field or with an effective atomic potential (e.g., a local version of the Hartree-Fock potential). In the last case the corresponding subtraction must be done in the interaction Hamiltonian to eliminate double accounting the interelectronic interaction corrections.

For a description of an N-electron atom in the framework of QED we introduce the Fourier transform of the two-time Green function by

$$g(E)\,\delta(E-E') = \frac{1}{2\pi i}\,\frac{1}{N!}\int dx'^0 dx^0 \exp(iE'x'^0 - iEx^0) \times \langle 0|T\psi(x'^0,\mathbf{x}'_1)\cdots\psi(x'^0,\mathbf{x}'_N) \times \psi^\dagger(x^0,\mathbf{x}_N)\cdots\psi^\dagger(x^0,\mathbf{x}_1)|0\rangle, \tag{14}$$

where $\psi(x)$ is the electron-positron field operator in the Heisenberg representation, and T is the time-ordered product operator. The bound states of the atom correspond to the poles of $g(E)$ in the complex E plane. Denoting the unperturbed wave function of the state under consideration by u_a, we introduce

$$g_a(E) = \langle u_a|g(E)|u_a\rangle. \tag{15}$$

The spectral representation of $g(E)$ gives

$$g_a(E) = \frac{A_a}{E-E_a} + (\text{terms that are regular by } E\sim E_a), \tag{16}$$

where E_a is the exact energy of the level and A_a is a constant. Choosing the contour Γ so that it surrounds the level a and does not surround other levels, we have

$$\frac{1}{2\pi i}\oint_\Gamma dE\; Eg_a(E) = E_a A_a, \tag{17}$$

$$\frac{1}{2\pi i}\oint_\Gamma dE\; g_a(E) = A_a, \tag{18}$$

where the contour is assumed to be traversed counterclockwise. Dividing Eq. (17) by Eq. (18) we obtain

$$E_a = \frac{\dfrac{1}{2\pi i}\oint_\Gamma dE\; Eg_a(E)}{\dfrac{1}{2\pi i}\oint_\Gamma dE\; g_a(E)}. \tag{19}$$

Taking into account that in the zero approximation

$$g_a^{(0)} = \frac{1}{E-E_a^{(0)}}, \tag{20}$$

where $E_a^{(0)}$ is the unperturbed energy (which is the sum of the one-electron Dirac energies), and denoting $\Delta g_a = g_a - g_a^{(0)}$, one can obtain for the energy shift

$$\Delta E_a \equiv E_a - E_a^{(0)} = \frac{\dfrac{1}{2\pi i}\oint_\Gamma dE(E-E_a^{(0)})\Delta g_a(E)}{1+\dfrac{1}{2\pi i}\oint_\Gamma dE\,\Delta g_a(E)}. \tag{21}$$

In the first order of the perturbation theory we have

$$\Delta E_a^{(1)} = \frac{1}{2\pi i}\oint_\Gamma dE(E-E_a^{(0)})\Delta g_a^{(1)}(E). \tag{22}$$

For the practical calculations it is convenient to express the Green function $g_a(E)$ in terms of the Fourier transform of the $2N$-time Green function

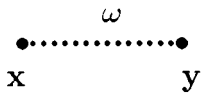
$$g_a(E)\,\delta(E-E') = \frac{2\pi}{i}\,\frac{1}{N!}\int_{-\infty}^{\infty} dp_1^0\cdots dp_N^0 dp_1'^0\cdots dp_N'^0 \times \delta(E-p_1^0-\cdots-p_N^0) \times \delta(E'-p_1'^0-\cdots-p_N'^0) \times \langle u_a|G(p_1'^0,\ldots,p_N'^0;p_1^0,\ldots,p_N^0) \times \gamma_1^0\cdots\gamma_N^0|u_a\rangle, \tag{23}$$

where

$$G(p_1'^0,\ldots,p_N'^0;p_1^0,\ldots,p_N^0) = (2\pi)^{-2N}\int_{-\infty}^{\infty} dx_1^0\cdots dx_N^0 dx_1'^0\cdots dx_N'^0 \times \exp(ip_1'^0x_1'^0+\cdots+ip_N'^0x_N'^0-ip_1^0x_1^0-\cdots-ip_N^0x_N^0) \times \langle 0|T\psi(x_1')\cdots\psi(x_N')\overline{\psi}(x_N)\cdots\overline{\psi}(x_1)|0\rangle, \tag{24}$$

