Zeeman effect of the hyperfine-structure levels in lithiumlike ions

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The fully relativistic theory of the Zeeman splitting of the $(1s)^22s$ hyperfine-structure levels in lithiumlike ions with Z=6-32 is considered for the magnetic field magnitude in the range from 1 to 10 T. The second-order corrections to the Breit-Rabi formula are calculated and discussed including the one-electron contributions as well as the interelectronic-interaction effects of order 1/Z. The 1/Z corrections are evaluated within a rigorous QED approach. These corrections are combined with other interelectronic-interaction, QED, nuclear recoil, and nuclear size corrections to obtain high-precision theoretical values for the Zeeman splitting in Li-like ions with nonzero nuclear spin. The results can be used for a precise determination of nuclear magnetic moments from g-factor experiments.

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I. INTRODUCTION

High-precision measurements of the g factor of low-Z H-like ions [1–3] have triggered theoretical investigations of this effect [4–22]. Besides a new possibility for tests of the magnetic sector of quantum electrodynamics (QED), these investigations have already provided a new determination of the electron mass (see Refs. [3,23], and references therein). Extensions of these experiments to systems with higher nuclear charge number Z and to ions with nonzero nuclear spin would also provide the basis for new determinations of the fine-structure constant [8,24,25], the nuclear magnetic moments [24], and the nuclear charge radii.

Extending theoretical description from an H-like to a Lilike ion, one encounters a serious complication due to the presence of additional electrons. A number of relativistic calculations of the g factor of Li-like ions were carried out previously [26–30]. However, to reach the accuracy comparable to the one for H-like ions, a systematic quantum electrodynamic (QED) treatment is required [16,31–35].

For both H- and Li-like heavy ions with nonzero nuclear spin the ground-state Zeeman splitting caused by the magnetic field in the range from 1 to 10 T is much smaller than the hyperfine splitting. Therefore, the consideration can be reduced to the g factor [19,35]. However, for H-like ions with Z=1-20, which are under current experimental investigations at Mainz University, the Zeeman splitting is comparable with the hyperfine splitting if the magnitude of the homogeneous magnetic field does not exceed 10 T. This demands constructing the perturbation theory for degenerate states. To a good accuracy, the well-known Breit-Rabi formula [36–39] gives the solution of the problem. However, the current experimental precision clearly shows the necessity for an improvement of the Breit-Rabi formula for H-like ions [21].

In the present paper, we consider the Breit-Rabi formula for the 2s hyperfine-structure levels in lithiumlike ions. Evaluations of the coefficients of this formula should include corrections depending on the nuclear g factor. Besides a simple one-electron lowest-order nuclear-spin-dependent contribution, one should also calculate the second-order cor-

rections caused by the hyperfine interaction and the interaction with the external magnetic field, taking into account the presence of the closed $(1s)^2$ electron shell. We perform such calculations in the range Z=6-32, where the 2s hyperfinestructure (HFS) splitting can be comparable with the Zeeman splitting if the magnitude of the homogeneous magnetic field is in the range under consideration. The calculations are based on perturbation theory in the parameter 1/Z within a rigorous QED approach. The contributions of zeroth and first orders in 1/Z are taken into account for the magnetic-dipole correction and the contribution of zeroth order is taken into consideration for the electric-quadrupole correction. Also, the B^2 -dependent correction is calculated, including the contributions of zeroth and first orders in 1/Z. The obtained results are combined with other corrections to get accurate theoretical predictions for the Breit-Rabi formula coefficients for lithiumlike ions with nonzero nuclear spin. These predictions will be important for experimental investigations that are anticipated in the near future at University of Mainz and GSI [40].

The calculations of the interelectronic-interaction corrections to the Zeeman splitting are the most labor-intensive part of the present paper. Nevertheless, to make the paper consistent and self-contained, in Sec. II some basic formulas for the one-electron case, which were mentioned by us in Ref. [21], are given.

Relativistic units $(\hbar = c = 1)$ and the Heaviside charge unit $(\alpha = e^2/4\pi, e < 0)$ are used in the paper. In some important cases, the final formulas contain \hbar and c explicitly to be applicable for arbitrary system of units.

II. BREIT-RABI FORMULA IN THE LOWEST-ORDER ONE-ELECTRON APPROXIMATION

We consider a lithiumlike ion with nonzero nuclear spin I in a state of the valence electron with the total electron angular momentum j=1/2. For such a state there are only two HFS levels $E(F)=E_{n\kappa}+\varepsilon_{\text{HFS}}(F)$ with the total atomic angular momentum $F=I\pm 1/2$. Here

$$E_{n\kappa} = \frac{\gamma + n_r}{N} m_e \tag{1}$$

is the one-electron energy of the valence electron Dirac state in the Coulomb field of the nucleus, $\varepsilon_{\rm HFS}(F)$ is the hyperfine-structure shift from this state, n is the principal quantum number, $l=j\pm\frac{1}{2}$ defines the parity of the state, $n_r=n-|\kappa|$ is the radial quantum number, $\gamma=\sqrt{\kappa^2-(\alpha Z)^2}$, $N=\sqrt{n_r^2+2n_r\gamma+\kappa^2}$, and m_e is the electron mass. The ion is placed in a homogeneous magnetic field \vec{B} directed along the z axis. In case $\Delta E_{\rm mag} \sim \Delta E_{\rm HFS}$, where $\Delta E_{\rm mag} = E-[E(I-1/2)+E(I+1/2)]/2$ is the Zeeman splitting and $\Delta E_{\rm HFS} = E(I+1/2)-E(I-1/2)$, we must take into account mixing the HFS sublevels with the same M_F , where $M_F = -F, -F+1, \ldots, F-1, F$ is the z projection of the total angular momentum. In what follows, we restrict our consideration to the ground state of the valence electron. One can obtain the Breit-Rabi formula (see, e.g., Refs. [21,36–39]) for the Zeeman splitting with the same $M_F = -I+1/2, \ldots, I-1/2$,

