Relativistic nuclear recoil corrections to the energy levels of hydrogenlike and high-Z lithiumlike atoms in all orders in αZ

A.N. Artemyev, V.M. Shabaev, and V.A. Yerokhin
Department of Physics, St. Petersburg State University, Oulianovskaya 1, Petrodvorets, St. Petersburg 198904, Russia
(Received 14 December 1994; revised manuscript received 20 March 1995)

The relativistic nuclear recoil corrections to the energy levels of low-lying states of hydrogenlike and high-Z lithiumlike atoms in all orders in αZ are calculated. The calculations are carried out using the B-spline method for the Dirac equation. For low Z the results of the calculation are in good agreement with the αZ-expansion results. It is found that the nuclear recoil contribution, in addition to Salpeter's contribution, to the Lamb shift ($n = 2$) of hydrogen is $-1.32(6)$ kHz. The total nuclear recoil correction to the energy of the $(1s)^2 2p_{\frac{1}{2}}$-$(1s)^2 2s$ transition in lithiumlike uranium constitutes -0.07 eV.

PACS number(s): 12.20.Ds, 31.30.Jv

I. INTRODUCTION

As is known, in the nonrelativistic approximation the nuclear recoil correction for a hydrogenlike atom can be taken into account by using the reduced mass $\mu = \frac{mM}{m+M}$. The relativistic corrections of order $(\alpha Z)^4 \frac{m}{M} mc^2$ can be found by employing the Breit equation [1]. A theory of the nuclear recoil effect in higher orders in αZ must be constructed in the framework of quantum electrodynamics (QED) on the basis of an exact relativistic equation for the hydrogenlike atom. Such an equation was proposed by Bethe and Salpeter [2] immediately after the creation of QED. On the basis of this equation the nuclear recoil corrections were calculated in [3] up to terms of order $(\alpha Z)^5 \frac{m}{M} mc^2$. It was shown in this work that the nuclear recoil effect in the case of a complex nucleus is calculated in a good approximation by assuming the nucleus is a Dirac particle with the charge $|e|Z$ and the mass M. Subsequently these corrections were recalculated by a number of authors [4–6]. Calculations of the nuclear recoil corrections of the next order in αZ were considered in [7–11].

In the theory of high-Z one-electron ions the parameter αZ can no longer be considered small. For this reason calculations of the nuclear recoil corrections for such systems must be carried out without expansion in αZ. In contrast to other QED effects in the region of strongly bound states ($\alpha Z \sim 1$), the calculation of the nuclear recoil effect at high Z demands using QED outside the external field approximation. [Calculations of QED effects in hydrogen, positronium, and muonium correspond to the case of weakly bound states ($\alpha Z \ll 1$).] In this connection a nontrivial problem of derivation of closed expressions for the nuclear recoil corrections in all orders in αZ arises. This problem was first discussed in [12,13]. The work [12] was based on the Bethe-Salpeter equation. This approach encountered serious technical difficulties, associated with summation of a complete sequence of irreducible diagrams. These difficulties were partly overcome only in the lowest orders in αZ. Complete αZ-dependence expressions were not found in this way. In [13] a general case of a relativistic few-electron atom was considered. An efficient method for summing the Feynman diagrams in the zeroth and first orders in $\frac{m}{M}$, based on an expansion of the nuclear propagator, was proposed in this paper. However, because the procedure of the derivation of the nuclear recoil corrections was not rigorously formulated, the method considered there gave several ambiguities in the expressions for the nuclear recoil corrections. In addition, certain errors were made in derivation of the formulas for the contributions with one and two transverse photons. As result, only a part of the expressions for the relativistic nuclear recoil corrections was found in this work. The complete expressions for the nuclear recoil corrections for hydrogenlike atoms were obtained in [14] (the overall sign of the two-transverse-photons contribution was corrected in [15,16]). The paper [14] was based on a version of the quasipotential approach that immediately gives the Dirac equation in the limit of infinite nuclear mass [17,18,5]. [The quasipotential approach was first introduced in quantum field theory by Logunov and Tavkhelidze [19] and was subsequently developed by many authors (see, e.g., [20]). This approach is absolutely rigorous and, in contrast to the Bethe-Salpeter equation, allows one to exclude the relative time (energy) in the wave function from the very beginning. The quasipotential equation can be represented in an evidently covariant form [20,17].] The relevant quasipotential equation in the center-of-mass system is (the relativistic units $\hbar = c = 1$ are used)

$$(E - \sqrt{\mathbf{p}^2 + M^2} - \boldsymbol{\alpha} \cdot \mathbf{p} - \beta m)\psi(\mathbf{p}) = \int V(E, \mathbf{p}, \mathbf{q})\psi(\mathbf{q}) d\mathbf{q} \ , \quad (1)$$

where $\boldsymbol{\alpha}$ and β are the Dirac matrices acting on the electron variables. The quasipotential $V(E)$ can be constructed by various methods [17,19,20]. One of the methods consists in using the relativistic scattering amplitude with one particle (nucleus) on mass shell [17,18,21]. In this method the quasipotential $V(E)$ may be defined by the Lippman-Schwinger equation

$$V = \tau(1 + F\tau)^{-1}\,, \tag{2}$$

where

$$F = [E - (\sqrt{\mathbf{p}^2 + M^2} + \boldsymbol{\alpha}\cdot\mathbf{p} + \beta m)(1 - i0)]^{-1}\,, \tag{3}$$

$$\begin{aligned}\tau(E,\mathbf{p},\mathbf{q}) &= -2\pi i\beta\overline{u}(-\mathbf{p})T(p_1,p_2;q_1,q_2)u(-\mathbf{q})\,,\\ \mathbf{p}_1 &= -\mathbf{p}_2 \equiv \mathbf{p},\ \ \mathbf{q}_1 = -\mathbf{q}_2 \equiv \mathbf{q}\,,\\ p_1^0 &= E - \sqrt{\mathbf{p}^2 + M^2}\ ,\ \ p_2^0 = \sqrt{\mathbf{p}^2 + M^2}\,,\\ q_1^0 &= E - \sqrt{\mathbf{q}^2 + M^2}\ ,\ \ q_2^0 = \sqrt{\mathbf{q}^2 + M^2}\,,\end{aligned} \tag{4}$$

p_1 and q_1 are the electron variables, p_2 and q_2 are the nucleus variables; T is the off-mass-shell relativistic scattering amplitude; $u(\mathbf{q})$ is the wave function of the free nucleus with the positive energy normalized by the condition $u^\dagger(\mathbf{q})u(\mathbf{q}) = 1$. In [14] the quasipotential $V(E)$ was constructed in the zeroth and first orders in $\frac{m}{M}$. So the closed expressions for the nuclear recoil corrections in the first order in $\frac{m}{M}$ and in all orders in αZ were obtained. The most detailed derivation was published in [22]. In [16] these results were generalized to the case of high-Z few-electron atoms. For that a more general method was developed. In the second section of the present paper we briefly formulate the results of [16]. In the third section the calculation of the nuclear recoil corrections for hydrogenlike atoms is considered. In the fourth section the corrections for high-Z lithiumlike atoms are calculated.

II. BASIC FORMULAS

We consider the system of Dirac particles: a nucleus with mass M and N electrons with mass m. Following the ideas of the quasipotential approach we introduce in the center-of-mass system the two-time Green function with the nucleus on the mass shell

$$\begin{aligned}G(t',t,\mathbf{p}',\mathbf{x}_1',\ldots,\mathbf{x}_N',\mathbf{p}',\mathbf{x}_1,\ldots,\mathbf{x}_N)\\ = \langle\mathbf{p}',\lambda|T\psi(t',\mathbf{x}_1')\cdots\psi(t',\mathbf{x}_N')\\ \times\psi^\dagger(t,\mathbf{x}_N)\cdots\psi^\dagger(t,\mathbf{x}_1)|\mathbf{p},\lambda\rangle\,,\end{aligned} \tag{5}$$

where $\psi(x)$ is the electron-positron field operator in the Heisenberg representation, T is the time ordered product operator,

$$|\mathbf{p},\lambda\rangle = a_{in}(\mathbf{p},\lambda)|0\rangle,\ \ |\mathbf{p}',\lambda\rangle = a_{out}(\mathbf{p}',\lambda)|0\rangle \tag{6}$$

are the in and out states of the nucleus, and $\mathbf{p}$ and λ are the momentum and polarization of the nucleus. Here we normalize the operators a_{in} and a_{out} by

$$\begin{aligned}\{a_{in}^\dagger(\mathbf{p},\lambda),\, a_{in}(\mathbf{p}',\lambda')\} &= \{a_{out}^\dagger(\mathbf{p},\lambda),\, a_{out}(\mathbf{p}',\lambda')\}\\ &= \delta_{\lambda\lambda'}\delta(\mathbf{p}-\mathbf{p}')\,.\end{aligned} \tag{7}$$