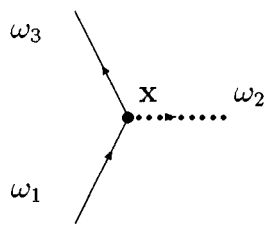
$\overline{\psi}(x) = \psi^\dagger(x)\gamma^0$. The Green function G is constructed using the Wick theorem after the transition in Eq. (24) to the interaction representation. The diagram technique rules for G, without the term H_M in the interaction Hamiltonian, were considered in detail in [15] and are summarized in the Appendix. Including H_M in the interaction Hamiltonian gives the following additional lines and vertices to the diagram technique rules.

(i) *Coulomb contribution.* An additional line (''Coulomb-recoil'' line) appears to be



$$\frac{i}{2\pi}\frac{\delta_{kl}}{M}\int_{-\infty}^{\infty} d\omega\,.$$

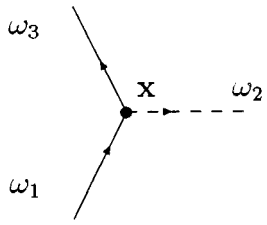
This line joins two vertices each of which corresponds to



$$-i2\pi\gamma_0\delta(\omega_1-\omega_2-\omega_3)\int d\mathbf{x}\,p_k\,,$$

where $\mathbf{p} = -i\nabla_{\mathbf{x}}$ and $k = 1,2,3$.

(ii) *One-transverse-photon contribution.* An additional vertex on an electron line appears to be



$$-i2\pi\gamma_0\delta(\omega_1-\omega_2-\omega_3)\frac{eZ}{M}\int d\mathbf{x}\,p_k\ ,$$

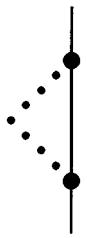
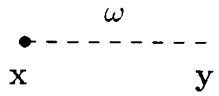


FIG. 1. Coulomb nuclear recoil diagram.

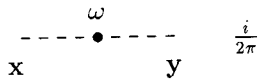
The transverse photon line attached to this vertex (at the point **x**) is



$$\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega D_{kl}(\omega,\mathbf{y})\,.$$

At the point **y** this line is to be attached to a usual vertex in which we have $-ie\gamma_0\alpha_l 2\pi\delta(\omega_1-\omega_2-\omega_3)\int d\mathbf{y}$ (see the Appendix), where α_l ($l=1,2,3$) are the usual Dirac matrices [we note here that in the notations of [15] $\alpha^\mu=(1,\boldsymbol{\alpha})$ and $\alpha_\mu=(1,-\boldsymbol{\alpha})$].

(iii) *Two-transverse-photon contribution.* An additional line (''two-transverse-photon-recoil'' line) appears to be



$$\frac{i}{2\pi}\frac{e^2Z^2}{M}\int_{-\infty}^{\infty}d\omega D_{il}(\omega,\mathbf{x})D_{lk}(\omega,\mathbf{y})\,.$$

This line joins usual vertices (see the previous item).

An important advantage of the approach considered here, in comparison with the one developed in [1,11], consists in the present method being suitable for arbitrary local potential $V(r)$ (e.g., a local version of the Hartree-Fock potential) used as the zero approximation. In addition, the transition to the formalism in which the role of the vacuum is played by closed shells can simply be realized by changing the sign of $i0$ in the electron propagator denominators corresponding to the closed shells.

III. ONE ELECTRON OVER CLOSED SHELLS

Let us consider an atom with one electron over closed shells. In the zero approximation the electrons of the atom interact with the potential $V(r)$, which can be chosen to include approximately the electron-electron interaction. In the formalism with the closed-shell states as well as the negative-energy states referred to the vacuum, the electron propagator is given by

$$S(\omega,\mathbf{x},\mathbf{y})=\sum_n\ \frac{\psi_n(\mathbf{x})\overline{\psi_n}(\mathbf{y})}{\omega-\varepsilon_n+i\,\eta_n 0}, \tag{25}$$

where $\eta_n=\varepsilon_n-\varepsilon_F$ and ε_F is the Fermi energy, which is chosen to be higher than the one-electron closed-shell energies and lower than the energies of the one-electron states over the closed shells. In the simplest case of a one-electron atom, $\eta_n=\varepsilon_n$.