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left(a_1 M_F x \pm \frac{1}{2} \sqrt{1 + \frac{4M_F}{2I + 1} c_1 x + c_2 x^2} \right), \tag{2}$$

where $x = \mu_0 B / \Delta E_{HFS}^{(2s)}$, $\mu_0 = |e| \hbar / (2m_e c)$ is the Bohr magneton,

$$a_1 = -g_1', \tag{3}$$

$$c_1 = g_i + g_I', \tag{4}$$

$$c_2 = (g_i + g_I')^2. (5)$$

 g_j is the ground-state bound-electron g factor of the lithium-like ion.

$$g_i = g_D + \Delta g_{\text{int}} + \Delta g_{\text{QED}} + \Delta g_{\text{rec}}^{(e)} + \Delta g_{\text{NS}} + \Delta g_{\text{NP}}, \quad (6)$$

 $g_{\rm D}$ is the one-electron Dirac value for a point-charge nucleus,

$$g_{\rm D} = \frac{2(\sqrt{2+2\gamma}+1)}{3} = 2 - \frac{(\alpha Z)^2}{6} + \cdots,$$
 (7)

 $\gamma = \sqrt{1 - (\alpha Z)^2}$, $\Delta g_{\rm int}$ is the interelectronic-interaction correction, $\Delta g_{\rm QED}$ is the QED correction, $\Delta g_{\rm rec}^{(e)}$ is the nuclear recoil correction to the bound-electron g factor, $\Delta g_{\rm NS}$ is the nuclear size correction, $\Delta g_{\rm NP}$ is the nuclear polarization correction, g_I' is the nuclear g factor expressed in the Bohr magnetons,

$$g_I' = \frac{m_e}{m_p} (g_I + \Delta g_{\text{rec}}^{(n)}), \tag{8}$$

 m_p is the proton mass, $g_I = \mu/(\mu_N I)$, $\mu = \langle II | \mu_z | II \rangle$ is the nuclear magnetic moment, μ_z is the z projection of the nuclear magnetic moment operator $\vec{\mu}$ acting in the space of

nuclear wave functions $|IM_I\rangle$ with the total angular momentum I and its projection M_I , $\mu_N = |e|\hbar/(2m_pc)$ is the nuclear magneton, and $\Delta g_{\rm rec}^{(n)}$ is the recoil correction to the bound-nucleus g factor. Since in all of the cases under consideration below $\Delta g_{\rm rec}^{(n)}$ is smaller than 10^{-11} [12] this correction can be neglected, and we actually have the following in Eq. (8): $g_I' = (m_e/m_p)g_I$. For $F = I + \frac{1}{2}$ and $M_F = \pm (I + \frac{1}{2})$ one obtains in the first order of perturbation theory,

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left(\frac{1}{2} \pm d_1 x \right), \tag{9}$$

where

$$d_1 = \frac{1}{2}g_j - Ig_I' \tag{10}$$

and the minus and plus signs refer to $M_F = -(I + \frac{1}{2})$ and $M_F = I + \frac{1}{2}$, respectively.

For Li-like ions with I=1/2 the Breit-Rabi formula takes the form

$$\Delta E_{\text{mag}}(x) = \pm \frac{\Delta E_{\text{HFS}}^{(2s)}}{2} \sqrt{1 + c_2 x^2}$$
 (11)

for M_F =0 and the effect is described by Eq. (9) with $d_1 = \frac{1}{2}(g_j - g_I')$ for $M_F = \pm 1$. In case $\Delta E_{\rm mag} \! \ll \! \Delta E_{\rm HFS}^{(2s)}$ we can express the linear-

In case $\Delta E_{\text{mag}} \ll \Delta E_{\text{HFS}}^{2.3}$ we can express the linear-dependent part of the Zeeman splitting in terms of the atomic g factor,

$$\Delta E_{\text{mag}} = \pm \frac{\Delta E_{\text{HFS}}^{(2s)}}{2} + g(F)\mu_0 B M_F,$$
 (12)

where, to the lowest-order approximation (see, e.g., Ref. [38]),

$$g(F) = g_{\rm D} Y_{\rm el}(F) - \frac{m_e}{m_p} g_I Y_{\rm nuc}^{(\mu)}(F),$$
 (13)

$$Y_{el}(F) = \frac{F(F+1) + 3/4 - I(I+1)}{2F(F+1)}$$

$$= \begin{cases} -\frac{1}{2I+1} & \text{for } F = I - \frac{1}{2}, \\ \frac{1}{2I+1} & \text{for } F = I + \frac{1}{2}, \end{cases}$$
(14)

$$Y_{\text{nuc}}^{(\mu)}(F) = \frac{F(F+1) + I(I+1) - 3/4}{2F(F+1)}$$

$$= \begin{cases} \frac{2(I+1)}{2I+1} & \text{for } F = I - \frac{1}{2}, \\ \frac{2I}{2I+1} & \text{for } F = I + \frac{1}{2}. \end{cases}$$
(15)

The total one-electron 2s g-factor value of a Li-like ion with nonzero nuclear spin can be written as