Let us introduce the Fourier transform of G:

$$\begin{aligned}&\delta(E-E')\delta(\mathbf{P}-\mathbf{P}')\overline{G}(E,\mathbf{p}',\mathbf{p}_1',\ldots,\mathbf{p}_N',\mathbf{p},\mathbf{p}_1,\ldots,\mathbf{p}_N)\\ &\quad= \frac{1}{2\pi i}\frac{1}{N!}\frac{1}{(2\pi)^{3N}}\int dtdt'd\mathbf{x}_1\cdots d\mathbf{x}_N d\mathbf{x}_1'\cdots d\mathbf{x}_N'\exp\left[i(\mathcal{E}'t'-\mathcal{E}t)\right]\\ &\quad\times\exp\left[-i\sum_{i=1}^N(\mathbf{p}_i'\cdot\mathbf{x}_i' - \mathbf{p}_i\cdot\mathbf{x}_i)\right]G(t',t,\mathbf{p}',\mathbf{x}_1',\ldots,\mathbf{x}_N',\mathbf{p}',\mathbf{x}_1,\ldots,\mathbf{x}_N)\,,\end{aligned} \tag{8}$$

where

$$\begin{aligned}&E = \mathcal{E} + \sqrt{\mathbf{p}^2 + M^2} - M,\ \ E' = \mathcal{E}' + \sqrt{\mathbf{p}'^2 + M^2} - M\,,\\ &\mathbf{P} = \mathbf{p} + \sum_{i=1}^N\mathbf{p}_i\ ,\ \ \mathbf{P}' = \mathbf{p}' + \sum_{i=1}^N\mathbf{p}_i'\,.\end{aligned} \tag{9}$$

In the center-of-mass system we have

$$\mathbf{p} = -\sum_{i=1}^N\mathbf{p}_i\,,\quad \mathbf{p}' = -\sum_{i=1}^N\mathbf{p}_i'\,.$$

We are interested in the energy of a bound state n of the atom. The spectral representation of $\overline{G}(E)$ gives

$$\begin{aligned}\overline{G}(E) = \frac{\Phi_n\Phi_n^\dagger}{E-E_n}\\ +(\text{terms that are regular at } E = E_n)\ ,\end{aligned} \tag{10}$$

where E_n is the bound state energy with the nucleus rest mass subtracted, and the wave function Φ_n is defined by the equation

$$\begin{aligned}&(2\pi)^{\frac{3}{2}}\delta(\mathbf{P})\Phi_n(\mathbf{p},\mathbf{p}_1,\ldots,\mathbf{p}_N)\\ &\quad= \frac{1}{\sqrt{N!}}\frac{1}{(2\pi)^{\frac{3N}{2}}}\int d\mathbf{x}_1\cdots d\mathbf{x}_N\exp\left[-\sum_{i=1}^N\mathbf{p}_i\cdot\mathbf{x}_i\right]\\ &\quad\times\langle\mathbf{p}|\psi(0,\mathbf{x}_1)\cdots\psi(0,\mathbf{x}_N)|n\rangle\ .\end{aligned} \tag{11}$$

The Green function $\overline{G}(E)$ is constructed by perturbation theory after transition in (5) to the interaction representation. Let the energy level n belong to an m-fold degenerate level $E_n^{(0)}$ in the limit $M \to \infty$ if the radiative and interelectronic interaction corrections are neglected. [The neglect of the interelectronic interaction in the zeroth approximation is justified for high-Z few-electron atoms ($N \ll Z$).] The m-dimensional subspace generated by the unperturbed eigenstates making up this level we designate as Ω. The projector on Ω is

$$P_0 = \sum_{k=1}^{m} u_k u_k^\dagger \,, \tag{12}$$

where

$$u_k = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \psi_{k_1}(P1) \cdots \psi_{k_N}(PN) \,, \tag{13}$$

and ψ_k are solutions of the Dirac equation in the Coulomb field of the nucleus:

$$H\psi_k = \varepsilon_k \psi_k \,, \quad H = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + V_c \,,$$
$$E_n^{(0)} = \sum_{i=1}^{N} \varepsilon_{k_i} \,. \tag{14}$$

Let us introduce the Green function g:

$$g = P_0 \overline{G} P_0 \,. \tag{15}$$

For this Green function, as for $\overline{G}(E)$, we have

$$g(E) = \frac{\phi_n \phi_n^\dagger}{E - E_n} + (\text{ terms that are regular at } E = E_n) \,, \tag{16}$$

where $\phi_n = P_0 \Phi_n$ belongs to the subspace Ω. Constructing $g(E)$ by the perturbation theory in the interaction representation we get it in the form of a series in powers in αZ. However, we are interested in an expansion in another parameter, namely, $\frac{m}{M}$. For this reason it is necessary to sum infinite sequences of the Feynman diagrams in the zeroth and first orders in $\frac{m}{M}$. We designate the contribution of the terms of zeroth order in $\frac{m}{M}$ by g_0. In [16] it was found that

$$g_0(E) = \frac{P_0}{E - E_n^{(0)}} \,. \tag{17}$$

From Eq. (16) and the identity

$$g^{-1} g = 1 \tag{18}$$

we obtain for $E = E_n$

$$g^{-1}(E_n)\phi_n = 0 \,. \tag{19}$$

Or, introducing the quasipotential operator

$$v(E) = g_0^{-1} - g^{-1} = g_0^{-1}\, \Delta g\, g_0^{-1} + g_0^{-1}\, \Delta g\, g_0^{-1}\, \Delta g\, g_0^{-1} + \cdots \,, \tag{20}$$

where $\Delta g \equiv g - g_0$, we obtain

$$[E_n^{(0)} + v(E_n)]\phi_n = E_n \phi_n \,. \tag{21}$$

The equation for determination of the energy levels follows as

$$\det\{(E - E_n^{(0)})\delta_{ik} - v_{ik}(E)\} = 0 \,. \tag{22}$$

It should be stressed that Eq. (22) is absolutely rigorous within QED and gives, in principle, the exact energies of the m levels arising from the m-fold degenerate level $E_n^{(0)}$. In [16] the quasipotential v_{ik} was found in the first order in $\frac{m}{M}$ and in the zeroth order in α (but in all orders in αZ) by summing infinite sequences of the Feynman diagrams in the Coulomb gauge. For that the expansion of the nuclear propagator from [13] was used. Only the following kinds of diagrams contribute in the considered order.

(i) The diagrams with only Coulomb photons.

(ii) The diagrams with one transverse and an arbitrary number of Coulomb photons.

(iii) The diagrams with two transverse and an arbitrary number of Coulomb photons.

The contribution from the diagrams with only Coulomb photons is

$$(v_c)_{ik} = (v_c^{(1)})_{ik} + (v_c^{(2)})_{ik} + (v_c^{(int)})_{ik} \,, \tag{23}$$

$$(v_c^{(1)})_{ik} = \sum_{s=1}^{N} \delta_{i_1 k_1} \cdots \overset{s}{\sqcap} \cdots \delta_{i_N k_N} \left\langle i_s \left| \frac{\mathbf{p}_s^2}{2M} \right| k_s \right\rangle , \tag{24}$$

$$(v_c^{(2)})_{ik} = \frac{2\pi i}{M} \sum_{s=1}^{N} \delta_{i_1 k_1} \cdots \overset{s}{\sqcap} \cdots \delta_{i_N k_N} \int_{-\infty}^{\infty} d\omega\, \delta_+^2(\omega) \times \langle i_s | [\mathbf{p}_s, v_s] G_s(\omega + \varepsilon_{i_s}) [\mathbf{p}_s, v_s] | k_s \rangle \,, \tag{25}$$

$$(v_c^{(int)})_{ik} = \frac{1}{M} \sum_{s<s'} \delta_{i_1 k_1} \cdots \overset{s}{\sqcap} \cdots \overset{s'}{\sqcap} \cdots \delta_{i_N k_N} \times \sum_P (-1)^P \langle P i_s P i_{s'} | \mathbf{p}_s \cdot \mathbf{p}_{s'} | k_s k_{s'} \rangle \,, \tag{26}$$