To find the Coulomb nuclear recoil correction we have to calculate the contribution of the diagram shown in Fig. 1. According to the diagram technique rules given in the previous section and in the Appendix, we obtain

$$\Delta g_a^{(1)}=\frac{1}{(E-E_a^{(0)})^2}\,\frac{1}{M}\,\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\sum_n\ \frac{\langle a|p_i|n\rangle\langle n|p_i|a\rangle}{\omega-\epsilon_n+i\,\eta_n 0}. \tag{26}$$

The formula (22) gives

$$\Delta E_c=\frac{1}{M}\,\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\sum_n\ \frac{\langle a|p_i|n\rangle\langle n|p_i|a\rangle}{\omega-\varepsilon_n+i\,\eta_n 0}. \tag{27}$$

Using the identities

$$\frac{1}{x+i0}=\frac{\pi}{i}\,\delta(x)+P\,\frac{1}{x}, \tag{28}$$

$$\frac{1}{x-i0}=\pi i\,\delta(x)+P\,\frac{1}{x}, \tag{29}$$

one can get

$$\Delta E_c=\frac{1}{2M}\sum_n\ \frac{\eta_n}{|\eta_n|}\,|\langle a|\mathbf{p}|n\rangle|^2$$

$$=\frac{1}{2M}\,\langle a|\mathbf{p}^2|a\rangle-\frac{1}{M}\sum_{\varepsilon_n<\varepsilon_F}|\langle a|\mathbf{p}|n\rangle|^2. \tag{30}$$

The one-transverse-photon nuclear recoil correction corresponds to the diagrams shown in Fig. 2. A similar calculation gives

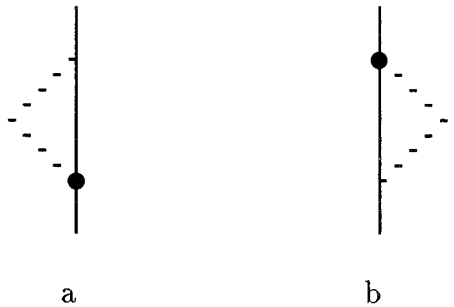


FIG. 2. One-transverse-photon nuclear recoil diagrams.

FIG. 3. Two-transverse-photon nuclear recoil diagram.

$$\Delta E_{\mathrm{tr}(1)}=\frac{4\pi\alpha Z}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega \times\sum_n\left\{\frac{\langle a|p_i|n\rangle\langle n|\alpha_k D_{ik}(\varepsilon_a-\omega)|a\rangle}{\omega-\varepsilon_n+i\eta_n 0}+\frac{\langle a|\alpha_k D_{ik}(\varepsilon_a-\omega)|n\rangle\langle n|p_i|a\rangle}{\omega-\varepsilon_n+i\eta_n 0}\right\}. \quad (31)$$

By using the identity

$$\frac{1}{\omega-\varepsilon_n+i\eta_n 0}=\frac{1}{\omega-\varepsilon_a+i0}+\frac{\varepsilon_n-\varepsilon_a}{(\omega-\varepsilon_a+i0)(\omega-\varepsilon_n+i\eta_n 0)}$$

and Eq. (28), the expression (31) can easily be transformed to the following:

$$\Delta E_{\mathrm{tr}(1)}=\Delta E^{(1)}_{\mathrm{tr}(1)}+\Delta E^{(2)}_{\mathrm{tr}(1)},$$

$$\Delta E^{(1)}_{\mathrm{tr}(1)}=\frac{4\pi\alpha Z}{2M}\langle a|[p_i\alpha_k D_{ik}(0)+\alpha_k D_{ik}(0)p_i]|a\rangle, \quad (32)$$

$$\Delta E^{(2)}_{\mathrm{tr}(1)}=\frac{4\pi\alpha Z}{M}\int_{-\infty}^{\infty}d\omega\ \delta_+(\omega-\varepsilon_a) \times\sum_n\left\{\frac{\langle a|[p_i,V]|n\rangle\langle n|\alpha_k D_{ik}(\varepsilon_a-\omega)|a\rangle}{\omega-\varepsilon_n+i\eta_n 0}-\frac{\langle a|\alpha_k D_{ik}(\varepsilon_a-\omega)|n\rangle\langle n|[p_i,V]|a\rangle}{\omega-\varepsilon_n+i\eta_n 0}\right\}. \quad (33)$$