¹In the present paper, the energy of a Zeeman sublevel $\Delta E_{\rm mag}$ is counted with respect to the mean energy [E(I-1/2)+E(I+1/2)]/2 of the hyperfine-structure doublet [38,39]. To count the energy from the hyperfine centroid of the doublet [36,37], one should use the relation $\Delta E_{\rm mag}^{\rm hc} = \Delta E_{\rm mag} - [\Delta E_{\rm HFS}/2(2I+1)]$.

$$g(F) = (g_{\rm D} + \Delta g_{\rm int} + \Delta g_{\rm QED} + \Delta g_{\rm rec}^{(e)} + \Delta g_{\rm NS} + \Delta g_{\rm NP}) Y_{\rm el}(F)$$
$$-\frac{m_e}{m_p} (g_I + \Delta g_{\rm rec}^{(n)}) Y_{\rm nuc}^{(\mu)}(F) + \delta g_{\rm HFS}^{(2s)}(F), \tag{16}$$

where the HFS correction $\delta g_{\rm HFS}^{(2s)}(F) = \delta g_{\rm HFS(\mu)}^{(2s)}(F) + \delta g_{\rm HFS(Q)}^{(2s)}(F)$ [35] is briefly discussed below.

III. HYPERFINE-INTERACTION CORRECTIONS TO THE GROUND-STATE g FACTOR

Let us start our consideration of the HFS correction to the ground-state g factor of a Li-like ion with the one-electron approximation. In this approximation, the interaction of the ion with the magnetic field can be represented as

$$\vec{V_B} = \vec{V_B^{(e)}} + \vec{V_B^{(n)}}.$$
 (17)

Here $V_{\tilde{B}}^{(e)}$ describes the interaction of the valence 2s electron with the homogeneous magnetic field,

$$V_{\vec{B}}^{(e)} = -e(\vec{\alpha} \cdot \vec{A}) = \frac{|e|}{2} (\vec{\alpha} \cdot [\vec{B} \times \vec{r}]), \tag{18}$$

where the vector $\vec{\alpha}$ incorporates the Dirac α matrices, and

$$V_{\vec{p}}^{(n)} = -(\vec{\mu} \cdot \vec{B}) \tag{19}$$

describes the interaction of the nuclear magnetic moment $\vec{\mu}$ with \vec{B} . The hyperfine-interaction operator is given by the sum

$$V_{\text{HFS}} = V_{\text{HFS}}^{(\mu)} + V_{\text{HFS}}^{(Q)},$$
 (20)

where $V_{\rm HFS}^{(\mu)}$ and $V_{\rm HFS}^{(Q)}$ are the magnetic-dipole and electric-quadrupole hyperfine-interaction operators, respectively. In the point-dipole approximation,

$$V_{\rm HFS}^{(\mu)} = \frac{|e|}{4\pi} \frac{(\vec{\alpha} \cdot [\vec{\mu} \times \vec{r}])}{r^3},\tag{21}$$

and, in the point-quadrupole approximation,

$$V_{\rm HFS}^{(Q)} = -\alpha \sum_{m=-2}^{m=2} Q_{2m} \eta_{2m}^*(\vec{n}). \tag{22}$$

Here $Q_{2m} = \sum_{i=1}^{Z} r_i^2 C_{2m}(\vec{n_i})$ is the operator of the electric-quadrupole moment of the nucleus, $\eta_{2m} = C_{2m}(\vec{n})/r^3$ is an operator that acts on electron variables, $\vec{n} = \vec{r}/r$, $\vec{n_i} = \vec{r_i}/r_i$, \vec{r} is the position vector of the electron, $\vec{r_i}$ is the position vector of the *i*th proton in the nucleus, $C_{lm} = \sqrt{4\pi/(2l+1)}Y_{lm}$, and Y_{lm} is a spherical harmonic. It must be stressed that the electric-quadrupole interaction should be taken into account only for ions with I > 1/2.

An unperturbed atomic eigenstate that corresponds to given values of F and M_F is a linear combination of products of electron and nuclear wave functions,

$$|nljIFM_F\rangle = \sum_{m_i,M_I} C_{jm_jIM_I}^{FM_F} |nljm_j\rangle |IM_I\rangle.$$
 (23)

Here $C_{jm_j JM_l}^{FM_F}$ are the Clebsch-Gordan coefficients, $|nljm_j\rangle$ are the unperturbed one-electron wave functions, which are four-

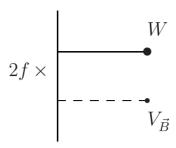


FIG. 1. The second-order diagrams contributing to $S_2^{(t)}(\alpha Z)$, $T_2^{(t)}(\alpha Z)$ (if f=1 and $W=V_{\rm HFS}^{(\mu)}$ or $W=V_{\rm HFS}^{(Q)}$), and $U_2^{(t)}(\alpha Z)$ (if $f=\frac{1}{2}$ and $W=V_{\tilde{B}}^{(e)}$).

component eigenvectors of the Dirac equation for the Coulomb field, with the total angular momentum j and its projection m_i .

In the one-electron approximation, the magnetic-dipole and electric-quadrupole hyperfine-interaction corrections to the ground-state g factor of the Li-like ion are given by

$$\begin{split} \delta g_{\mathrm{HFS}(\mu,\mathcal{Q})}^{\mathrm{one-el}(2s)} &= \frac{2}{\mu_0 B M_F} \sum_{m_j M_I} \sum_{m_j' M_I'} C_{1/2m_j' I M_I}^{F M_F} C_{1/2m_j' I M_I'}^{F M_F} \\ &\times \langle I M_I | \sum_{n}^{(\varepsilon_n \neq \varepsilon_v)} \frac{\langle v | V_B^{(e)} | n \rangle \langle n | V_{\mathrm{HFS}}^{(\mu,\mathcal{Q})} | v' \rangle}{\varepsilon_v - \varepsilon_n} | I M_I' \rangle, \end{split}$$

where $|v\rangle = |20\frac{1}{2}m_j\rangle$ and $|v'\rangle = |20\frac{1}{2}m_j'\rangle$ are the 2s states of the valence electron with the angular momentum projections m_j and m_j' , respectively, $|n\rangle \equiv |nljm_j\rangle$, $\varepsilon_v = E_{2,-1}$, and $\varepsilon_n \equiv E_{n\kappa}$. The summation in Eq. (24) runs over discrete as well as continuum states. The corresponding diagrams are presented in Fig. 1.

