Interelectronic interaction contribution to the hyperfine structure of highly charged lithiumlike ions

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The hyperfine structure of highly charged lithiumlike ions is considered within QED using the $\frac{1}{Z}$ perturbation theory (Z is the nuclear charge). The interelectronic interaction contribution of the order of $\frac{1}{Z}$ to the hyperfine splitting of the ground state is calculated in the range $Z = 5$–100. The hyperfine splitting values are found for the ground state of $^{57}Fe^{23+}$ and $^{209}Bi^{80+}$.

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I. INTRODUCTION

Several years ago it was noted [1] that study of the radio lines in the millimeter region, corresponding to the transitions between the hyperfine structure components of multicharged ions, could be a method of investigation of chemical composition of hot astrophysical plasma. The search conditions of this transition for $^{57}Fe^{23+}$ required the prediction of the wavelength with an accuracy $\sim 0.2\%$. It gave rise to the calculations of the hyperfine structure of highly charged lithiumlike ions by various methods [2–5]. So, in [2] the multiconfiguration Hartree-Fock (MCHF) method with the relativistic correction was used. The Hartree-Fock-Dirac (HFD) method and the model potential method were employed in [3] and [4], respectively. The most precise calculation for $^{57}Fe^{23+}$ was done in [5] where the $\frac{1}{Z}$ perturbation theory had been used.

In the present paper we refine the result of [5] and extend the calculation of the interelectronic interaction contribution to higher Z. We evaluate the hyperfine structure of $^{209}Bi^{80+}$ that can be of interest for the experimental investigations at GSI (Darmstadt) [6,7].

In the zeroth order of the $\frac{1}{Z}$ perturbation theory the hyperfine structure of the lithiumlike ions is defined by the same formulas as for the one-electron ions [8]. Taking account of the interelectronic interaction in the first order of the perturbation theory gives the corrections of the order of $\frac{1}{Z}$. These corrections are calculated within quantum electrodynamics (QED) in the range $Z = 5$–100 in Sec. II of the present paper. The calculations of the hyperfine splitting of the ground state of $^{57}Fe^{23+}$ and $^{209}Bi^{80+}$ are presented in Sec. III.

The relativistic units ($\hbar = c = m = 1$) and the Heaviside charge unit ($\alpha = \frac{e^2}{4\pi}$, $e < 0$) are used throughout the paper.

II. BASIC FORMULAS AND CALCULATIONS

We consider the hyperfine splitting of the ground state of highly charged lithiumlike ions. It is convenient to represent the energy difference between the hyperfine splitting components in the form

$$\Delta E_{2s} = \frac{1}{6}\alpha(\alpha Z)^3 \frac{m}{m_p}\frac{\mu}{\mu_N}\frac{2I+1}{2I}mc^2 \times\Big\{[A(\alpha Z)(1-\delta)(1-\varepsilon)+x_{\rm rad}] +\frac{1}{Z}B(\alpha Z)+\frac{1}{Z^2}C(\alpha Z)+\cdots\Big\}, \quad (1)$$

where α is the fine structure constant, I is the nuclear spin, μ is the nuclear magnetic moment, μ_N is the nuclear magneton, and m_p is the proton mass. $A(\alpha Z)$ is the one-electron relativistic factor [9,5]

$$A(\alpha Z) = \frac{2[2(1+\gamma)+\sqrt{2(1+\gamma)}]}{(1+\gamma)^2\gamma(4\gamma^2-1)} = 1+\frac{17}{8}(\alpha Z)^2+\frac{449}{128}(\alpha Z)^4+\cdots, \quad (2)$$

$\gamma = \sqrt{1-(\alpha Z)^2}$; δ and ε denote the nuclear charge and magnetization distribution corrections. $x_{\rm rad}$ is the one-electron radiative correction. In the lowest orders in α and αZ this correction is [10,11]

$$x_{\rm rad} = \frac{\alpha}{2\pi}+\left(\ln 2-\frac{5}{2}\right)\alpha(\alpha Z)-\frac{8}{3\pi}\ln^2\Big(\frac{1}{\alpha Z}\Big)\alpha(\alpha Z)^2 +\frac{2}{\pi}\Big(-\frac{16}{3}\ln 2+\frac{37}{72}+\frac{4}{15}+\frac{7}{2}\Big)\ln\Big(\frac{1}{\alpha Z}\Big)\alpha(\alpha Z)^2 +(3.12\pm 0.09)\alpha(\alpha Z)^2. \quad (3)$$

Thus, the one-electron contribution is enclosed in the square brackets of Eq. (1). The other terms in the curly brackets of (1) correspond to two- and three-electron contributions.

To calculate the function $B(\alpha Z)$ we need, first of all, to derive the calculation expression for this contribution. For that we use the Green function technique in the Furry picture for the case when the closed $(1s)^2$ shell is considered as the vacuum. The Fourier transform of the QED Green function of the considered system is defined by

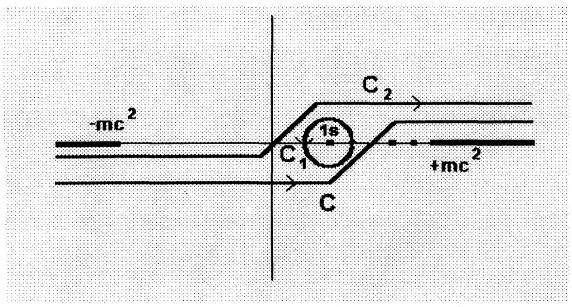

FIG. 1. C is the original contour of the integration over the electron energy variable when the closed $(1s)^2$ shell is considered as the vacuum. C_1+C_2 is the transformed contour.