The two-transverse-photon nuclear recoil correction is defined by the diagram shown in Fig. 3. We find

$$\Delta E_{\mathrm{tr}(2)}=\frac{(4\pi\alpha Z)^2}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega \times\sum_n\frac{\langle a|\alpha_i D_{il}(\varepsilon_a-\omega)|n\rangle\langle n|\alpha_k D_{lk}(\varepsilon_a-\omega)|a\rangle}{\omega-\varepsilon_n+i\eta_n 0}. \quad (34)$$

As follows from the Eqs. (27), (31), and (34), the sum of all the contributions can be written in the following compact form:

$$\Delta E_{\mathrm{tot}}=\frac{1}{M}\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\langle a|[p_i+4\pi\alpha Z\alpha_l D_{li}(\omega)]G(\omega+\varepsilon_a) \times[p_i+4\pi\alpha Z\alpha_m D_{mi}(\omega)]|a\rangle, \quad (35)$$

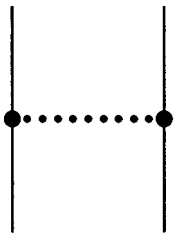


FIG. 4. Two-electron Coulomb nuclear recoil diagram.

where $G(\varepsilon)=\Sigma_n(\varepsilon-\varepsilon_n+i\eta_n 0)^{-1}|n\rangle\langle n|$ is the electron Green function. In the case of a hydrogenlike atom, the expressions derived here coincide with the ones given in Sec. I.

IV. TWO ELECTRONS OVER CLOSED SHELLS

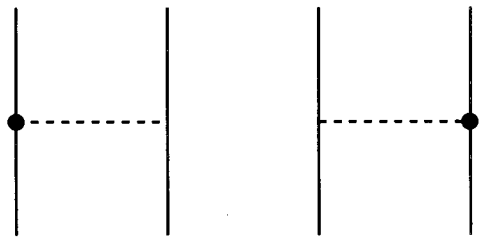
Consider now an atom with two electrons over closed shells (a general case of N electrons over closed shells can be considered in the same way). For simplicity, we take as the unperturbed wave function the one-determinant wave function

$$u=\frac{1}{\sqrt{2}}\sum_P(-1)^P\psi_{Pa}(\mathbf{x}_1)\psi_{Pb}(\mathbf{x}_2). \quad (36)$$

The nuclear recoil correction is the sum of the one-electron and two-electron contributions. Using the diagram technique rules from the Appendix and Sec. II and the formula (22), one easily finds that the one-electron contribution is equal to the sum of the expressions (35) for the a and b states. The two-electron contributions correspond to the diagrams shown in Figs. 4–6. The two-electron Coulomb contribution is

$$\Delta E^{(\mathrm{int})}_c=\frac{1}{M}\frac{1}{2\pi i}\oint_\Gamma dE(E-E^{(0)}) \times\left\{\left(\frac{i}{2\pi}\right)^2\int_{-\infty}^{\infty}dp^0dp'^0\sum_P(-1)^P\frac{1}{p'^0-\varepsilon_{Pa}+i0} \times\frac{1}{E-p'^0-\varepsilon_{Pb}+i0}\frac{1}{p^0-\varepsilon_a+i0}\frac{1}{E-p^0-\varepsilon_b+i0} \times\langle Pa|p_i|a\rangle\langle Pb|p_i|b\rangle\right\}. \quad (37)$$

Integrating over p^0, p'^0, and E we get



a b

FIG. 5. Two-electron one-transverse-photon nuclear recoil diagrams.