The total hyperfine-interaction correction to the groundstate *g* factor of the Li-like ion is given by

$$\delta g_{\rm HFS}^{(2s)} = \delta g_{\rm HFS(\mu)}^{(2s)} + \delta g_{\rm HFS(Q)}^{(2s)} \tag{25}$$

with

$$\delta g_{\rm HFS(\mu)}^{(2s)} = \alpha^2 Z \frac{1}{12} \frac{\mu}{\mu_N} \frac{m_e}{m_p} \frac{1}{I} Y_{\rm nuc}^{(\mu)}(F) \left(S_2(\alpha Z) + \frac{1}{Z} B_{\mu}(\alpha Z) + \frac{1}{Z^2} C_{\mu}(\alpha Z) + \cdots \right)$$
(26)

and

$$\delta g_{\text{HFS}(Q)}^{(2s)} = \alpha^4 Z^3 \frac{23}{2160} Q \left(\frac{m_e c}{\hbar} \right)^2 Y_{\text{nuc}}^{(Q)}(F) \left(T_2(\alpha Z) + \frac{1}{Z} B_Q(\alpha Z) + \frac{1}{Z^2} C_Q(\alpha Z) + \cdots \right). \tag{27}$$

Here the angular factor is

$$Y_{\text{nuc}}^{(Q)}(F) = \begin{cases} -\frac{(I+1)(2I+3)}{I(2I-1)(2I+1)} & \text{for } F = I - \frac{1}{2}, \\ \frac{1}{2I+1} & \text{for } F = I + \frac{1}{2}, \end{cases}$$
 (28)

and $Q=2\langle II|Q_{20}|II\rangle$ is the electric-quadrupole moment of the nucleus. The functions

$$S_2(\alpha Z) = \frac{12}{\alpha^2 Z \frac{m_e}{m_p} g_I Y_{\text{nuc}}^{(\mu)}(F)} \delta g_{\text{HFS}(\mu)}^{\text{one-el}(2s)}$$
(29)

and

$$T_2(\alpha Z) = \frac{2160}{23\alpha^4 Z^3 Q \left(\frac{m_e c}{\hbar}\right)^2 Y_{\text{nuc}}^{(Q)}(F)} \delta g_{\text{HFS}(Q)}^{\text{one-el}(2s)}$$
(30)

determine the one-electron contributions, which are discussed in detail in Ref. [19]. For the point-charge nucleus, the functions $S_2(\alpha Z)$ and $T_2(\alpha Z)$ are [19,35]

$$S_{2}(\alpha Z) = \frac{8}{3N} \left[\frac{1}{N+2} \left(N + \frac{10(N+1)}{3N} \right) + \frac{(\alpha Z)^{2}}{\gamma(\gamma+1)} \left(\frac{2(N+1)}{3-4(\alpha Z)^{2}} + 1 \right) - \frac{1}{\gamma} \right]$$

$$= 1 + \frac{229}{144} (\alpha Z)^{2} + \cdots$$
(31)

and

$$T_2(\alpha Z)$$

$$=\frac{192[(N+\gamma+1)(18+24\gamma-12N+8\gamma N^2)+15(1+\gamma)]}{23\gamma N^3[15-16(\alpha Z)^2](N+\gamma+1)^2}$$

$$=1+\frac{427}{276}(\alpha Z)^2+\cdots,$$
 (32)

where $N = \sqrt{2(1+\gamma)}$.

The interelectronic-interaction correction $B_{\mu}(\alpha Z)$ can be calculated within the rigorous QED approach [35]. The interaction of the electrons with the Coulomb field of the nucleus is included in the unperturbed Hamiltonian, i.e., the Furry picture is used. The perturbation theory is formulated with the technique of the two-time Green function (TTGF) [41,42]. To simplify the calculations, the closed $(1s)^2$ shell is regarded as belonging to a redefined vacuum. With this vacuum, the Fourier transform of TTGF can be introduced by

$$\mathcal{G}(E; \vec{x'}; \vec{x}) \,\delta(E - E') = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dx^0 dx'^0 \, \exp(iE'x'^0 - iEx^0)$$

$$\times \langle 0_{(1s)^2} | T\psi(x'^0, \vec{x'}) \psi^{\dagger}(x^0, \vec{x}) | 0_{(1s)^2} \rangle,$$
(33)

where $\psi(x^0, \vec{x})$ is the electron-positron field operator in the Heisenberg representation and T is the time-ordered product

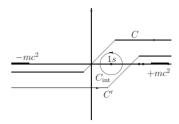


FIG. 2. C is the original contour of the integration over the electron energy variable in the formalism with the standard vacuum. C' is the integration contour for the vacuum with the $(1s)^2$ shell included. The integral along the contour $C_{\text{int}} = C' - C$ describes the interaction of the valent electron with the $(1s)^2$ -shell electrons.