where $|i_s\rangle$ and $|k_s\rangle$ are the one-electron unperturbed states of the Dirac electron in the Coulomb field of the nucleus, belonging to the N-electron states i and k, respectively, $\mathbf{p}$ is the momentum operator, $v_s \equiv V_c(r_s) = -\frac{\alpha Z}{r_s}$, the symbol $\overset{s}{\sqcap}$ means that the factor $\delta_{i_s k_s}$ is omitted in the product, $\delta_+(\omega) = \frac{i}{2\pi}(\omega + i0)^{-1}$, and $G(\omega) = [\omega - H(1 - i0)]^{-1}$ is the relativistic Coulomb Green function. [Formally, the matrix element in Eq. (25) at fixed ω is infinite, due to the strong Coulomb singularity at $r = 0$. This means that the integration over ω must be carried out at an intermediate stage of the calculation, depending on which representation of G is used.] The contribution from the diagrams with one transverse and an arbitrary number of Coulomb photons consists of two terms. The first term depends on the spin of the nucleus and coincides with the Fermi-Breit expression for the hyperfine interaction [23]. The second term is

$$(v_{tr(1)})_{ik} = (v_{tr(1)}^{(1)})_{ik} + (v_{tr(1)}^{(2)})_{ik} + (v_{tr(1)}^{(int)})_{ik} \,, \tag{27}$$

$$(v_{tr(1)}^{(1)})_{ik} = -\frac{1}{2M} \sum_{s=1}^{N} \delta_{i_1 k_1} \cdots \overset{s}{\sqcap} \cdots \delta_{i_N k_N} \times \langle i_s | [\mathbf{D}_s(0) \cdot \mathbf{p}_s + \mathbf{p}_s \cdot \mathbf{D}_s(0)] | k_s \rangle \,, \tag{28}$$

$$(v_{tr(1)}^{(2)})_{ik} = -\frac{1}{M} \sum_{s=1}^{N} \delta_{i_1 k_1} \cdots \overset{s}{\sqcap} \cdots \delta_{i_N k_N} \int_{-\infty}^{\infty} d\omega\, \delta_+(\omega) \times \langle i_s | \{[\mathbf{p}_s, v_s] G_s(\omega + \varepsilon_{i_s}) \mathbf{D}_s(\omega) - \mathbf{D}_s(\omega) G_s(\omega + \varepsilon_{i_s}) [\mathbf{p}_s, v_s]\} | k_s \rangle \,, \tag{29}$$

$$(v_{tr(1)}^{(int)})_{ik} = -\frac{1}{M}\sum_{s<s'} \delta_{i_1k_1}\cdots \overset{s}{\sqcap}\cdots\overset{s'}{\sqcap}\cdots\delta_{i_Nk_N} \times \sum_P (-1)^P \langle Pi_sPi_{s'}|[\mathbf{D}_s(\varepsilon_{Pi_s}-\varepsilon_{k_s})\cdot\mathbf{p}_{s'} +\mathbf{p}_s\cdot\mathbf{D}_{s'}(\varepsilon_{Pi_{s'}}-\varepsilon_{k_{s'}})]|k_sk_{s'}\rangle\,, \tag{30}$$

where

$$D_m(\omega) = -4\pi\alpha Z\alpha_l D_{lm}(\omega)\,, \tag{31}$$

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

$$D_{ik}(\omega,\mathbf{r}) = -\frac{1}{4\pi}\Big\{\frac{\exp{(i|\omega|r)}}{r}\delta_{ik} +\nabla_i\nabla_k\frac{[\exp{(i|\omega|r)}-1]}{\omega^2 r}\Big\}\,. \tag{32}$$

The contribution from the diagrams with two transverse and an arbitrary number of Coulomb photons is

$$(v_{tr(2)})_{ik} = (v_{tr(2)}^{(1)})_{ik} + (v_{tr(2)}^{(int)})_{ik}\,, \tag{33}$$

$$(v_{tr(2)}^{(1)})_{ik} = \frac{i}{2\pi M}\sum_{s=1}^{N}\delta_{i_1k_1}\cdots\overset{s}{\sqcap}\cdots\delta_{i_Nk_N} \times\int_{-\infty}^{\infty}d\omega\langle i_s|\mathbf{D}_s(\omega)G_s(\omega+\varepsilon_{i_s}) \times\mathbf{D}_s(\omega)|k_s\rangle\,, \tag{34}$$

$$(v_{tr(2)}^{(int)})_{ik} = \frac{1}{M}\sum_{s<s'}\delta_{i_1k_1}\cdots\overset{s}{\sqcap}\cdots\overset{s'}{\sqcap}\cdots\delta_{i_Nk_N}\sum_P(-1)^P \times\langle Pi_sPi_{s'}|\mathbf{D}_s(\varepsilon_{Pi_s}-\varepsilon_{k_s})\cdot\mathbf{D}_{s'}(\varepsilon_{Pi_{s'}} -\varepsilon_{k_{s'}})|k_sk_{s'}\rangle\,. \tag{35}$$

The formulas (23)–(35) were derived in [16]. The corresponding formulas for the case of a one-electron atom were first obtained in [14] (the overall sign of the contribution $\Delta E_{tr(2)}$ was corrected in [15,16]) and recently reproduced in [24,10].

The contributions $v_c^{(1)}$, $v_c^{(int)}$, $v_{tr(1)}^{(1)}$, and $v_{tr(1)}^{(int)}$ are leading for low αZ and completely define the nuclear recoil corrections within the $\frac{m^2}{M}(\alpha Z)^4$ approximation. It follows that within the $\frac{m^2}{M}(\alpha Z)^4$ approximation the nuclear recoil corrections can be obtained by evaluating the expectation values with the Dirac wave functions of the operator

$$H_M = \frac{1}{2M}\sum_{s,s'}\left[\mathbf{p}_s\cdot\mathbf{p}_{s'} - \frac{\alpha Z}{r_s}\left(\boldsymbol{\alpha}_s + \frac{(\boldsymbol{\alpha}_s\cdot\mathbf{r}_s)\mathbf{r}_s}{r_s^2}\right)\cdot\mathbf{p}_{s'}\right]\,. \tag{36}$$

In [25] the relativistic nuclear recoil corrections of order $\frac{m^2}{M}(\alpha Z)^4$ to the energy levels of two- and three-electron multicharged ions were calculated using this operator. The expression (36) can be found by reformulating the Stone's theory as well [26].

III. HYDROGENLIKE ATOMS

For hydrogenlike atoms the nuclear recoil corrections to the energy of a state a are defined by the diagonal matrix elements [$\Delta E = (v)_{aa}$] of the one-electrons contributions (24), (25), (28), (29), and (34). The terms $\Delta E_c^{(1)}$ and $\Delta E_{tr(1)}^{(1)}$ are leading at low Z. These terms can easily be calculated by using the virial relations for the Dirac equation [27–29]. Such a calculation gives [14]

$$\Delta E_c^{(1)} = \frac{m^2}{2M}\left\{1-\frac{(\gamma+n_r)^2}{N^2}+\frac{2(\alpha Z)^4}{N^4\gamma(4\gamma^2-1)} \times\{\kappa[2\kappa(\gamma+n_r)-N]+n_r(4\gamma^2-1)\}\right\}\,, \tag{37}$$

$$\Delta E_{tr(1)}^{(1)} = -\frac{m^2}{M}\frac{(\alpha Z)^4}{N^4\gamma(4\gamma^2-1)}\{\kappa[2\kappa(\gamma+n_r)-N] +n_r(4\gamma^2-1)\}\,, \tag{38}$$

$$\Delta E^{(1)} \equiv \Delta E_c^{(1)}+\Delta E_{tr(1)}^{(1)} = \frac{m^2-\varepsilon_a^2}{2M} = \frac{m^2}{M}\frac{(\alpha Z)^2}{2N^2}\,, \tag{39}$$

where

$$\kappa = (-1)^{j+l+\frac{1}{2}}(j+\tfrac{1}{2})\,,\quad \gamma=\sqrt{\kappa^2-(\alpha Z)^2}\,,$$

$$N=\sqrt{n^2-2n_r(|\kappa|-\gamma)}\,,\qquad n=n_r+|\kappa|\,,$$

j is the total electron moment, l is the orbital moment, n is the principal quantum number, and n_r is the radial quantum number. Only these terms contribute within the $\frac{m^2}{M}(\alpha Z)^4$ approximation. Expanding (39) in power series in αZ we find

$$\Delta E^{(1)} = \frac{m^2}{M}\left\{\frac{(\alpha Z)^2}{2n^2}+\frac{(\alpha Z)^4}{2n^3}\left(\frac{1}{j+\frac{1}{2}}-\frac{1}{n}\right) +\frac{(\alpha Z)^6 n_r}{2n^4(j+\frac{1}{2})^2}\left(\frac{1}{4(j+\frac{1}{2})}+\frac{n_r}{n^2}\right)+\cdots\right\}\,. \tag{40}$$

The terms $\Delta E_c^{(2)}$, $\Delta E_{tr(1)}^{(2)}$, and $\Delta E_{tr(2)}^{(1)}$ [Eqs. (25), (29), and (34)] are given in a form that allows one to use the relativistic Coulomb Green function for their calculations. In addition, this form is convenient for αZ-expansion calculations [10]. However, in the present paper we transform these equations to ones that are most convenient for calculations using the finite basis set methods [30–32].