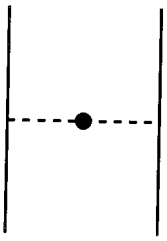


FIG. 6. Two-electron two-transverse-photon nuclear recoil diagram.

$$\Delta E_c^{(\mathrm{int})}=\frac{1}{M}\sum_P\,(-1)^P\langle Pa|p_i|a\rangle\langle Pb|p_i|b\rangle. \qquad (38)$$

A similar calculation of the one-transverse-photon contribution gives

$$\begin{aligned}\Delta E_{\mathrm{tr}(1)}^{(\mathrm{int})}=&\frac{4\pi\alpha Z}{M}\sum_P\,(-1)^P[\langle Pa|p_i|a\rangle\\ &\times\langle Pb|\alpha_k D_{ki}(\varepsilon_{Pb}-\varepsilon_b)|b\rangle\\ &+\langle Pa|\alpha_k D_{ki}(\varepsilon_{Pa}-\varepsilon_a)|a\rangle\\ &\times\langle Pb|p_i|b\rangle]. \qquad (39)\end{aligned}$$

Finally, for the two-transverse-photon contribution we find

$$\begin{aligned}\Delta E_{\mathrm{tr}(2)}^{(\mathrm{int})}=&\frac{(4\pi\alpha Z)^2}{M}\sum_P\,(-1)^P[\langle Pa|\alpha_k D_{ki}(\varepsilon_{Pa}-\varepsilon_a)|a\rangle\\ &\times\langle Pb|\alpha_m D_{mi}(\varepsilon_{Pb}-\varepsilon_b)|b\rangle. \qquad (40)\end{aligned}$$

The sum of the two-electron contributions (38)–(40) can be written in the following compact form:

$$\begin{aligned}\Delta E_{\mathrm{tot}}^{(\mathrm{int})}=&\frac{1}{M}\sum_P\,(-1)^P\langle Pa|p_i+4\pi\alpha Z\alpha_l D_{li}(\varepsilon_{Pa}-\varepsilon_a)|a\rangle\\ &\times\langle Pb|p_i+4\pi\alpha Z\alpha_m D_{mi}(\varepsilon_{Pb}-\varepsilon_b)|b\rangle. \qquad (41)\end{aligned}$$

The formulas (38)–(41) coincide with the related expressions found for high-Z few-electron atoms in [11] (see also [7]). The only difference is that the present expressions (38)–(41) are not restricted to the case of the pure Coulomb zero approximation.

V. COMPOSITE NUCLEAR STRUCTURE

The problem of the composite nuclear structure in the nuclear recoil theory was first discussed by Salpeter [6]. In Ref. [6], it was shown that the calculations based on the assumption that the nucleus is a point Dirac particle of electric charge $|e|Z$ and mass M are valid for composite nuclei (independently of the nuclear spin), if the distance between the nuclear levels is large compared with the distance between the atomic (electrons plus field) levels contributing to the nuclear recoil effect. In this section we consider how this result [which is not quite obvious for the term quadratic in $\mathbf{A}(\mathbf{0})$] can be derived within the approach developed in the present paper.

Let us assume, for simplicity, that the nucleus is a bound state of a two-particle system (e.g., a core with a mass m_1 and a charge e_1 and a valent nucleon with a mass m_2 and a charge e_2). In this case the sum of the last three terms in Eq. (9) must be replaced by $H_1+H_2+H_3$, where

$$H_1=\frac{e}{4\pi}\int d\mathbf{x}\;\rho_e(\mathbf{x})\left(\frac{e_1}{|\mathbf{x}-\mathbf{x}_1|}+\frac{e_2}{|\mathbf{x}-\mathbf{x}_2|}\right), \qquad (42)$$

$$\begin{aligned}H_2=&\frac{1}{2m_1}\,[\mathbf{p}_1-e_1\mathbf{A}(\mathbf{x}_1)]^2+\frac{1}{2m_2}\,[\mathbf{p}_2-e_2\mathbf{A}(\mathbf{x}_2)]^2\\ &+U(\mathbf{x}_1-\mathbf{x}_2), \qquad (43)\end{aligned}$$

$$H_3=-\boldsymbol{\mu}_s^{(1)}\cdot\boldsymbol{\mathcal{H}}(\mathbf{x}_1)-\boldsymbol{\mu}_s^{(2)}\cdot\boldsymbol{\mathcal{H}}(\mathbf{x}_2). \qquad (44)$$