operator. The energy shift of a state a can be expressed in terms of the TTGF defined by

$$g_{aa}(E) = \langle u_a | \mathcal{G}(E) | u_a \rangle \equiv \int d\vec{x} d\vec{x'} u_a^{\dagger}(\vec{x'}) \mathcal{G}(E; \vec{x'}; \vec{x}) u_a(\vec{x}),$$
(34)

where $u_a(\vec{x})$ is the unperturbed Dirac wave function of the state a. Using the Nagy and Kato technique [43], one can derive for the total energy shift $\Delta E_a = E_a - E_a^{(0)}$ [41,42],

$$\Delta E_{a} = \frac{\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{aa}(E)}{1 + \frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g_{aa}(E)},$$
(35)

where $\Delta E \equiv E - E_a^{(0)}$, $\Delta g_{aa}(E) \equiv g_{aa}(E) - g_{aa}^{(0)}(E)$, and $g_{aa}^{(0)}(E) = (E - E_a^{(0)})^{-1}$. The integrals in the complex E plane are taken along the contour Γ which surrounds the pole of $g_{aa}(E)$ corresponding to the level a and keeps outside all other singularities. The contour Γ is oriented counterclockwise.

To first three orders of the perturbation theory, the energy shift is given by

$$\Delta E_a^{(1)} = \frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{aa}^{(1)}(E), \qquad (36)$$

$$\Delta E_{a}^{(2)} = \frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{aa}^{(2)}(E) - \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{aa}^{(1)}(E)\right) \times \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g_{aa}^{(1)}(E)\right), \tag{37}$$

$$\begin{split} \Delta E_{a}^{(3)} &= \frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{aa}^{(3)}(E) - \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{aa}^{(2)}(E) \right) \\ &\times \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g_{aa}^{(1)}(E) \right) - \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{aa}^{(1)}(E) \right) \\ &\times \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g_{aa}^{(2)}(E) \right) + \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{aa}^{(1)}(E) \right) \end{split}$$

$$\begin{pmatrix} & & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & &$$

FIG. 3. The third-order diagrams contributing to $S_2^{(t)}(\alpha Z)$ (if f=1 and $W=V_{\rm HFS}^{(\mu)}$) and $U_2^{(t)}(\alpha Z)$ (if $f=\frac{1}{2}$ and $W=V_{\tilde{B}}^{(e)}$) being combined with products of the lower-order diagrams presented in Figs. 4 and 5.

$$\times \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g_{aa}^{(1)}(E)\right)^{2}.$$
 (38)

The redefinition of the vacuum changes i0 to -i0 in the electron propagator denominators corresponding to the closed $(1s)^2$ shell. In other words, it means replacing the standard Feynman contour of integration over the electron energy C with a new contour C' (Fig. 2). The second-order contribution is defined by the diagrams presented in Fig. 1. Its evaluation according to Eq. (37) yields formula (24). In the formalism under consideration, the lowest-order interelectronicinteraction and the radiative corrections to Eq. (24) are described by the third-order diagrams presented in Fig. 3 and, according to Eq. (38), by some products of the loworder diagrams depicted in Figs. 4 and 5. According to Fig. 2, to separate the interelectronic-interaction corrections, the contour C' must be divided into two parts, C and C_{int} . The integral along the standard Feynman contour C gives the one-electron radiative correction. The integral along the contour C_{int} describes the interaction of the valence electron with the closed shell electrons. Formula (38) allows one to evaluate the interelectronic-interaction correction $B_{\mu}(\alpha Z)$ [35]. The results of this evaluation will be presented in the next section together with other related corrections to the Breit-Rabi formula.

IV. CORRECTIONS TO THE BREIT-RABI FORMULA FOR THE GROUND STATE

Now we assume that the Zeeman splitting $\Delta E_{\rm mag}$ of the 2s HFS levels F = I - 1/2 and F' = I + 1/2 is much smaller than the distance to other levels but is comparable with $\Delta E_{\rm HFS}^{(2s)}$. The unperturbed eigenstates form a two-dimensional subspace $\Omega = \{|1^{(0)}\rangle, |2^{(0)}\rangle\}$, where $|1^{(0)}\rangle = |20\frac{1}{2}IFM_F\rangle, |2^{(0)}\rangle = |20\frac{1}{2}IF'M_F\rangle$. Employing the perturbation theory for degenerate states [42] with energy ε_v we denote the projector on Ω by

$$P^{(0)} = \sum_{i=1}^{2} |i^{(0)}\rangle\langle i^{(0)}|. \tag{39}$$

We project the Green function $\mathcal{G}(E)$ on the subspace Ω ,

$$g(E) = P^{(0)}\mathcal{G}(E)P^{(0)},$$
 (40)

where, as in Eq. (34), the integration over the electron coordinates is implicit. In this case we can choose a contour Γ in the complex E plane in a way that it surrounds all g(E) poles, which correspond to the states under consideration, and keeps outside all other singularities of g(E). As in the case of a single level, to the zeroth-order approximation one easily finds

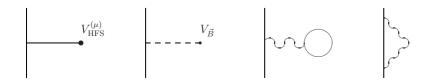


FIG. 4. The first-order diagrams contributing to $S_2^{(t)}(\alpha Z)$ and $U_2^{(t)}(\alpha Z)$ being multiplied by the second-order diagrams presented in Fig. 5.