Integrating over ω in (25) we find

$$\Delta E_c^{(2)} = -\frac{1}{M}\sum_{\varepsilon_n<0}\langle a|\mathbf{p}|n\rangle\langle n|\mathbf{p}|a\rangle\,. \tag{41}$$

[It should be noted here that the formula (41) was first found in [13]. Its derivation was refined in [14]. A similar formula but with the projector on the negative energy states of a free electron was obtained in the lowest order in αZ in [12].] The matrix elements of the momentum operator are easily calculated using the identity [25]

$$\mathbf{p} = \frac{1}{2}(\boldsymbol{\alpha} H + H\boldsymbol{\alpha}) - \boldsymbol{\alpha} V_c \,. \tag{42}$$

Rotating in (29) the integration contour in the complex ω plane we find

$$\Delta E^{(2)}_{tr(1)} = \Delta E^{(2,a)}_{tr(1)} + \Delta E^{(2,b)}_{tr(1)} + \Delta E^{(2,c)}_{tr(1)} \,, \tag{43}$$

$$\Delta E^{(2,a)}_{tr(1)} = \frac{1}{2M} \sum_{\varepsilon_n \neq \varepsilon_a} \Big\{ \langle a|\mathbf{p}|n\rangle\langle n|\mathbf{D}(0)|a\rangle + \langle a|\mathbf{D}(0)|n\rangle\langle n|\mathbf{p}|a\rangle \Big\} \,, \tag{44}$$

$$\Delta E^{(2,b)}_{tr(1)} = \frac{2}{\pi M} \mathrm{Re} \int_0^\infty dy \sum_{\varepsilon_n \neq \varepsilon_a} \frac{\varepsilon_a - \varepsilon_n}{y^2 + (\varepsilon_a - \varepsilon_n)^2} \times \langle a|\mathbf{p}|n\rangle\langle n|\mathbf{S}(y)|a\rangle \,, \tag{45}$$

$$\Delta E^{(2,c)}_{tr(1)} = -\frac{1}{M} \sum_{|\varepsilon_n| < \varepsilon_a} \Big\{ \langle a|\mathbf{p}|n\rangle\langle n|\mathbf{D}(\varepsilon_a - \varepsilon_n)|a\rangle + \langle a|\mathbf{D}(\varepsilon_a - \varepsilon_n)|n\rangle\langle n|\mathbf{p}|a\rangle \Big\} \,, \tag{46}$$

where

$$\mathbf{S}(y) = \mathbf{S}_1(y) + \mathbf{S}_2(y) \,,$$

$$\mathbf{S}_1(y) = \alpha Z \boldsymbol{\alpha} \frac{\exp(-yr)}{r} \,,$$

$$\mathbf{S}_2(y) = i\alpha Z [H, \tilde{f}(y,r)\mathbf{n}] \,,$$

$$\tilde{f}(y,r) = \frac{\exp(-yr)(1+yr) - 1}{y^2 r^2} \,,$$

$$\mathbf{D}(\omega) = \mathbf{D}_1(\omega) + \mathbf{D}_2(\omega) \,,$$

$$\mathbf{D}_1(\omega) = \alpha Z \boldsymbol{\alpha} \frac{\exp(i|\omega|r)}{r} \,,$$

$$\mathbf{D}_2(\omega) = i\alpha Z [H, f(\omega,r)\mathbf{n}] \,,$$

$$f(\omega,r) = \frac{1 - \exp(i|\omega|r)(1 - i|\omega|r)}{\omega^2 r^2} \,,$$

$$\mathbf{D}(0) = \alpha Z \frac{\boldsymbol{\alpha}}{r} - \frac{i\alpha Z}{2}[H, \mathbf{n}] \,,$$

$\mathbf{n} = \frac{\mathbf{r}}{|\mathbf{r}|}$. The term $\Delta E^{(2,c)}_{tr(1)}$ has real and imaginary parts. The imaginary part gives a small correction to the width of the level. Integrating over y in (45) and uniting the contributions $\Delta E^{(2,a)}_{tr(1)}$, $\Delta E^{(2,b)}_{tr(1)}$, and the real part of $\Delta E^{(2,c)}_{tr(1)}$ we find

$$\Delta E^{(2)}_{tr(1)} = \frac{2\alpha Z}{\pi M} \mathrm{Re} \sum_{\varepsilon_n \neq \varepsilon_a} (\varepsilon_n - \varepsilon_a) \langle a|i\boldsymbol{\alpha}\phi(r)|n\rangle \times \langle n|[i\boldsymbol{\alpha}\Phi_1(r) + \mathbf{n}\Phi_2(r)]|a\rangle \,, \tag{47}$$

where

$$\phi = \frac{\varepsilon_a + \varepsilon_n}{2} + \frac{\alpha Z}{r} \,, \tag{48}$$

$$\Phi_1(r) = \frac{1}{\Delta_n r}\left[\mathrm{ci}(\Delta_n r)\sin(\Delta_n r) - \mathrm{si}(\Delta_n r)\cos(\Delta_n r) + \mathrm{sgn}(\varepsilon_a - \varepsilon_n)\frac{\pi}{2}\right] - \theta(\varepsilon_a - |\varepsilon_n|)\frac{\pi}{\Delta_n}\frac{\exp(i\Delta_n r)}{r} \,, \tag{49}$$

$$\begin{aligned}\Phi_2(r) = {} & -\mathrm{sgn}(\varepsilon_a - \varepsilon_n)\frac{1}{(\Delta_n r)^2}\Big\{ -\mathrm{si}(\Delta_n r)\cos(\Delta_n r) - \frac{\pi}{2} + \Delta_n r + \mathrm{ci}(\Delta_n r)[\sin(\Delta_n r) - (\Delta_n r)\cos(\Delta_n r)] \\ & -(\Delta_n r)\,\mathrm{si}(\Delta_n r)\sin(\Delta_n r)\Big\} - \frac{\pi}{4} - \theta(\varepsilon_a - |\varepsilon_n|)\pi f(\Delta_n, r) \,, \end{aligned} \tag{50}$$

$$\Delta_n = |\varepsilon_a - \varepsilon_n|, \;\; \theta(x) = (x + |x|)/2x \,.$$

The contribution $\Delta E_{tr(2)}$ is equal to

$$\Delta E^{(1)}_{tr(2)} = \Delta E^{(1,a)}_{tr(2)} + \Delta E^{(1,b)}_{tr(2)} + \Delta E^{(1,c)}_{tr(2)} \,, \tag{51}$$

$$\Delta E^{(1,a)}_{tr(2)} = -\frac{1}{\pi M} \int_0^\infty dy \sum_{\varepsilon_n \neq \varepsilon_a} \frac{\varepsilon_a - \varepsilon_n}{y^2 + (\varepsilon_a - \varepsilon_n)^2} \times \langle a|\mathbf{S}(y)|n\rangle\langle n|\mathbf{S}(y)|a\rangle \,, \tag{52}$$

$$\Delta E^{(1,b)}_{tr(2)} = \frac{1}{2M} \sum_{\varepsilon_n = \varepsilon_a} \langle a|\mathbf{D}(0)|n\rangle\langle n|\mathbf{D}(0)|a\rangle \,, \tag{53}$$

$$\Delta E^{(1,c)}_{tr(2)} = \frac{1}{M} \sum_{|\varepsilon_n| < \varepsilon_a} \langle a|\mathbf{D}(\varepsilon_a - \varepsilon_n)|n\rangle \times \langle n|\mathbf{D}(\varepsilon_a - \varepsilon_n)|a\rangle \,. \tag{54}$$

The term $\Delta E^{(1,c)}_{tr(2)}$, like $\Delta E^{(2,c)}_{tr(1)}$, has an imaginary part which gives a small contribution to the width of the level.