Here $U(\mathbf{x}_1-\mathbf{x}_2)$ describes the interaction between the nuclear particles (for simplicity, we assume that U does not depend on the spins) and $\boldsymbol{\mu}_s^{(1)}$ and $\boldsymbol{\mu}_s^{(2)}$ are the intrinsic magnetic moments of the nuclear particles. Introducing the center-of-nucleus-mass variables

$$\mathbf{X}_n=\frac{m_1\mathbf{x}_1+m_2\mathbf{x}_2}{m_1+m_2},\quad \mathbf{x}_n=\mathbf{x}_1-\mathbf{x}_2, \qquad (45)$$

we have

$$\mathbf{p}_1=\frac{m_1}{m_1+m_2}\,\mathbf{P}_n+\mathbf{p}_n,\quad \mathbf{p}_2=\frac{m_2}{m_1+m_2}\,\mathbf{P}_n-\mathbf{p}_n, \qquad (46)$$

where $\mathbf{P}_n=-\nabla_{\mathbf{X}_n}$ and $\mathbf{p}_n=-\nabla_{\mathbf{x}_n}$. As in the Sec. II, we can restrict our consideration to the center-of-atom-mass system ($\mathbf{P}=\mathbf{P}_n+\mathbf{P}_e+\mathbf{P}_f=0$). So, the total nuclear momentum $\mathbf{P}_n$ is given by Eq. (11). In terms of the variables $\mathbf{X}_n$ and $\mathbf{x}_n$ the operator H_2 can be represented in the form

$$H_2=H_\mu+H_M, \qquad (47)$$

where

$$H_\mu=\frac{\mathbf{p}_n^2}{2\mu}+U(\mathbf{x}_n), \qquad (48)$$

and $\mu=(m_1m_2)/(m_1+m_2)$. The Hamiltonian H_μ describes the intrinsic states of the nucleus. Let us denote the wave function of the nuclear state that is under the consideration by $\phi_a(\mathbf{x}_n)$. The wave function of the whole system in the zero approximation is the product of $\phi_a(\mathbf{x}_n)$ and the atomic wave function calculated using the operator $\langle\phi_a|H_1|\phi_a\rangle$ as the interaction with the nucleus (we assume here and subsequently that the distance between the nuclear energy levels is large compared with the distance between the atomic levels). The operator $\langle\phi_a|H_1|\phi_a\rangle$ describes the interaction of electrons with the extended nucleus charge. The m/M corrections are calculated by perturbation theory. Using the fact that the nuclear size ($\sim|\mathbf{x}_n|$) is much smaller than the atomic size, we expand the vector $\mathbf{A}$ in powers of $\mathbf{x}_n$. Taking into account that $\phi_a(\mathbf{x}_n)$ is of a definite parity we find to the lowest orders

$$\langle\phi_a|H_M|\phi_a\rangle=\langle\phi_a|\Bigg\{\frac{\mathbf{P}_n^2}{2M}-\frac{(e_1+e_2)}{2M}\,[\mathbf{P}_n\cdot\mathbf{A}(\mathbf{X}_n)+\mathbf{A}(\mathbf{X}_n)\cdot\mathbf{P}_n]+\left(\frac{e_1^2}{2m_1}+\frac{e_2^2}{2m_2}\right)\mathbf{A}^2(\mathbf{X}_n)-\frac{1}{2M}\left(\frac{e_1m_2}{m_1}+\frac{e_2m_1}{m_2}\right)[\mathbf{p}_n(\mathbf{x}_n\cdot\nabla_{\mathbf{X}_n})\mathbf{A}(\mathbf{X}_n)+(\mathbf{x}_n\cdot\nabla_{\mathbf{X}_n})\mathbf{A}(\mathbf{X}_n)\mathbf{p}_n]\Bigg\}|\phi_a\rangle. \tag{49}$$