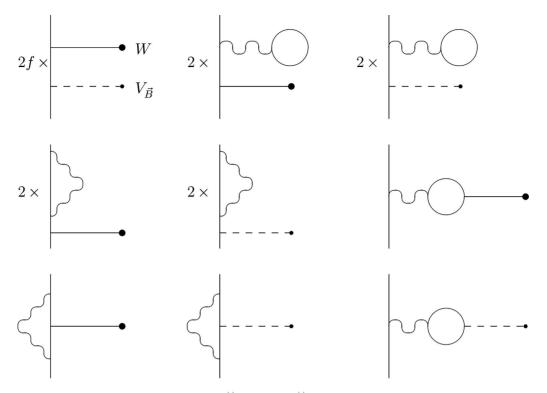


FIG. 5. The second-order diagrams contributing to $S_2^{(t)}(\alpha Z)$ and $U_2^{(t)}(\alpha Z)$ being multiplied by the first-order diagrams presented in Fig. 4.

$$g^{(0)}(E) = \sum_{i=1}^{2} \frac{|i^{(0)}\rangle\langle i^{(0)}|}{E - E_i^{(0)}}.$$
 (41)

We introduce the operators K and P by

$$K \equiv \frac{1}{2\pi i} \oint_{\Gamma} dE E g(E), \tag{42}$$

$$P = \frac{1}{2\pi i} \oint_{\Gamma} dE g(E). \tag{43}$$

As it is shown in Ref. [42], the energy levels are determined from the equation

$$\det(H - E) = 0, (44)$$

where

$$H = P^{-1/2}KP^{-1/2}. (45)$$

The operators K and P are constructed by formulas (42) and (43),

$$K = K^{(0)} + K^{(1)} + K^{(2)} + K^{(3)} + \cdots,$$
 (46)

$$P = P^{(0)} + P^{(1)} + P^{(2)} + P^{(3)} + \cdots, \tag{47}$$

where the superscript indicates the order of the perturbation theory in a small parameter. The operator H is

$$H = H^{(0)} + H^{(1)} + H^{(2)} + H^{(3)} + \cdots,$$
 (48)

where

$$H^{(0)} = K^{(0)}, (49)$$

$$H^{(1)} = K^{(1)} - \frac{1}{2}P^{(1)}K^{(0)} - \frac{1}{2}K^{(0)}P^{(1)}, \tag{50}$$

$$H^{(2)} = K^{(2)} - \frac{1}{2}P^{(2)}K^{(0)} - \frac{1}{2}K^{(0)}P^{(2)} - \frac{1}{2}P^{(1)}K^{(1)} - \frac{1}{2}K^{(1)}P^{(1)} + \frac{3}{8}P^{(1)}P^{(1)}K^{(0)} + \frac{3}{8}K^{(0)}P^{(1)}P^{(1)} + \frac{1}{4}P^{(1)}K^{(0)}P^{(1)}, \quad (51)$$

$$\begin{split} H^{(3)} &= K^{(3)} - \frac{1}{2}P^{(3)}K^{(0)} - \frac{1}{2}K^{(0)}P^{(3)} - \frac{1}{2}P^{(1)}K^{(2)} - \frac{1}{2}K^{(2)}P^{(1)} - \frac{1}{2}P^{(2)}K^{(1)} - \frac{1}{2}K^{(1)}P^{(2)} + \frac{3}{8}P^{(1)}P^{(2)}K^{(0)} + \frac{3}{8}K^{(0)}P^{(1)}P^{(2)} \\ &+ \frac{3}{8}P^{(2)}P^{(1)}K^{(0)} + \frac{3}{8}K^{(0)}P^{(2)}P^{(1)} + \frac{1}{4}P^{(1)}K^{(0)}P^{(2)} + \frac{1}{4}P^{(2)}K^{(0)}P^{(1)} + \frac{3}{8}P^{(1)}P^{(1)}K^{(1)} + \frac{3}{8}K^{(1)}P^{(1)}P^{(1)} + \frac{1}{4}P^{(1)}K^{(1)}P^{(1)} \\ &+ \frac{3}{8}P^{(1)}P^{(1)}K^{(1)} + \frac{3}{8}P^{($$

$$-\frac{5}{16}P^{(1)}P^{(1)}P^{(1)}K^{(0)} - \frac{5}{16}K^{(0)}P^{(1)}P^{(1)}P^{(1)} - \frac{3}{16}P^{(1)}P^{(1)}K^{(0)}P^{(1)} - \frac{3}{16}P^{(1)}K^{(0)}P^{(1)}P^{(1)}.$$

$$(52)$$

Taking into account only the relevant contributions of kind $\alpha(\mu/\mu_N)B$ and $\alpha \times B \times B$, where α comes from the interelectronic interaction, we obtain for the third-order term in Eq. (48),

$$\begin{split} H_{jk}^{(3)} &= \frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{jk}^{(3)}(E) - \frac{1}{2} \sum_{l=1}^{2} \left[\left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g_{jl}^{(1)}(E) \right) \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{lk}^{(2)}(E) \right) + \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{jl}^{(2)}(E) \right) \right. \\ & \times \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g_{lk}^{(1)}(E) \right) \left] - \frac{1}{2} \sum_{l=1}^{2} \left[\left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g_{jl}^{(2)}(E) \right) \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{lk}^{(1)}(E) \right) + \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta E \Delta g_{jl}^{(1)}(E) \right) \right. \\ & \times \left(\frac{1}{2\pi i} \oint_{\Gamma} dE \Delta g_{lk}^{(2)}(E) \right) \right], \end{split}$$

where $\Delta E = E - \varepsilon_v$, j, k=1, 2.