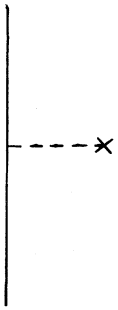

FIG. 2. The lowest-order diagram contributing to the hyperfine structure.

$$g(E,\mathbf{x},\mathbf{x}')\delta(E-E') = \frac{1}{2\pi i}\int_{-\infty}^{\infty} dt dt' \ \exp(iEt - iE't') \times \langle 0_{(1s)^2}|T\psi(t,\mathbf{x})\psi^\dagger(t',\mathbf{x}')|0_{(1s)^2}\rangle, \tag{4}$$

where $\psi(x)$ is the electron-positron field operator in the Heisenberg representation and T is the time-ordered product operator. Introducing $g_{nn}(E)$ by

$$g_{nn}(E) = \int d\mathbf{x} d\mathbf{x}' \ u_n^\dagger(\mathbf{x}) g(E,\mathbf{x},\mathbf{x}') u_n(\mathbf{x}') \ , \tag{5}$$

where u_n is the unperturbed wave function of a state n, and using the Sz.-Nagy and Kato technique [12] we get the energy shift [13]

$$\Delta E_n \equiv E_n - E_n^{(0)} = \frac{\frac{1}{2\pi i}\oint_\Gamma dE \ (E-E_n^{(0)})\Delta g_{nn}(E)}{1+\frac{1}{2\pi i}\oint_\Gamma dE \ \Delta g_{nn}(E)} \ , \tag{6}$$

where $\Delta g_{nn} \equiv g_{nn} - g_{nn}^{(0)}$, $g_{nn}^{(0)} = (E-E_n^{(0)})^{-1}$. The integration contour Γ surrounds the level $E_n^{(0)}$ and does not surround the other levels. The Green function $g_{nn}(E)$ is constructed using Wick's theorem after the transition in (4) to the interaction representation. Because we consider the closed $(1s)^2$ shell as the vacuum, in the diagram technique rules [13] the electron propagator denominators corresponding to the $1s$ states have the same sign of $i0$ as the denominators corresponding to the negative energy states. In other words, the integration over the intermediate electron energy variable is carried out along the contour C represented in Fig. 1. In the first order of the perturbation theory according to (6) we have

$$\Delta E_n^{(1)} = \frac{1}{2\pi i}\oint_\Gamma dE \ (E-E_n^{(0)})\Delta g_{nn}^{(1)}(E) \ . \tag{7}$$

In the second order

$$\Delta E_n^{(2)} = \frac{1}{2\pi i}\oint_\Gamma dE \ (E-E_n^{(0)})\Delta g_{nn}^{(2)}(E) - \frac{1}{2\pi i}\oint_\Gamma dE \ (E-E_n^{(0)})\Delta g_{nn}^{(1)}(E) \times \frac{1}{2\pi i}\oint_\Gamma dE \ \Delta g_{nn}^{(1)}(E) \ . \tag{8}$$

We are interested here only in the hyperfine splitting. Therefore, in the first order of the perturbation theory we calculate only the contribution from the diagram represented in Fig. 2 where the dotted line denotes the hyperfine interaction. It corresponds to averaging the Fermi-Breit operator

$$W_\mu = \frac{|e|}{4\pi}\frac{\boldsymbol{\alpha}(\boldsymbol{\mu}\times\mathbf{r})}{r^3} \ , \tag{9}$$

where $\boldsymbol{\alpha}$ are the Dirac matrices, with the Dirac Coulomb wave functions and gives the relativistic one-electron contribution. In the technique considered here the interelectronic interaction corrections and the one-electron radiative corrections to the hyperfine splitting are the result of the diagrams represented in Fig. 3. To divide the contributions of these diagrams into the interelectronic interaction ones and the one-electron radiative ones we represent the intermediate electron energy integration along the contour C (Fig. 1) in the form of the sum of the integrals along the contours C_1 and C_2 shown in Fig. 1. The integration along C_2 gives the one-electron radiative corrections that are determined by (3) in the lowest orders in αZ. The contribution from the contour C_1 corresponding to the interelectronic interaction corrections in the Feynman gauge is (see the Appendix)

$$\Delta E_F^{(2)} = \sum_{M_I\, m}\sum_{M_I'\, m'} C^{FM_F}_{IM_I'\frac{1}{2}m'} C^{FM_F}_{IM_I\frac{1}{2}m} \chi^\dagger_{IM_I'}(I^{(2a)}+I^{(2b)}+I^{(2c)}+I^{(2d)})\chi_{IM_I} \ , \tag{10}$$