The last term in Eq. (49) can be transformed to

$$-\frac{1}{2M}\left(\frac{e_1m_2}{m_1}+\frac{e_2m_1}{m_2}\right)\int d\mathbf{x}_n\phi_a^*(\mathbf{x}_n)\times(\mathbf{x}_n\times\mathbf{p}_n)\phi_a(\mathbf{x}_n)\boldsymbol{\mathcal{H}}(\mathbf{X}_n)=-\left(\frac{e_1}{2m_1}\langle\boldsymbol{l}_1\rangle+\frac{e_2}{2m_2}\langle\boldsymbol{l}_2\rangle\right)\boldsymbol{\mathcal{H}}(\mathbf{X}_n), \tag{50}$$

where $\boldsymbol{l}_1$ and $\boldsymbol{l}_2$ are the orbital moments of the nuclear particles in the center-of-nucleus-mass system. Adding this term to the term H_3 gives the total operator of the hyperfine interaction $-\boldsymbol{\mu}\cdot\boldsymbol{\mathcal{H}}(\mathbf{X}_n)$, where $\boldsymbol{\mu}=\boldsymbol{\mu}_l^{(1)}+\boldsymbol{\mu}_s^{(1)}+\boldsymbol{\mu}_l^{(2)}+\boldsymbol{\mu}_s^{(2)}$ is the total magnetic moment of the nucleus and $\boldsymbol{\mu}_l^{(i)}=(e_i/2m_i)\boldsymbol{l}_i$. Since the operator H_M contains the term

$$H_M'=-\left(\frac{e_1}{m_1}-\frac{e_2}{m_2}\right)\mathbf{p}_n\cdot\mathbf{A}(\mathbf{X}_n), \tag{51}$$

there is a contribution of the order m/M from the second order of the perturbation theory. For a state a of the whole system we have

$$\Delta E_a'=\left(\frac{e_1}{m_1}-\frac{e_2}{m_2}\right)^2\sum_{n\neq a}\frac{\langle a|\mathbf{p}_n\cdot\mathbf{A}(\mathbf{X}_n)|n\rangle\langle n|\mathbf{p}_n\cdot\mathbf{A}(\mathbf{X}_n)|a\rangle}{E_a-E_n}. \tag{52}$$

Assuming that the energy difference between the nuclear state that is under the consideration and the other nuclear states contributing to the sum in Eq. (52) is large compared with the corresponding energy differences between the atomic (electrons plus field) states that give a dominant contribution to $\Delta E_a'$, we replace E_a-E_n in Eq. (52) with $\varepsilon_a-\varepsilon_n$, where ε_a and ε_n are the nuclear energies. Using the identity $\mathbf{p}_n=i\mu[H_\mu,\mathbf{x}_n]$, we find

$$\begin{aligned}\Delta E_a'&=\left(\frac{e_1}{m_1}-\frac{e_2}{m_2}\right)^2\langle\Phi_a|\mathbf{A}^2(\mathbf{X}_n)|\Phi_a\rangle\,\frac{i}{2}\,\mu\sum_{n\neq a}\frac{1}{\varepsilon_a-\varepsilon_n}[\langle\phi_a|[H_\mu,\mathbf{x}_n]|\phi_n\rangle\langle\phi_n|\mathbf{p}_n|\phi_a\rangle+\langle\phi_a|\mathbf{p}_n|\phi_n\rangle\langle\phi_n|[H_\mu,\mathbf{x}_n]|\phi_a\rangle]\\&=\left(\frac{e_1}{m_1}-\frac{e_2}{m_2}\right)^2\langle\Phi_a|\mathbf{A}^2(\mathbf{X}_n)|\Phi_a\rangle\,\frac{i}{2}\,\mu\sum_{n\neq a}[\langle\phi_a|\mathbf{x}_n|\phi_n\rangle\langle\phi_n|\mathbf{p}_n|\phi_a\rangle-\langle\phi_a|\mathbf{p}_n|\phi_n\rangle\langle\phi_n|\mathbf{x}_n|\phi_a\rangle]\\&=\left(\frac{e_1}{m_1}-\frac{e_2}{m_2}\right)^2\langle\Phi_a|\mathbf{A}^2(\mathbf{X}_n)|\Phi_a\rangle\,\frac{i}{2}\,\mu\langle\phi_a|[\mathbf{x}_n,\mathbf{p}_n]|\phi_a\rangle\\&=-\frac{1}{2}\left(\frac{e_1}{m_1}-\frac{e_2}{m_2}\right)^2\mu\langle\Phi_a|\mathbf{A}^2(\mathbf{X}_n)|\Phi_a\rangle,\end{aligned} \tag{53}$$