Keeping only the three lowest-order terms in B, we get the following equation for the perturbed energies:

$$\begin{vmatrix} h_0(F) + h_1(F)B + h_2(F)B^2 - E & \widetilde{h}_1(F, F')B + \widetilde{h}_2(F, F')B^2 \\ \widetilde{h}_1(F', F)B + \widetilde{h}_2(F', F)B^2 & h_0(F') + h_1(F')B + h_2(F')B^2 - E \end{vmatrix} = 0.$$
 (54)

Here $F = I - \frac{1}{2}$, $F' = I + \frac{1}{2}$,

$$h_0(k) = E(k) \tag{55}$$

is the energy of the HFS level,

$$h_{1}(k) = \frac{1}{B} \left[\Delta E_{(B)}^{(1)}(k,k) + \Delta E_{(\mu)}^{(2)}(k,k) + \Delta E_{(Q)}^{(2)}(k,k) + \Delta E_{(\mu)}^{(3)}(k,k) + \Delta E_{(Q)}^{(3)}(k,k) \right] + (\Delta g_{\text{int}} + \Delta g_{\text{QED}} + \Delta g_{\text{rec}}^{(e)} + \Delta g_{\text{NS}} + \Delta g_{\text{NS}} + \Delta g_{\text{NP}} Y_{\text{el}}(k) \mu_{0} M_{F} - \Delta g_{\text{rec}}^{(n)} Y_{\text{nuc}}^{(\mu)}(k) \mu_{N} M_{F} = g(k) \mu_{0} M_{F},$$
(56)

$$h_2(k) = \frac{1}{B^2} \left[\Delta E_{(B)}^{(2)}(k,k) + \Delta E_{(B)}^{(3)}(k,k) \right], \tag{57}$$

$$\widetilde{h}_{1}(j,k) = \frac{1}{B} \left[\Delta E_{(B)}^{(1)}(j,k) + \Delta E_{(\mu)}^{(2)}(j,k) + \Delta E_{(Q)}^{(2)}(j,k) + \Delta E_{(\mu)}^{(2)}(j,k) + \Delta E_{(\mu)}^{(3)}(j,k) + \Delta E_{(Q)}^{(3)}(j,k) \right] + (\Delta_{\text{int}} + \Delta_{\text{QED}} + \Delta_{\text{rec}}^{(e)} + \Delta_{\text{NS}} + \Delta_{\text{NP}}) \mu_{0} - \Delta_{\text{rec}}^{(n)} \mu_{N}, \tag{58}$$

$$\tilde{h}_2(j,k) = \frac{1}{R^2} \left[\Delta E_{(B)}^{(2)}(j,k) + \Delta E_{(B)}^{(3)}(j,k) \right], \tag{59}$$

where j,k=F,F'. $\Delta_{\rm int},~\Delta_{\rm QED},~\Delta_{\rm rec}^{(e)},~\Delta_{\rm NS}$, and $\Delta_{\rm NP}$ are the interelectronic-interaction, QED, nuclear recoil, nuclear size, and nuclear polarization corrections. They are similar to the corresponding corrections to $h_1(k)$ but have a different angular factor as well as $\Delta_{\rm rec}^{(n)}$. Here both $\Delta g_{\rm rec}^{(n)}$ and $\Delta_{\rm rec}^{(n)}$ can be neglected as it was mentioned in Sec. II. It should be noted that we have also neglected here terms describing virtual transitions into excited nuclear states via the direct interaction of the nucleus with the magnetic field [22]. The energy shifts are

$$\Delta E_{(\vec{B})}^{(1)}(j,k) = \sum_{m_j M_I} \sum_{m'_i M'_I} C_{1/2m'_j I M_I}^{j M_F} C_{1/2m'_j I M'_I}^{k M_F} \langle I M_I | \langle v | V_{\vec{B}} | v' \rangle | I M'_I \rangle, \tag{60}$$

$$\Delta E_{(\mu,Q,\vec{B})}^{(2)}(j,k) = \sum_{m_j M_I} \sum_{m'_l M'_l} C_{1/2m'_j IM_I}^{jM_F} C_{1/2m'_j IM'_l}^{kM_F} \langle IM_I | I_{\mu,Q,\vec{B}}^{(2)} | IM'_I \rangle, \tag{61}$$

$$\Delta E_{(\mu,Q,\vec{B})}^{(3)}(j,k) = \sum_{m_j M_I} \sum_{m_j' M_I'} C_{1/2m_j' IM_I}^{jM_F} C_{1/2m_j' IM_I'}^{kM_F} \langle IM_I | I_{\mu,Q,\vec{B}}^{(3a)} + I_{\mu,Q,\vec{B}}^{(3b)} + I_{\mu,Q,\vec{B}}^{(3c)} + I_{\mu,Q,\vec{B}}^{(3d)} | IM_I \rangle, \tag{62}$$

where

$$I_{\mu,Q,\vec{B}}^{(2)} = 2f \sum_{n}^{(\varepsilon_n \neq \varepsilon_v)} \frac{\langle v | V_{\vec{B}}^{(e)} | n \rangle \langle n | W | v' \rangle}{\varepsilon_v - \varepsilon_n}, \tag{63}$$