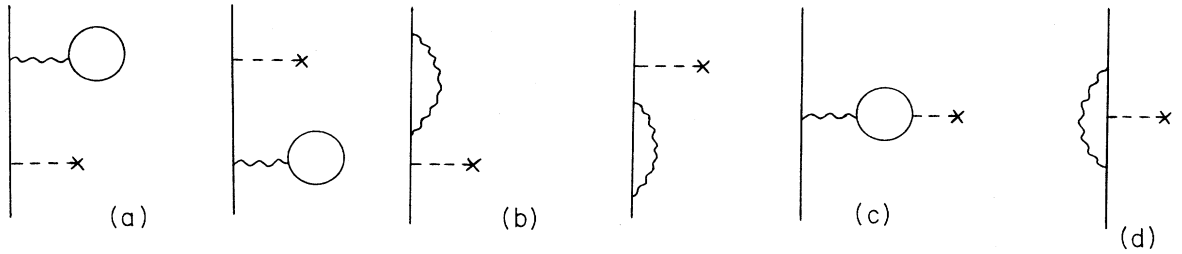

FIG. 3. The second-order diagrams contributing to the hyperfine structure.

$$I^{(2a)} = \alpha \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \sum_{\varepsilon_c=\varepsilon_{1s}} \psi^\dagger_{v'}(\mathbf{x}_3)\psi^\dagger_c(\mathbf{x}_2) \times \Big(\frac{1-\boldsymbol{\alpha}_2\cdot\boldsymbol{\alpha}_3}{r_{23}} G^R_{2s}(3,1) W_\mu(1) + W_\mu(3) G^R_{2s}(3,1) \frac{1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2}{r_{12}} \Big) \psi_v(\mathbf{x}_1)\psi_c(\mathbf{x}_2) \,, \tag{11}$$

$$I^{(2b)} = -\alpha \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \sum_{\varepsilon_c=\varepsilon_{1s}} \Big(\psi^\dagger_c(\mathbf{x}_3)\psi^\dagger_{v'}(\mathbf{x}_2) \frac{(1-\boldsymbol{\alpha}_2\cdot\boldsymbol{\alpha}_3)\cos\Delta r_{23}}{r_{23}} G^R_{2s}(3,1) W_\mu(1)\psi_v(\mathbf{x}_1)\psi_c(\mathbf{x}_2)$$
$$+\psi^\dagger_c(\mathbf{x}_1)\psi^\dagger_{v'}(\mathbf{x}_3) W_\mu(3) G^R_{2s}(3,2) \frac{(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\cos\Delta r_{12}}{r_{12}} \psi_v(\mathbf{x}_1)\psi_c(\mathbf{x}_2) - [\psi^\dagger_{v'}(\mathbf{x}_1) W_\mu(1)\psi_v(\mathbf{x}_1)]$$
$$\times \psi^\dagger_c(\mathbf{x}_3)\psi^\dagger_v(\mathbf{x}_2)(1-\boldsymbol{\alpha}_2\cdot\boldsymbol{\alpha}_3)\sin(\Delta r_{23})\,\psi_v(\mathbf{x}_3)\psi_c(\mathbf{x}_2)\Big) \,, \tag{12}$$

$$I^{(2c)} = \alpha \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \sum_{\varepsilon_c=\varepsilon_{1s}} \psi^\dagger_{v'}(\mathbf{x}_1)\psi^\dagger_c(\mathbf{x}_3) \times \Big(\frac{1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_3}{r_{13}} G^R_{1s}(3,2) W_\mu(2) + W_\mu(3) G^R_{1s}(3,2) \frac{1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2}{r_{12}} \Big) \psi_v(\mathbf{x}_1)\psi_c(\mathbf{x}_2) \,, \tag{13}$$

$$I^{(2d)} = -\alpha \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \sum_{\varepsilon_c=\varepsilon_{1s}} \Big(\psi^\dagger_c(\mathbf{x}_1)\psi^\dagger_{v'}(\mathbf{x}_3) \frac{(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_3)\cos\Delta r_{13}}{r_{13}} G^R_{1s}(3,2) W_\mu(2)\psi_v(\mathbf{x}_1)\psi_c(\mathbf{x}_2)$$
$$+\psi^\dagger_c(\mathbf{x}_3)\psi^\dagger_{v'}(\mathbf{x}_2) W_\mu(3) G^R_{1s}(3,1) \frac{(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\cos\Delta r_{12}}{r_{12}} \psi_v(\mathbf{x}_1)\psi_c(\mathbf{x}_2) + \sum_{\varepsilon_{c'}=\varepsilon_{1s}} \psi^\dagger_c(\mathbf{x}_3) W_\mu(3)\psi_{c'}(\mathbf{x}_3)$$
$$\times \psi^\dagger_{v'}(\mathbf{x}_2)\psi^\dagger_{c'}(\mathbf{x}_1)(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\sin(\Delta r_{12})\,\psi_v(\mathbf{x}_1)\psi_c(\mathbf{x}_2)\Big) \,, \tag{14}$$

where

$$G^R_k(1,2) = \sum_{\varepsilon_n\neq\varepsilon_k} \frac{\psi_n(\mathbf{x}_1)\psi^\dagger_n(\mathbf{x}_2)}{\varepsilon_k - \varepsilon_n} \,, \tag{15}$$

$v \equiv (2\tfrac{1}{2}0m)$, $v' \equiv (2\tfrac{1}{2}0m')$, $C^{FM_F}_{IM_I\frac{1}{2}m}$ is the Clebsch-Gordan coefficient, χ_{IM_I} is the nuclear wave function, $\Delta = \varepsilon_{2s} - \varepsilon_{1s}$, and ε_n is the energy of the n state in the Coulomb field of the nucleus.