After integration over angles that is easily carried out using formulas presented in the Appendix, the calculation of the expressions (41), (47), and (52)–(54) was done using the B-spline method for the Dirac equation, developed in [31]. The zero boundary conditions and the grid selection algorithm proposed in [33] were used. However, we used the grid $r_i = \frac{\rho_i^4 \gamma_0}{Z}$, where $\gamma_0 = \sqrt{1-(\alpha Z)^2}$, instead of the grid $r_i = \frac{\rho_i^4}{Z}$ [33]. The radial integration caused no problems and was carried out with high accuracy using the Gauss-Legendre quadratures. The integration over y in (52) was also done by the Gauss-Legendre quadratures with a suitable transformation to map the infinite integration range to a finite one. The uncertainty of the integration was estimated from the stability of the result with respect to change of the number of integration points and the grid parameters and was found to be much smaller than the uncertainty due to the finiteness of the basis set. The size of the box was chosen to be sufficiently large so as not to affect the results. The uncertainty due to the finiteness of the basis set was estimated by changing the number of splines from 40 to 90. In addition, to make an independent estimate of the uncertainty of the numerical results we calculated the corrections $\Delta E_c^{(2)}$ and $\Delta E_{tr(1)}^{(2)}$ using two different representations for them. So the correction $\Delta E_c^{(2)}$ was calculated by the formula (41) as well as by

$$\Delta E_c^{(2)} = -\frac{1}{M}\left\{\langle a|\mathbf{p}^2|a\rangle - \sum_{\varepsilon_n>0}\langle a|\mathbf{p}|n\rangle\langle n|\mathbf{p}|a\rangle\right\}. \quad (55)$$

We found that the results of both calculations coincided with each other with good precision, and this coincidence improved when the number of splines increased. The correction $\Delta E_{tr(1)}^{(2)}$ was calculated by Eq. (47) as well as by (43)–(45). The results of both calculations coincided with each other with high accuracy.

Tables I, II, and III show the results of the numerical calculation for the $1s$, $2s$, and $2p_{\frac{1}{2}}$ states, respectively, expressed in terms of the function $P(\alpha Z)$ defined by

$$\Delta E^{(2)} = \Delta E_c^{(2)} + \Delta E_{tr(1)}^{(2)} + \Delta E_{tr(2)}^{(1)} = \frac{m}{M}\frac{(\alpha Z)^5}{\pi n^3}P(\alpha Z)mc^2 . \quad (56)$$

The functions P_c, $P_{tr(1)}$, and $P_{tr(2)}$ correspond to the contributions $\Delta E_c^{(2)}$, $\Delta E_{tr(1)}^{(2)}$, and $\Delta E_{tr(2)}^{(1)}$, respectively. For comparison, in the last columns of the tables Salpeter's contributions [3–6]

$$P_S^{(1s)}(\alpha Z) = -\frac{2}{3}\ln(\alpha Z) - \frac{8}{3}2.984\,129 + \frac{14}{3}\ln 2 + \frac{62}{9}, \quad (57)$$

$$P_S^{(2s)}(\alpha Z) = -\frac{2}{3}\ln(\alpha Z) - \frac{8}{3}2.811\,769 + \frac{187}{18}, \quad (58)$$

$$P_S^{(2p_{\frac{1}{2}})} = \frac{8}{3}0.030\,017 - \frac{7}{18} \quad (59)$$

are given. The uncertainties given in the tables correspond only to errors of the numerical calculation. In addition, there is an uncertainty due to deviation from the point-single-particle model of the nucleus, used here.

TABLE I. The results of the numerical calculation of the one-electron nuclear recoil corrections to the $1s$ state energy expressed in terms of the function $P(\alpha Z)$ defined by Eq. (56). $P_S(\alpha Z)$ is the Salpeter contribution defined by Eq. (57). The numbers in parentheses are the uncertainties of the calculations.

Z	$P_c(\alpha Z)$	$P_{tr(1)}(\alpha Z)$	$P_{tr(2)}(\alpha Z)$	$P(\alpha Z)$	$P_S(\alpha Z)$
1	-1.3111(2)	12.568(2)	-5.8267(3)	5.430(2)	5.4461
5	-1.2345(1)	8.5854(3)	-3.0476(2)	4.3033(4)	4.3731
10	-1.1586	6.9974(1)	-2.0438	3.7950(1)	3.9110
15	-1.0994	6.1340(1)	-1.5373	3.4973(1)	3.6407
20	-1.0537	5.5678(1)	-1.2201	3.2940(1)	3.4489
25	-1.0192	5.1671(1)	-0.9996	3.1483(1)	3.3001
30	-0.9946	4.8744(1)	-0.8362	3.0437(1)	3.1786
35	-0.9790	4.6598(1)	-0.7094	2.9714(1)	3.0758
40	-0.9721	4.5065(1)	-0.6076	2.9268(1)	2.9868
45	-0.9740	4.4048(1)	-0.5231	2.9077(1)	2.9083
50	-0.9849	4.3496(1)	-0.4510	2.9137(1)	2.8380
55	-1.0059	4.3389(1)	-0.3874	2.9456(1)	2.7745
60	-1.0383	4.3739(2)	-0.3295	3.0061(2)	2.7165
65	-1.0845(1)	4.4588(2)	-0.2746	3.0997(2)	2.6631
70	-1.1479(2)	4.6014(3)	-0.2201	3.2334(4)	2.6137
75	-1.2339(3)	4.8153(7)	-0.1631	3.4183(8)	2.5677
80	-1.3506(5)	5.122(1)	-0.0996(1)	3.672(1)	2.5247
85	-1.512(1)	5.558(4)	-0.0237(2)	4.022(4)	2.4843
90	-1.741(3)	6.186(7)	0.0743(9)	4.519(8)	2.4462
92	-1.861(5)	6.51(1)	0.123(1)	4.77(1)	2.4315
95	-2.084(9)	7.12(3)	0.212(1)	5.25(3)	2.4101
100	-2.64(3)	8.6(1)	0.428(6)	6.4(1)	2.3759

TABLE II. The results of the numerical calculation of the one-electron nuclear recoil corrections to the $2s$ state energy expressed in terms of the function $P(\alpha Z)$ defined by Eq. (56). $P_S(\alpha Z)$ is the Salpeter contribution defined by Eq. (58). The numbers in parentheses are the uncertainties of the calculations.

Z	$P_c(\alpha Z)$	$P_{tr(1)}(\alpha Z)$	$P_{tr(2)}(\alpha Z)$	$P(\alpha Z)$	$P_S(\alpha Z)$
1	-1.3112(2)	13.177(1)	-5.7103(3)	6.155(1)	6.1710
5	-1.2351(1)	9.1911(2)	-2.9225(1)	5.0335(2)	5.0980
10	-1.1612	7.6075(1)	-1.9080	4.5383(1)	4.6359
15	-1.1055	6.7562	-1.3908	4.2599	4.3656
20	-1.0647	6.2093	-1.0621	4.0825	4.1738
25	-1.0367	5.8352	-0.8294	3.9691	4.0251
30	-1.0202	5.5767	-0.6528	3.9037	3.9035
35	-1.0147	5.4047	-0.5115	3.8785	3.8008
40	-1.0202	5.3037	-0.3935	3.8900	3.7117
45	-1.0372	5.2656	-0.2908	3.9376	3.6332
50	-1.0668	5.2876(1)	-0.1980	4.0228(1)	3.5630
55	-1.1108	5.3711(1)	-0.1105	4.1498(1)	3.4994
60	-1.1723(1)	5.5218(1)	-0.0247	4.3248(2)	3.4414
65	-1.2554(1)	5.7504(2)	0.0634	4.5584(2)	3.3881
70	-1.3668(2)	6.0743(4)	0.1581(1)	4.8656(5)	3.3387
75	-1.5164(4)	6.5211(7)	0.2651(1)	5.2698(8)	3.2927
80	-1.7199(7)	7.135(2)	0.3921(2)	5.807(2)	3.2496
85	-2.003(1)	7.988(4)	0.5516(4)	6.537(4)	3.2092
90	-2.413(4)	9.205(8)	0.7645(6)	7.557(9)	3.1711
92	-2.630(7)	9.84(1)	0.872(1)	8.08(2)	3.1565
95	-3.04(2)	11.02(2)	1.070(2)	9.05(3)	3.1351
100	-4.07(5)	13.9(1)	1.55(1)	11.4(2)	3.1009

TABLE III. The results of the numerical calculation of the one-electron nuclear recoil corrections to the $2p_{\frac{1}{2}}$ state energy expressed in terms of the function $P(\alpha Z)$ defined by Eq. (56). $P_S(\alpha Z)$ is the Salpeter contribution defined by Eq. (59). The numbers in parentheses are the uncertainties of the calculations.