where $|\phi_a\rangle$ is the nuclear wave function and $|\Phi_a\rangle$ is the atomic (electrons plus field) wave function. Combining this term with Eq. (49), we find that the nuclear recoil correction of the first order in m/M is defined by the operator

$$H_M=\frac{\mathbf{P}_n^2}{2M}-\frac{(e_1+e_2)}{2M}\,[\mathbf{P}_n\cdot\mathbf{A}(\mathbf{X}_n)+\mathbf{A}(\mathbf{X}_n)\cdot\mathbf{P}_n]+\frac{(e_1+e_2)^2}{2M}\,\mathbf{A}^2(\mathbf{X}_n)=\frac{1}{2M}\,[\mathbf{P}_n-|e|Z\mathbf{A}(\mathbf{X}_n)]^2. \tag{54}$$

So, within the approximations made above, we may consider the nucleus as a structureless particle of mass M. The error due to these approximations depends on the specific nuclear structure. In the case of deuterium it was estimated by Salpeter [6] to be about 10%.

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APPENDIX: FEYNMAN RULES FOR *G*

(i) The external electron line

$$\overbrace{\mathbf{x}\qquad\qquad\mathbf{y}}\qquad \frac{i}{2\pi}S(\omega,\mathbf{x},\mathbf{y}),$$

where, in the formalism with the usual vacuum,

$$S(\omega,\mathbf{x},\mathbf{y})=\sum_n\frac{\psi_n(\mathbf{x})\overline{\psi}_n(\mathbf{y})}{\omega-\varepsilon_n(1-i0)},$$

$\psi_n(\mathbf{x})$ are the solutions of the Dirac equation

$$(\boldsymbol{\alpha}\cdot\mathbf{p}+\beta m+V)\psi_n=\varepsilon_n\psi_n\,.$$

(ii) The internal electron line

$\mathbf{x}$ ——— $\mathbf{y}$ $\quad \frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\; S(\omega,\mathbf{x},\mathbf{y})\,.$

(iii) The separate electron line, which is not connected with others

$\mathbf{x}$ ——— $\mathbf{y}$ $\quad \frac{i}{2\pi}S(\omega,\mathbf{x},\mathbf{y})\delta(\omega-\omega')\,.$

(iv) The internal photon line

$\cdots\cdots$ $\quad \frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega D_{\mu\nu}(\omega,\mathbf{x}-\mathbf{y})\,,$

where

$$D_{\mu\nu}(\omega,\mathbf{x}-\mathbf{y})=-g_{\mu\nu}\int\frac{d\mathbf{k}}{(2\pi)^3}\,\frac{\exp\left[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})\right]}{\omega^2-\mathbf{k}^2+i0}$$

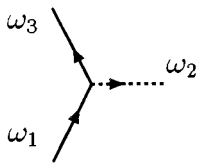
in the Feynman gauge and

$$D_{00}(\omega,\mathbf{x}-\mathbf{y})=\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\,,\quad D_{i0}=D_{0i}=0\qquad(i=1,2,3)\,,$$

$$D_{il}(\omega,\mathbf{x}-\mathbf{y})=\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{\exp\left[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})\right]}{\omega^2-\mathbf{k}^2+i0}\left(\delta_{il}-\frac{k_ik_l}{\mathbf{k}^2}\right)\qquad(i,l=1,2,3)$$

in the Coulomb gauge.

(v) The vertex



$$-ie\gamma^{\mu}2\pi\delta(\omega_1-\omega_2-\omega_3)\int d\mathbf{x}\,,$$

where $\gamma^{\mu}=(\beta,\beta\alpha)$; β, α are Dirac's matrices.

(vi) The symmetry factor $(-1)^P$, where P is the parity of the permutation of the final electron coordinates with respect to the initial ones. For every closed electron loop a minus sign is added.

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