After the integration over the angular variables in (10)–(14), in the case of a point nucleus the summation over the intermediate electron states coming from G^R_k is carried out analytically using the method of the generalized virial relations for the Dirac equation [14]. This method allows one to calculate by simple algebraic relations the sums of kind

$$|\xi\rangle \equiv \sum_{n'}{}' \frac{|n'\kappa'\rangle\langle n'\kappa'|R|n\kappa\rangle}{\varepsilon_{n\kappa} - \varepsilon_{n'\kappa'}} \,. \tag{16}$$

Here the prime over the summation means that it is carried out over all n' (κ' is fixed) for which $\varepsilon_{n'\kappa'} \neq \varepsilon_{n\kappa}$; $\kappa = (-1)^{j+l+\frac{1}{2}}(j+\frac{1}{2})$, j and l are the total and orbital electron moments, respectively; n is the principal quantum number;

$$|n\kappa\rangle \equiv \begin{pmatrix} rg_{n\kappa}(r) \\ rf_{n\kappa}(r) \end{pmatrix} , \quad \langle n\kappa|n\kappa\rangle = \int_0^\infty (g_{n\kappa}^2 + f_{n\kappa}^2) r^2 \, dr = 1 ,$$

$g_{n\kappa}$ and $f_{n\kappa}$ denote the upper and lower radial components of the Dirac Coulomb wave function:

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

R is one of the following operators: r^s, $\sigma_z r^s$, $\sigma_x r^s$, $i\sigma_y r^s$, where σ_x, σ_y, σ_z are the Pauli matrices, $s = -2, -3, -4, \ldots$. [For $\kappa' = \kappa$ the method allows the calculation of the sums (16) for arbitrary integer s.] So, for the case $R = \sigma_x r^{-2}$ that appears in our calculation one can find for $\kappa \neq \pm\kappa'$

$$\begin{aligned} \sum_{n'} \frac{|n'\kappa'\rangle\langle n'\kappa'|\sigma_x r^{-2}|n\kappa\rangle}{\varepsilon_{n\kappa} - \varepsilon_{n'\kappa'}} &= \{[1-(\kappa-\kappa')^2][1-(\kappa+\kappa')^2] + 4(\alpha Z)^2\}^{-1} \\ &\times \Big[[1-(\kappa+\kappa')^2]\Big(\frac{4\alpha Z m}{\kappa^2-\kappa'^2} + (\kappa'-\kappa)r^{-1} + r^{-1}\sigma_z \\ &- \frac{2}{\kappa+\kappa'}(m\sigma_x + \varepsilon_{n\kappa} i\sigma_y)\Big) + \frac{4\alpha Z[(\kappa'+\kappa)m - \varepsilon_{n\kappa}]}{\kappa-\kappa'} \\ &+ 2\alpha Z[\sigma_x r^{-1} + (\kappa'+\kappa)r^{-1} i\sigma_y]\Big]|n\kappa\rangle . \end{aligned} \tag{17}$$

For $\kappa' = \kappa$

$$\begin{aligned} \sum_{n'}{}' \frac{|n'\kappa\rangle\langle n'\kappa|\sigma_x r^{-2}|n\kappa\rangle}{\varepsilon_{n\kappa} - \varepsilon_{n'\kappa}} &= \frac{1}{4(\alpha Z)^2 + (1-4\kappa^2)}\Big[2\alpha Z\sigma_x r^{-1} + 4\alpha Z\kappa i\sigma_y r^{-1} \\ &+ (1-4\kappa^2)\sigma_z r^{-1} + \frac{(1-4\kappa^2)}{\kappa}(\varepsilon_{n\kappa} i\sigma_y - m\sigma_x) \\ &- \frac{2(\alpha Z)^3 \kappa m}{N^3\gamma}\Big]|n\kappa\rangle - \frac{2\alpha Z(2\varepsilon_{n\kappa} - \frac{m}{\kappa})}{4(\alpha Z)^2 + (1-4\kappa^2)} \frac{d}{d\kappa}|n\kappa\rangle , \end{aligned} \tag{18}$$

where $\gamma = \sqrt{\kappa^2 - (\alpha Z)^2}$, $N = \sqrt{n_r^2 + 2\gamma n_r + \kappa^2}$, n_r is the radial quantum number ($n = n_r + |\kappa|$). The derivative $\frac{d}{d\kappa}|n\kappa\rangle$ is calculated at the fixed radial quantum number n_r. For the $1s$ state:

$$\frac{d}{d\kappa}|n\kappa\rangle = \begin{pmatrix} G_{1s}(r) \\ F_{1s}(r) \end{pmatrix} , \tag{19}$$