Z	$P_c(\alpha Z)$	$P_{tr(1)}(\alpha Z)$	$P_{tr(2)}(\alpha Z)$	$P(\alpha Z)$	$P_S(\alpha Z)$
1	-0.0000	-0.1440	-0.1571	-0.3011	-0.3088
5	-0.0007	-0.1492	-0.1194	-0.2692	-0.3088
10	-0.0024	-0.1526	-0.0727	-0.2277	-0.3088
15	-0.0051	-0.1535	-0.0258	-0.1845	-0.3088
20	-0.0088	-0.1524	0.0218	-0.1393	-0.3088
25	-0.0133	-0.1493	0.0706	-0.0920	-0.3088
30	-0.0189	-0.1444	0.1212	-0.0421	-0.3088
35	-0.0255	-0.1375	0.1742	0.0112	-0.3088
40	-0.0335	-0.1284	0.2304	0.0685	-0.3088
45	-0.0432	-0.1165	0.2906	0.1310	-0.3088
50	-0.0548	-0.1012	0.3560	0.2000	-0.3088
55	-0.0691	-0.0814	0.4278	0.2774	-0.3088
60	-0.0868	-0.0555	0.5078	0.3655	-0.3088
65	-0.1091	-0.0211	0.5982	0.4680	-0.3088
70	-0.1376	0.0252	0.7018	0.5894	-0.3088
75	-0.1750	0.0891(1)	0.8229	0.7370(1)	-0.3088
80	-0.2253(1)	0.1796(1)	0.9671	0.9214(2)	-0.3088
85	-0.2954(2)	0.3123(3)	1.1429(1)	1.1598(4)	-0.3088
90	-0.3972(6)	0.515(1)	1.3632(1)	1.481(1)	-0.3088
92	-0.451(1)	0.626(1)	1.468(2)	1.643(3)	-0.3088
95	-0.554(2)	0.842(3)	1.649(3)	1.937(5)	-0.3088
100	-0.816(9)	1.41(1)	2.040(3)	2.63(2)	-0.3088

To make a more detailed comparison with the αZ-expansion calculations we represent the functions P_c, $P_{tr(1)}$, and $P_{tr(2)}$ for the s states in the form

$$\begin{aligned} P_c &= a_1 + a_2\alpha Z + a_3(\alpha Z)^2 \ln(\alpha Z) + a_4(\alpha Z)^2 , \\ P_{tr(1)} &= b_1 \ln(\alpha Z) + b_2 + b_3\alpha Z \ln(\alpha Z) \\ &\quad + b_4\alpha Z + b_5(\alpha Z)^2 \ln(\alpha Z) \\ &\quad + b_6(\alpha Z)^2 + b_7(\alpha Z)^3 , \\ P_{tr(2)} &= c_1 \ln(\alpha Z) + c_2 + c_3\alpha Z \ln(\alpha Z) \\ &\quad + c_4\alpha Z + c_5(\alpha Z)^2 \ln(\alpha Z) \\ &\quad + c_6(\alpha Z)^2 + c_7(\alpha Z)^3 . \end{aligned} \tag{60}$$

The coefficients a_i, b_i, and c_i can be calculated from our numerical results for the $P(\alpha Z)$ functions. Such a calculation for the $2s$ state using the values of the $P(\alpha Z)$ functions for Z =1,2,3,5,8,15,30 gives

$$\begin{aligned} &a_1 = -1.3333, \quad a_2 = 3.156, \\ &b_1 = -2.6662, \quad b_2 = -0.091, \\ &b_3 = -6.02, \quad b_4 = -9.98, \\ &c_1 = 2.0031, \quad c_2 = 4.338, \\ &c_3 = 6.46, \quad c_4 = 5.92 . \end{aligned} \tag{61}$$

The coefficients a_1, $b_{1,2}$, and $c_{1,2}$ are in good agreement with Salpeter's results,

$$\begin{aligned} &a_1 = -1.3333 , \quad b_1 = -2.6666 , \quad b_2 = -0.094 , \\ &c_1 = 2.0000 , \quad c_2 = 4.318 . \end{aligned} \tag{62}$$

Within the errors of the numerical procedure our values b_3 and c_3 are in good agreement with the analytical result of [8,9],

$$b_3 = -c_3 = -2\pi = -6.2832 , \quad b_3 + c_3 = 0 \tag{63}$$

(the coefficient b_3 was first found in [7]). The coefficient a_2 coincides, within the numerical errors, with the corresponding coefficient ($a_2 = \pi = 3.1459$) obtained in [7]. The coefficients b_4 and c_4 are in satisfactory agreement with the results of [10],

$$b_4 = -10.996 , \quad c_4 = 5.569 . \tag{64}$$

For the $1s$ state we have found a similar agreement.

To make a similar comparison for the $2p_{\frac{1}{2}}$ state we represent the functions $P_{tr(1)}$ and $P_{tr(2)}$ for this state in the form

$$\begin{aligned} P_{tr(1)} &= b_1 + b_2\alpha Z + b_3(\alpha Z)^2 \ln(\alpha Z) \\ &\quad + b_4(\alpha Z)^2 + b_5(\alpha Z)^3 \ln(\alpha Z) \\ &\quad + b_6(\alpha Z)^3 + b_7(\alpha Z)^4 , \\ P_{tr(2)} &= c_1 + c_2\alpha Z + c_3(\alpha Z)^2 \ln(\alpha Z) \\ &\quad + c_4(\alpha Z)^2 + c_5(\alpha Z)^3 \ln(\alpha Z) \\ &\quad + c_6(\alpha Z)^3 + c_7(\alpha Z)^4 . \end{aligned} \tag{65}$$

Using our values of $P(\alpha Z)$ for $Z = 1, 2, 3, 5, 8, 15, 30$ we have found

$$\begin{aligned} &b_1 = -0.142\,178 , \quad b_2 = -0.261\,66 , \\ &c_1 = -0.166\,666 , \quad c_2 = 1.308\,81 . \end{aligned} \tag{66}$$

The coefficients b_1 and c_1 are in excellent agreement with Salpeter's results: $b_1 = -0.142\,178$ and $c_1 = -0.166\,667$. Adding to the sum $b_2 + c_2$ the corresponding coefficient from the equation (40), we find that the total coefficient of the $\frac{m^2}{M}\frac{(\alpha Z)^6}{n^3\pi}$ contribution for the $2p_{\frac{1}{2}}$ state is 1.439 85. The related analytical result obtained in [11] is $\frac{11}{24}\pi =$ 1.439 90.

The term $\Delta E^{(1)}$ does not contribute to the Lamb shift of hydrogenlike atoms. The contribution of the difference between $\Delta E^{(2)}$ and the Salpeter's correction to the Lamb shift ($n = 2$) of hydrogen is $-1.32(6)$ kHz. The corresponding result for the ground state is $-7.1(9)$ kHz. These results are in good agreement with analytical calculations of the $\frac{m^2}{M}(\alpha Z)^6$ contributions [10,11]. So according to [10] the total $\frac{m^2}{M}(\alpha Z)^6$ correction, including the related term from Eq. (40), is -7.4 kHz and -0.77 kHz for the $1s$ and $2s$ state, respectively. The $\frac{m^2}{M}(\alpha Z)^6$ correction for the $2p_{\frac{1}{2}}$ state found in [11] is 0.58 kHz.[We note that in [11] a correction of order $\frac{m^2}{M}(\alpha)^2(\alpha Z)^4$ for p states is also calculated.]