where

$$G_{1s}(r) = \frac{k}{\sqrt{1-\gamma}} \exp(-t/2) t^\gamma \Big(\frac{\psi(2\gamma+1)}{\gamma} + (\gamma+1) - \frac{1}{2\gamma} - \frac{t}{2} - \frac{1}{\gamma}\ln t\Big) , \tag{20}$$

$$F_{1s}(r) = -\frac{k}{\sqrt{1+\gamma}} \exp(-t/2) t^\gamma \Big(\frac{\psi(2\gamma+1)}{\gamma} + (\gamma+1) + \frac{1}{2\gamma} - \frac{t}{2} - \frac{1}{\gamma}\ln t\Big) , \tag{21}$$

$$t = \frac{2\alpha Z m r}{N} , \quad k = \frac{(2\alpha Z)^{\frac{3}{2}} m^{\frac{1}{2}}}{2\sqrt{2\Gamma(2\gamma+1)}} ,$$

$\Gamma(x)$ is the gamma function, $\psi(x) = \frac{d}{dx}\ln\Gamma(x)$. For the $2s$ state:

$$\frac{d}{d\kappa}|n\kappa\rangle = \begin{pmatrix} G_{2s}(r) \\ F_{2s}(r) \end{pmatrix} , \tag{22}$$

where

$$\begin{aligned} G_{2s}(r) = k' \exp\Big(-\frac{t}{2}\Big) t^\gamma \frac{\sqrt{2+N}}{N^2-2} \Big\{ &\frac{t^2}{2(N-1)} - \Big(\frac{2N^4 - 4N^3 + 5N^2 - 3N + 2}{2N(N-1)^2} + \frac{2\psi(2\gamma+1)}{N-1}\Big)t \\ &+ \frac{N^4 - 2N^3 + N - 2}{2(N-1)} + 2N\psi(2\gamma+1) + \frac{2}{N-1} t\ln t - 2N\ln t\Big\} , \end{aligned} \tag{23}$$

$$F_{2s}(r) = -k' \exp\left(-\frac{t}{2}\right) t^{\gamma} \frac{\sqrt{2-N}}{N^2-2} \left\{ \frac{t^2}{2(N-1)} - \left(\frac{2N^4 - 2N^3 + N^2 + 3N - 2}{2N(N-1)^2} + \frac{2\psi(2\gamma+1)}{N-1} \right) t \right.$$
$$\left. + \frac{N^5 + 5N^2 - 8N - 4}{2N(N-1)} + 2(N+2)\psi(2\gamma+1) + \frac{2}{N-1} t \ln t - 2(N+2)\ln t \right\}, \quad (24)$$

$$t = \frac{2\alpha Z m r}{N}, \quad k' = \frac{\sqrt{\Gamma(2\gamma+2)}}{\Gamma(2\gamma+1)} \frac{1}{\sqrt{8N(N+1)}} \left(\frac{2\alpha Z m}{N}\right)^{\frac{1}{2}}.$$

The results of the calculation of $B(\alpha Z)$ are given in Table I. The functions $B^{(a)}(\alpha Z)$, $B^{(b)}(\alpha Z)$, $B^{(c)}(\alpha Z)$, and $B^{(d)}(\alpha Z)$ denote the contributions from the diagrams a, b, c, and d represented in Fig. 3. For low Z it is convenient to represent the function $B(\alpha Z)$ in the αZ expansion form

$$B(\alpha Z) = b_0 + b_2(\alpha Z)^2 + \cdots . \quad (25)$$

To calculate the coefficients b_0 and b_2, Eqs. (12) and (14) can be restricted to the two lowest terms in the expansion of $\cos \Delta r$ and the lowest term in the expansion of $\sin \Delta r$. After that, the total expression for $\Delta E_F^{(2)}$ can be transformed to the one which is obtained if the Coulomb-Breit operator is used for the interelectronic interaction

$$V^{C-B} = V^C + V^B, \quad (26)$$

where

$$V^C = \frac{\alpha}{r_{12}}, \quad V^B = -\frac{1}{2}\alpha \left(\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r_{12}} + \frac{(\boldsymbol{\alpha}_1 \cdot \mathbf{r}_{12})(\boldsymbol{\alpha}_2 \cdot \mathbf{r}_{12})}{r_{12}^3} \right).$$

The contributions to b_0 and b_2 from the diagrams represented in Fig. 3 are given in Table II. [In the Coulomb gauge the Coulomb-Breit interaction (26) is implied for the photon line in Fig. 3.] Here we have corrected a numerical error that was made in the calculation of the Breit part of b_2 in [5] (the numerical error was made in the calculation of a term equally contributing in both gauges). As one can see from Table II, the contributions from the separate diagrams in the Feynman and Coulomb gauges, generally speaking, do not coincide with each other but, in accordance with the gauge invariance, the total contributions from the gauge-invariant sets of the diagrams coincide with each other.

Because the function $B(\alpha Z)$ is calculated for a point nucleus, the nuclear size corrections to this function must be calculated separately. As one can see from Tables I and II, the function $B(\alpha Z)$ is largely made up of the contribution $B^{(a)}(\alpha Z)$ which corresponds to the direct Coulomb interaction of the $2s$ electron with the closed $1s$ shell. It means that the main part of the $\frac{1}{Z}$ contribution can be taken into account by averaging the Fermi-Breit operator (9) with the Dirac wave function of the electron in the spherically symmetric potential of the closed shell. In this case (see, e.g., [15]) the relative value of the nuclear charge distribution correction is mainly defined by behavior of the wave function at small r, where the Coulomb potential is to be, and is approximately the same as for the one-electron atom. (The interaction with the closed $1s$ shell changes mainly the normalization factor of the wave function at small r.) So, we suppose that a main contribution of this correction to $\frac{B(\alpha Z)}{Z}$, which we denote by $\Delta_{NS}\left[\frac{B(\alpha Z)}{Z}\right]$, can be estimated roughly by

$$\Delta_{NS}\left[\frac{B(\alpha Z)}{Z}\right] \approx -\delta \frac{B(\alpha Z)}{Z}, \quad (27)$$

where δ is the one-electron nuclear charge distribution correction. This formula is confirmed by the HFD calculations as well [16].

The term $\frac{C(\alpha Z)}{Z^2}$ in (1) is considerable only for low Z where the nonrelativistic approximation $C(\alpha Z) \approx c_0$ is valid. We can roughly estimate c_0 from the nonrelativistic calculation of the hyperfine splitting done in [17,18]. Proceeding from the nonrelativistic splitting values for $Z = 8, 9$ [18] and taking into account $b_0 = -2.6557$ [5] we obtain $c_0 = 0.9(4)$.

III. APPLICATIONS

A. Hyperfine structure of $^{57}Fe^{23+}$

Using the results of the preceding section and the formulas for δ and ε from [8], we evaluate the wavelength of the transition between the hyperfine structure components of the ground state of $^{57}Fe^{23+}$ which is necessary for the astrophysical search [1,19]. Because there is a discrepancy in the experimental values of μ, we calculate λ for all μ given in [20]. For $\frac{\mu}{\mu_N}$=0.090 623, 0.090 764, and 0.090 44(7) we find λ=0.3073(5) cm, 0.3068(5) cm, and 0.3079(5) cm, respectively. The values of the individual terms enclosed in the curly brackets of formula (1) are listed in Table III. For comparison, the results obtained with other methods are also given in this table. The nuclear charge distribution correction δ is found from Table I of [8] by interpolation. The uncertainty of δ is about 2% of δ. The Bohr-Weisskopf correction ε [21,22] is calculated within the single-particle model of the nucleus, taking into account the angular asymmetry of the spin distribution. For that the analytical formulas from [8] are employed. (It should be noted that taking account of the angular asymmetry changes ε by 75% in comparison with the calculation neglecting it.) The radial part of the probability density of the odd neutron is assumed to be homogeneously distributed within the nucleus. We

TABLE I. The contributions to the interelectronic interaction correction $B(\alpha Z)$, defined by (1), from the diagrams represented in Fig. 3.

Z	$B^{(a)}(\alpha Z)$	$B^{(b)}(\alpha Z)$	$B^{(c)}(\alpha Z)$	$B^{(d)}(\alpha Z)$	$B(\alpha Z)$
5	-2.94569	-0.376832	5.73790×10^{-4}	0.657978	-2.66397
10	-2.97773	-0.382178	2.31248×10^{-3}	0.668508	-2.68909
15	-3.03220	-0.391226	5.26916×10^{-3}	0.686408	-2.73175
20	-3.11082	-0.404194	9.53611×10^{-3}	0.712229	-2.79325
25	-3.21610	-0.421404	1.52510×10^{-2}	0.746792	-2.87547
30	-3.35163	-0.443301	2.26066×10^{-2}	0.791249	-2.98107
35	-3.52224	-0.470483	3.18650×10^{-2}	0.847170	-3.11369
40	-3.73451	-0.503743	4.33791×10^{-2}	0.916671	-3.27820
45	-3.99730	-0.544126	5.76232×10^{-2}	1.00261	-3.48119
50	-4.32266	-0.593015	7.52391×10^{-2}	1.10886	-3.73158
55	-4.72720	-0.652263	9.71064×10^{-2}	1.24074	-4.04162
60	-5.23417	-0.724378	0.124450	1.40570	-4.42840
65	-5.87690	-0.81282	0.159013	1.61438	-4.91633
70	-6.70440	-0.922491	0.203343	1.88241	-5.54114
75	-7.79119	-1.06049	0.261287	2.23347	-6.35692
80	-9.25523	-1.23751	0.338886	2.70496	-7.44889
85	-11.2927	-1.47040	0.446111	3.35898	-8.95803
90	-14.2514	-1.78723	0.600489	4.30529	-11.1328
95	-18.8006	-2.23850	0.835486	5.75477	-14.4488
100	-26.3862	-2.92560	1.22277	8.16191	-19.9271

suppose that the uncertainty of ε, due to mainly a deviation from the single-particle model of the nucleus, is about 50% of ε. The one-electron radiative correction is calculated according to formula (3). The uncertainty of this correction, determined by the uncalculated terms in the expansion (3), is about 30% of $x_{\rm rad}$. The nuclear size correction $\Delta_{NS}\left[\frac{B(\alpha Z)}{Z}\right]$ is estimated by Eq. (27). We assume that the uncertainty of this correction is about 50% of the value.