Let us consider the nuclear recoil corrections for hydrogenlike uranium. According to the formula (39) the first correction is

$$\Delta E_{1s}^{(1)} = 0.26 \text{ eV} , \quad \Delta E_{2s}^{(1)} = \Delta E_{2p_{\frac{1}{2}}}^{(1)} = 0.08 \text{ eV}. \tag{67}$$

The second correction defined by (56) is

$$\begin{aligned} \Delta E_{1s}^{(2)} = 0.24 \text{ eV} , \quad &\Delta E_{2s}^{(2)} = 0.05 \text{ eV} , \\ &\Delta E_{2p_{\frac{1}{2}}}^{(2)} = 0.01 \text{ eV} . \end{aligned} \tag{68}$$

In the next section we use these results to find the total nuclear recoil contribution to the energy of the $2p_{\frac{1}{2}}$-$2s$ transition in lithiumlike uranium.

IV. HIGH-Z LITHIUMLIKE ATOMS

The wave function of a high-Z lithiumlike atom with one electron over the closed $(1s)^2$ shell in the zeroth approximation is

$$u = \frac{1}{\sqrt{3!}} \sum_P (-1)^P \psi_{1s\uparrow}(P1)\psi_{1s\downarrow}(P2)\psi_a(P3) . \tag{69}$$

The nuclear recoil correction for the lithiumlike atom is the sum of the one- and two-electron corrections. The one-electron correction is obtained by summing all the one-electron contributions considered in the preceding section over all the one-electron states that are occupied. According to (26), (30), and (35) the two-electron corrections for the state considered here are

$$\Delta E_c^{(int)} = -\frac{1}{M} \sum_{\varepsilon_n = \varepsilon_{1s}} \langle a|\mathbf{p}|n\rangle\langle n|\mathbf{p}|a\rangle , \tag{70}$$

$$\Delta E^{(int)}_{tr(1)} = \frac{1}{M} \sum_{\varepsilon_n=\varepsilon_{1s}} \Big\{ \langle a|\mathbf{p}|n\rangle\langle n|\mathbf{D}(\varepsilon_a-\varepsilon_n)|a\rangle + \langle a|\mathbf{D}(\varepsilon_a-\varepsilon_n)|n\rangle\langle n|\mathbf{p}|a\rangle \Big\}, \quad (71)$$

$$\Delta E^{(int)}_{tr(2)} = -\frac{1}{M} \sum_{\varepsilon_n=\varepsilon_{1s}} \langle a|\mathbf{D}(\varepsilon_a-\varepsilon_n)|n\rangle \times\langle n|\mathbf{D}(\varepsilon_a-\varepsilon_n)|a\rangle\,. \quad (72)$$

The terms $\Delta E^{(int)}_{tr(1)}$ and $\Delta E^{(int)}_{tr(2)}$ have real and imaginary parts and are canceled by the part of the one-electron terms $\Delta E^{(2,c)}_{tr(1)}$ and $\Delta E^{(1,c)}_{tr(2)}$ which corresponds to the $1s$ states. So for the $(1s)^2 2s$ and $(1s)^2 2p_{\frac{1}{2}}$ states the imaginary parts of the one- and two-electron contributions are completely canceled.

We note here that the nuclear recoil corrections for a high-Z lithiumlike atom with one electron over the closed $(1s)^2$ shell can be obtained from the nuclear recoil corrections for the hydrogenlike atom by changing the sign of $i0$ in the denominators of the electron propagator in the Coulomb field of the nucleus, corresponding to the states of the closed shell. It follows, in particular, that the sum of the one- and two-electron Coulomb contributions can be represented in a simple form:

$$\Delta E_c = \frac{1}{2M}\left\{ \sum_{\varepsilon_n>\varepsilon_{1s}} |\langle a|\mathbf{p}|n\rangle|^2 - \sum_{\varepsilon_n\leq\varepsilon_{1s}} |\langle a|\mathbf{p}|n\rangle|^2 \right\}. \quad (73)$$

Table IV shows the results of the calculation of the corrections (70)–(72) for the $(1s)^2 2p_{\frac{1}{2}}$ state [for the $(1s)^2 2s$ states these corrections are equal to zero], expressed in terms of the function $Q(\alpha Z)$ defined by

$$\Delta E^{int} \equiv \Delta E^{(int)}_c + \Delta E^{(int)}_{tr(1)} + \Delta E^{(int)}_{tr(2)} = -\frac{2^9}{3^8}\frac{m^2}{M}(\alpha Z)^2 Q(\alpha Z)\,. \quad (74)$$

Here we have taken into account the known nonrelativistic limit of this correction [34]. Within the $\frac{m^2}{M}(\alpha Z)^4$ approximation the function $Q(\alpha Z)$ that we denote by $Q_L(\alpha Z)$ is [25]

$$Q_L(\alpha Z) = 1 + (\alpha Z)^2\Big(-\frac{29}{48} + \ln\frac{9}{8}\Big)\,. \quad (75)$$

For comparison, this function is given in the table as well. The functions $Q_c(\alpha Z)$, $Q_{tr(1)}(\alpha Z)$, and $Q_{tr(2)}(\alpha Z)$ correspond to the corrections $\Delta E^{(int)}_c$, $\Delta E^{(int)}_{tr(1)}$, and $\Delta E^{(int)}_{tr(2)}$, respectively. In leading orders in αZ they are

$$Q_c(\alpha Z) = 1 + (\alpha Z)^2\Big(\frac{55}{48} + \ln\frac{9}{8}\Big)\,, \quad (76)$$

$$Q_{tr(1)}(\alpha Z) = -\frac{7}{4}(\alpha Z)^2\,, \quad (77)$$

$$Q_{tr(2)}(\alpha Z) = \frac{49}{64}(\alpha Z)^4\,. \quad (78)$$

For low Z, in addition to the corrections considered here, the Coulomb electron-electron interaction corrections to the nonrelativistic nuclear recoil contribution must be calculated separately. The main contribution from these corrections is of order $\frac{1}{Z}(\alpha Z)^2\frac{m^2}{M}$.

Sometimes, to estimate the nuclear recoil corrections for high Z the nonrelativistic nuclear recoil operator is averaged with the Dirac wave functions. But, as one can see from the formulas (75)–(77) and Table IV, as in the one-electron case [see the formulas (37)–(40)], this contribution is considerably canceled by the one-transverse-photon contribution.

TABLE IV. The results of the numerical calculation of the two-electron nuclear recoil corrections $\Delta E^{(int)}$ for the $(1s)^2 2p_{\frac{1}{2}}$ state of lithiumlike ions expressed in terms of the function $Q(\alpha Z)$ defined by Eq. (74). $Q_L(\alpha Z)$ is the leading contribution defined by Eq. (75).

Z	$Q_c(\alpha Z)$	$Q_{tr(1)}(\alpha Z)$	$Q_{tr(2)}(\alpha Z)$	$Q(\alpha Z)$	$Q_L(\alpha Z)$
5	1.00168	-0.00233	0.00000	0.99935	0.99935
10	1.00677	-0.00938	0.00002	0.99741	0.99741
15	1.01533	-0.02129	0.00011	0.99416	0.99417
20	1.02753	-0.03830	0.00036	0.98959	0.98964
25	1.04359	-0.06077	0.00088	0.98370	0.98381
30	1.06378	-0.08920	0.00186	0.97645	0.97669
35	1.08851	-0.12422	0.00353	0.96782	0.96827
40	1.11827	-0.16669	0.00617	0.95776	0.95856
45	1.15370	-0.21767	0.01019	0.94622	0.94755
50	1.19560	-0.27853	0.01607	0.93313	0.93525
55	1.24500	-0.35105	0.02447	0.91841	0.92165
60	1.30322	-0.43751	0.03625	0.90195	0.90676
65	1.37198	-0.54091	0.05254	0.88361	0.89057
70	1.45352	-0.66521	0.07488	0.86320	0.87309
75	1.55087	-0.81573	0.10538	0.84052	0.85431
80	1.66810	-0.99980	0.14699	0.81529	0.83424
85	1.81092	-1.22771	0.20395	0.78716	0.81287
90	1.98751	-1.51431	0.28250	0.75570	0.79021
92	2.07014	-1.65003	0.32196	0.74206	0.78078
95	2.21001	-1.88186	0.39221	0.72035	0.76625
100	2.49719	-2.36503	0.54826	0.68041	0.74099

According to [35] the experimental value of the energy of the $(1s)^2 2p_{\frac{1}{2}}$-$(1s)^2 2s$ transition in lithiumlike uranium is 280.59(10) eV. Let us find the total nuclear recoil contribution to the energy of this transition. According to our calculation the term ΔE^{int} is -0.03 eV. Adding to this value the one-electron contribution defined by (68) we find

$$\Delta E_{(1s)^2 2p_{\frac{1}{2}}} - \Delta E_{(1s)^2 2s} = -0.07 \text{ eV}.$$

This correction is comparable with the uncertainty of the experimental value and, hence, will be important for comparison of theory with experiment, when calculations of all diagrams in the second order in α are completed.