The difference of the values of λ obtained in this paper from our previous value ($\lambda = 0.3071$ cm) [5] is mainly determined by the change of μ and ε. (In [5] we used $\mu = 0.090\,61$ and $\varepsilon = 0.0021$. This value of ε was found neglecting the angular asymmetry of the spin distribution and taking the average between two distributions of the nuclear magnetization, homogeneous over the volume and homogeneous over the surface.)

B. Hyperfine structure of $^{209}Bi^{80+}$

In connection with the experiments at GSI (Darmstadt), in [23,24] the hyperfine splitting of the ground state of $^{209}Bi^{80+}$ was calculated. The calculation of the present paper, without taking account of the one-electron radiative corrections, gives $\lambda = 1.543(11)$ μm, for $\frac{\mu}{\mu_N} = 4.1106(2)$ [20]. The values of the individual effects are given in Table IV. The Bohr-Weisskopf correction ε is calculated within the single-particle model of the nucleus by taking the average between two distributions of the radial part of the probability density of the odd proton, homogeneous over the nuclear volume and homogeneous over the nuclear surface. Thereby we have taken into account that the real distribution is an intermediate between these two [25]. For comparison, in Table IV the results of the previous calculations [23,24] are also presented. The difference of our value from the result of Panigrahy *et al.* [23], obtained with the relativistic many body perturbation theory, is defined mainly by the fact that the nuclear magnetization distribution correction was omitted in [23]. According to our calculation this correction contributes $-0.037(15)$ to the total value given in the table. The deviation of the present result from the result of [24] is caused mainly by the fact that the nuclear size correction $\Delta_{NS}\left[\frac{B(\alpha Z)}{Z}\right]$ was neglected in [24]. In addition, in [23] and [24] only the Coulomb part of the interelectronic interaction contribution was

TABLE II. The contributions to the coefficients b_0 and b_2, defined by (25), from the diagrams represented in Fig. 3.

Diagrams	b_0	Feynman gauge	Coulomb gauge		
		b_2	b_2^C	b_2^B	$b_2^C + b_2^B$
a	-2.9351	-7.9225	-7.9225	0	-7.9225
b	-0.3751	-1.3255	-0.5174	-0.2365	-0.7539
c	0	0.4299	0	0.4299	0.4299
d	0.6545	2.6043	1.7626	0.2701	2.0327
total	-2.6557	-6.2138	-6.6773	0.4635	-6.2138

TABLE III. The terms enclosed in the braces of formula (1) for $^{57}Fe^{23+}$. The wavelength of the transition between the hyperfine structure components is found to be $\lambda = 0.3073(5)cm$, $0.3068(5)cm$, and $0.3079(5)cm$ for $\mu/\mu_N = 0.090623$, 0.090764, and 0.09044(7) [20], respectively.

Term	Value
$A(\alpha Z)$	1.0813
δ	0.0045(1)
ε	0.0028(14)
$A(\alpha Z)(1-\delta)(1-\varepsilon)$	1.0734(14)
x_{rad}	-0.0010(3)
$\frac{B(\alpha Z)}{Z}$	-0.1113
$\Delta_{NS}\left[\frac{B(\alpha Z)}{Z}\right]$	0.0005(3)
$\frac{c_0}{Z^2}$	0.0013(6)
Total	0.9629(16)
Fermi-Segre formula [1]	0.966
MCHF with rel. cor. [2]	0.9662
HFD [3]	0.9410
Model potential [4]	0.955

calculated. According to our calculation the complete $\frac{1}{Z}$ contribution for the point nucleus is

$$\left.\frac{B(\alpha Z)}{Z}\right|_{Z=83} = -0.100$$

while the Coulomb part gives [24]

$$\left.\frac{B^C(\alpha Z)}{Z}\right|_{Z=83} = -0.105\,.$$

So, the Breit part contributes 0.005 to the total value given in the table and is small enough in comparison with what one could expect.

IV. CONCLUSION

In the present paper the interelectronic interaction contribution of the order of $\frac{1}{Z}$ to the hyperfine splitting of the ground state of lithiumlike ions has been calculated. The hyperfine splitting values for $^{57}Fe^{23+}$ and $^{209}Bi^{80+}$ are evaluated. At the present time an astrophysical search of the radio lines in the millimeter region corresponding to the transitions between the hyperfine structure components of lithiumlike ions with $Z < 20$ is also planned [19]. For that the prediction of the wavelengths with accuracy $\sim 0.1\%$ is required. We think that the method considered here in combination with the nonrelativistic MCHF method is most suitable for this purpose, since it allows one to find consistently various corrections to the hyperfine splitting and their uncertainties. Such calculations are underway and will be published elsewhere.

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APPENDIX

We consider how Eqs. (11)–(13) are derived on the example of the contribution from diagrams (b) represented in the Fig. 3. The contribution from these diagrams is to be considered together with the corresponding contribution of the second term in (8). According to (8) and the diagram technique rules [13] we have

TABLE IV. The terms enclosed in the braces of formula (1) for $^{209}Bi^{80+}$. The wavelength of the transition between the hyperfine structure components, without the one-electron radiative corrections, is found to be $\lambda = 1.543(11)\mu m$ for $\mu/\mu_N = 4.1106(2)$ [20].

Term	Value
$A(\alpha Z)$	2.790
δ	0.117(2)
ε	0.015(6)
$A(\alpha Z)(1-\delta)(1-\varepsilon)$	2.427(16)
$\frac{B(\alpha Z)}{Z}$	-0.100
$\Delta_{NS}\left[\frac{B(\alpha Z)}{Z}\right]$	0.012(6)
Total	2.340(17)
Panigrahy et al. [23]	2.387
Shabaeva [24]	2.321

$$\Delta E_F^{(2,b)} = \sum_{M_I m} \sum_{M_I' m'} C^{FM_F}_{IM_I' \frac{1}{2} m'} C^{FM_F}_{IM_I \frac{1}{2} m} \chi^{\dagger}_{IM_I'} (I^{(2b)}) \chi_{IM_I} , \tag{A1}$$

$$I^{(b)} = \frac{1}{2\pi i} \oint_\Gamma dE (E-\varepsilon_v)^{-1} \sum_n \Big\{ \langle v'|\Sigma(E)|n\rangle \frac{1}{E-\varepsilon_n} \langle n|W_\mu|v\rangle + \langle v'|W_\mu|n\rangle \frac{1}{E-\varepsilon_n} \langle n|\Sigma(E)|v\rangle \Big\}$$
$$- \frac{1}{2\pi i} \oint dE\, (E-\varepsilon_v)^{-1} \langle v'|W_\mu|v\rangle \frac{1}{2\pi i} \oint dE\, (E-\varepsilon_v)^{-2} \langle v|\Sigma(E)|v\rangle , \tag{A2}$$

where

$$\langle a|\Sigma(E)|b\rangle = \frac{i}{2\pi} \int_C dp^0 \sum_n \frac{\langle ab|I(E-p^0)|nb\rangle}{p^0-\varepsilon_n} , \tag{A3}$$

$$I(\omega) = \alpha(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2) \frac{\exp\left(i\sqrt{\omega^2-\mu^2+i\delta}\, r_{12}\right)}{r_{12}} , \tag{A4}$$

μ is a small photon mass that allows one to separate the pole at the point $E = \varepsilon_v$ from the corresponding cut [13,26]. Calculating the E residues we obtain

$$I^{(b)} = \sum_{\varepsilon_n \neq \varepsilon_v} \Big\{ \langle v'|\Sigma(\varepsilon_v)|n\rangle \frac{1}{\varepsilon_v-\varepsilon_n} \langle n|W_\mu|v\rangle + \langle v'|W_\mu|n\rangle \frac{1}{\varepsilon_v-\varepsilon_n} \langle n|\Sigma(\varepsilon_v)|v\rangle \Big\}$$
$$+ \langle v'|W_\mu|v\rangle \Big[\frac{d}{dE}\langle v|\Sigma(E)|v\rangle\Big]_{E=\varepsilon_v} . \tag{A5}$$

Let us represent the integral along C in (A3) in the form of the sum of the integrals along C_1 and C_2 (Fig. 1). We obtain

$$\langle v'|\Sigma(\varepsilon_v)|n\rangle = - \sum_{\varepsilon_c=\varepsilon_{1s}} \langle v'c|I(\varepsilon_v-\varepsilon_c)|cn\rangle + \langle v'|\Sigma^{\rm rad}(\varepsilon_v)|n\rangle , \tag{A6}$$

$$\langle n|\Sigma(\varepsilon_v)|v\rangle = - \sum_{\varepsilon_c=\varepsilon_{1s}} \langle nc|\hat{I}(\varepsilon_v-\varepsilon_c)|cv\rangle + \langle n|\Sigma^{\rm rad}(\varepsilon_v)|v\rangle , \tag{A7}$$

$$\Big[\frac{d}{dE}\langle v|\Sigma(E)|v\rangle\Big]_{E=\varepsilon_v} = - \sum_{\varepsilon_c=\varepsilon_{1s}} \langle vc|I'(\varepsilon_v-\varepsilon_c)|cv\rangle + \Big[\frac{d}{dE}\langle v|\Sigma^{\rm rad}(E)|v\rangle\Big]_{E=\varepsilon_v} , \tag{A8}$$

where

$$\langle a|\Sigma^{\rm rad}(E)|b\rangle = \frac{i}{2\pi} \int_{-\infty}^{\infty} dp^0 \sum_n \frac{\langle ab|I(E-p^0)|nb\rangle}{p^0-\varepsilon_n(1-i0)} \tag{A9}$$

is the matrix element of the usual self-energy operator, $I'(\omega) \equiv \frac{d}{dE} I(\omega)$. The first terms in the right side of (A6)–(A8) correspond to the interaction of the $2s$ electron with the $1s$ electrons. The last terms in (A6)–(A8) correspond to the one-electron radiative contributions. Taking the real part of the first terms we get the expression (12). The imaginary part of these terms is canceled with the imaginary part of the one-electron radiative corrections.

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