ACKNOWLEDGMENTS

We wish to thank I. B. Khriplovich and S. G. Karshenboim for stimulating discussions and K. Pachucki for making the results of [10] available for us prior to publication. The research described in this publication was made possible in part by Grant No. NWU000 from the International Science Foundation and Grant No. 95-02-05571a from the Russian Foundation for Fundamental Investigations. A.N.A. thanks I. V. Konovalov for financial support.

APPENDIX

The integration over angles in the expressions considered here is carried out using the formula

$$\sum_{m_2}\langle n_1j_1l_1m_1|\mathbf{A}|n_2j_2l_2m_2\rangle\langle n_2j_2l_2m_2|\mathbf{B}|n_1j_1l_1m_1\rangle$$

$$= (-1)^{j_1+j_2-2m_1}\frac{1}{2j_1+1}(n_1j_1l_1||A^1||n_2j_2l_2)(n_2j_2l_2||B^1||n_1j_1l_1)\,, \quad \text{(A1)}$$

where $(n_1j_1l_1||A^1||n_2j_2l_2)$ and $(n_2j_2l_2||B^1||n_1j_1l_1)$ are the reduced matrix elements [36]. For $\mathbf{A} = \boldsymbol{\alpha}\phi(r), \mathbf{n}\phi(r)$ one can find

$$(n_1j_1l_1||\boldsymbol{\alpha}\phi(r)||n_2j_2l_2) = (-1)^{j_1-\frac{1}{2}}i\sqrt{6}\sqrt{2j_1+1}\sqrt{2j_2+1}\left[(-1)^{l_1}\delta_{l_1l_2'}\begin{Bmatrix} j_1 & j_2 & 1 \\ \frac{1}{2} & \frac{1}{2} & l_1 \end{Bmatrix}\int_0^\infty g_{n_1j_1l_1}(r)f_{n_2j_2l_2}(r)\phi(r)r^2dr \right.$$
$$\left. -(-1)^{l_1'}\delta_{l_1'l_2}\begin{Bmatrix} j_1 & j_2 & 1 \\ \frac{1}{2} & \frac{1}{2} & l_1' \end{Bmatrix}\int_0^\infty f_{n_1j_1l_1}(r)g_{n_2j_2l_2}(r)\phi(r)r^2dr\right]\,, \quad \text{(A2)}$$

$$(n_1j_1l_1||\mathbf{n}\phi(r)||n_2j_2l_2) = (-1)^{j_2-\frac{1}{2}}\left[Z^{j_1j_2}_{l_1l_2}\int_0^\infty g_{n_1j_1l_1}(r)g_{n_2j_2l_2}(r)\phi(r)r^2dr + Z^{j_1j_2}_{l_1'l_2'}\int_0^\infty f_{n_1j_1l_1}(r)f_{n_2j_2l_2}(r)\phi(r)r^2dr\right]\,, \quad \text{(A3)}$$

where

$$Z^{j_1j_2}_{l_1l_2} = \sqrt{(2l_1+1)(2l_2+1)(2j_1+1)(2j_2+1)}\begin{pmatrix} l_1 & 1 & l_2 \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} j_1 & 1 & j_2 \\ l_2 & \frac{1}{2} & l_1 \end{Bmatrix}\,, \quad \text{(A4)}$$

$l' = 2j - l$; and $g_{njl}(r)$ and $f_{njl}(r)$ are the upper and lower radial components of the Dirac wave function [37]:

$$\psi_{njlm}(\mathbf{r}) = \begin{pmatrix} g_{njl}(r)\Omega_{jlm}(\mathbf{n}) \\ if_{njl}(r)\Omega_{jl'm}(\mathbf{n}) \end{pmatrix}\,.$$

[1] H.A. Bethe and E.E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer, Berlin, 1957).

[2] E.E. Salpeter and H.A. Bethe, Phys. Rev. **84**, 1232 (1951).

[3] E.E. Salpeter, Phys. Rev. **87**, 328 (1952).

[4] T. Fulton and P. C. Martin, Phys. Rev. **95**, 811 (1954).

[5] H. Grotch and D.R. Yennie, Rev. Mod. Phys. **41**, 350 (1969).

[6] G.W. Erickson and D.R. Yennie, Ann. Phys. (N.Y.) **35**, 271 (1965); G.W. Erickson, in *Physics of One- and Two-Electron Atoms*, edited by F. Bopp and H. Kleinpoppen (North-Holland, Amsterdam, 1970).

[7] M. Doncheski, H. Grotch, and G.W. Erickson, Phys. Rev. A **43**, 2152 (1991).

[8] I.B. Khriplovich, A.I. Milstein, and A.S. Yelkhovsky, Phys. Scr. **T46**, 252 (1993).

[9] R.N. Fell, I.B. Khriplovich, A.I. Milstein, and A.S. Yelkhovsky, Phys. Lett. A **181**, 172 (1993).

[10] K. Pachucki and H. Grotch, Phys. Rev. A **51**, 1854 (1995).

[11] E.A. Golosov, I.B. Khriplovich, A.I. Milstein, and A.S. Yelkhovsky, Zh. Eksp. Teor. Fiz. **107**, 393 (1995).

[12] L.N. Labzowsky, in *Papers at 17th All-Union Symposium on Spectroscopy* (Astrosovet, Moscow, 1972), Pt. 2, pp. 89–93.

[13] M.A. Braun, Zh. Eksp. Teor. Fiz. **64**, 413 (1973).

[14] V.M. Shabaev, Teor. Mat. Fiz. **63**, 394 (1985) [Theor. Math. Phys. **63**, 588 (1985)].

[15] V.M. Shabaev, in *Papers at First Soviet-British Symposium on Spectroscopy of Multicharged Ions* (Academy of Sciences, Troitsk, 1986), pp. 238–240.

[16] V.M. Shabaev, Yad. Fiz. **47**, 107 (1988) [Sov. J. Nucl. Phys. **47**, 69 (1988)].

[17] L.S. Dul'yan and R.N. Faustov, Teor. Mat. Fiz. **22**, 314 (1975).

[18] F. Gross, Phys. Rev. **186**, 1448 (1969).

[19] A.A. Logunov and A.N. Tavkhelidze, Nuovo Cimento **29**, 380 (1963).

[20] R.N. Faustov, Fiz. Elem. Chasits At. Yadra **3**, 238 (1972).

[21] G.P. Lepage, Phys. Rev. A **16**, 863 (1977).

[22] V.M. Shabaev, in *Many-Particle Effects in Atoms*, edited by U.I. Safronova (Academy of Sciences, Moscow, 1985), pp. 118–144.

[23] G. Breit, Phys. Rev. **35**, 1447 (1930).

[24] A.S. Yelkhovsky, Budker Institute of Nuclear Physics, Novosibirsk, Report No. BINP 94-27, 1994 (unpub-

lished).
[25] V.M. Shabaev and A.N. Artemyev, J. Phys. B **27**, 1307 (1994).
[26] C.W. Palmer, J. Phys. B **20**, 5987 (1987).
[27] J. Epstein and S. Epstein, Am. J. Phys. **30**, 266 (1962).
[28] V.M. Shabaev, Vestn. Leningr. Univ. No. 4, 15 (1984).
[29] V.M. Shabaev, J. Phys. B **24**, 4479 (1991).
[30] I.P. Grant and H.M. Quiney, Adv. At. Mol. Phys. **23**, 37 (1988).
[31] W.R. Johnson, S.A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).
[32] S. Salomonson and P. Öster, Phys. Rev. A **40**, 5548 (1989).
[33] C. Froese Fisher and F.A. Parpia, Phys. Lett. A **179**, 198 (1993).
[34] D.S. Hughes and C. Eckart, Phys. Rev. **36**, 694 (1930).
[35] J. Schweppe, A. Belkacem, L. Blumenfeld, N. Claytor, B. Feinberg, H. Gould, V.E. Kostroun, L. Levy, S. Misawa, J.R. Mowat, and M.H. Prior, Phys. Rev. Lett. **66**, 1434 (1991).
[36] I.I. Sobel'man, *Introduction to Theory of Atomic Spectra* (Nauka, Moscow, 1977).
[37] A.I. Akhiezer and V.B. Berestetsky, *Quantum Electrodynamics* (Nauka, Moscow, 1969).