$$\begin{split} I_{\mu,Q,\tilde{B}}^{(3a)} &= f \sum_{\varepsilon_{c} = E_{1,-1}} \left(\sum_{n_{1},n_{2}}^{(\varepsilon_{n_{1}} \neq \varepsilon_{v}, \varepsilon_{n_{2}} \neq \varepsilon_{v})} \frac{2}{(\varepsilon_{v} - \varepsilon_{n_{1}})(\varepsilon_{v} - \varepsilon_{n_{2}})} \left[\langle v | V_{\tilde{B}}^{(e)} | n_{1} \rangle \langle n_{1} | W | n_{2} \rangle \langle n_{2} c | I(0) | v' c \rangle + \langle v | V_{\tilde{B}}^{(e)} | n_{1} \rangle \langle n_{1} c | I(0) | n_{2} c \rangle \langle n_{2} | W | v' \rangle \right. \\ &\quad + \langle v | W | n_{1} \rangle \langle n_{1} | V_{\tilde{B}}^{(e)} | n_{2} \rangle \langle n_{2} c | I(0) | v' c \rangle \right] - \sum_{\varepsilon_{\tilde{v}} = \varepsilon_{v}} \sum_{n}^{(\varepsilon_{n} \neq \varepsilon_{v})} \frac{2}{(\varepsilon_{v} - \varepsilon_{n})^{2}} \left[\langle v | V_{\tilde{B}}^{(e)} | n \rangle \langle n | W | \tilde{v} \rangle \right. \\ &\quad \times \langle \tilde{v}c | I(0) | v' c \rangle + \langle v | V_{\tilde{B}}^{(e)} | n \rangle \langle n c | I(0) | \tilde{v}c \rangle \langle \tilde{v} | W | v' \rangle + \langle v | V_{\tilde{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} | W | n \rangle \langle n c | I(0) | v' c \rangle \right], \tag{64} \end{split}$$

$$I_{\mu,Q,\vec{B}}^{(3b)} = -f \sum_{\varepsilon_{c}=E_{1,-1}} \left(\sum_{n_{1},n_{2}}^{(\varepsilon_{n_{1}} \neq \varepsilon_{v},\varepsilon_{n_{2}} \neq \varepsilon_{v})} \frac{2}{(\varepsilon_{v} - \varepsilon_{n_{1}})(\varepsilon_{v} - \varepsilon_{n_{2}})} [\langle v | V_{\vec{B}}^{(e)} | n_{1} \rangle \langle n_{1} | W | n_{2} \rangle \langle n_{2} c | I(\omega) | cv' \rangle + \langle v | V_{\vec{B}}^{(e)} | n_{1} \rangle \langle n_{1} c | I(\omega) | cn_{2} \rangle \langle n_{2} | W | v' \rangle \right. \\ + \langle v | W | n_{1} \rangle \langle n_{1} | V_{\vec{B}}^{(e)} | n_{2} \rangle \langle n_{2} c | I(\omega) | cv' \rangle] - \sum_{\varepsilon_{\vec{v}} = \varepsilon_{v}} \sum_{n}^{(\varepsilon_{n} \neq \varepsilon_{v})} \frac{2}{(\varepsilon_{v} - \varepsilon_{n})^{2}} [\langle v | V_{\vec{B}}^{(e)} | n \rangle \langle n | W | \tilde{v} \rangle \langle \tilde{v} c | I(\omega) | cv' \rangle + \langle v | V_{\vec{B}}^{(e)} | n \rangle \langle n c | I(\omega) | c\tilde{v} \rangle \\ \times \langle \tilde{v} | W | v' \rangle + \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} | W | n \rangle \langle n c | I(\omega) | cv' \rangle] + \sum_{\varepsilon_{\vec{v}} = \varepsilon_{v}} \sum_{n}^{(\varepsilon_{n} \neq \varepsilon_{v})} \frac{2}{\varepsilon_{v} - \varepsilon_{n}} [\langle v | V_{\vec{B}}^{(e)} | n \rangle \langle n | W | \tilde{v} \rangle \langle \tilde{v} c | I'(\omega) | cv' \rangle + \langle v | V_{\vec{B}}^{(e)} | n \rangle \langle n c | I'(\omega) \rangle \\ \times |c\tilde{v} \rangle \langle \tilde{v} | W | v' \rangle + \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} | W | n \rangle \langle n c | I'(\omega) | cv' \rangle] + \sum_{\varepsilon_{\vec{v}} = \varepsilon_{v}} \sum_{n} \sum_{\vec{b} \in \varepsilon_{n}} \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} c | I''(\omega) | c\tilde{v} \rangle \langle \tilde{v} | W | v' \rangle \\ + \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} | W | v' \rangle + \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} | W | n \rangle \langle n c | I'(\omega) | cv' \rangle] + \sum_{\varepsilon_{\vec{v}} = \varepsilon_{n}} \sum_{\vec{b} \in \varepsilon_{n}} \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} c | I''(\omega) | c\tilde{v} \rangle \langle \tilde{v} | W | v' \rangle \\ + \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} | W | n \rangle \langle n c | I'(\omega) | cv' \rangle] + \sum_{\varepsilon_{\vec{v}} = \varepsilon_{n}} \sum_{\vec{b} \in \varepsilon_{n}} \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} c | I''(\omega) | c\tilde{v} \rangle \langle \tilde{v} | W | v' \rangle \\ + \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} | W | n \rangle \langle n c | I'(\omega) | cv' \rangle] + \sum_{\vec{b} \in \varepsilon_{n}} \sum_{\vec{b} \in \varepsilon_{n}} \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} c | I''(\omega) | c\tilde{v} \rangle \langle \tilde{v} | W | v' \rangle \\ + \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} | W | v' \rangle + \langle v | V_{\vec{B}}^{(e)} | \tilde{v} \rangle \langle \tilde{v} | W | v' \rangle \langle \tilde{v} | W | v' \rangle$$

$$\begin{split} I_{\mu,Q,B}^{(3c)} &= f \sum_{\varepsilon_{c} = E_{1,-1}} \left(\sum_{n_{1},n_{2}}^{(\varepsilon_{n_{1}} \neq \varepsilon_{v}, \varepsilon_{n_{2}} \neq \varepsilon_{c})} \frac{2}{(\varepsilon_{v} - \varepsilon_{n_{1}})(\varepsilon_{c} - \varepsilon_{n_{2}})} [\langle v | V_{B}^{(e)} | n_{1} \rangle \langle c | W | n_{2} \rangle \langle n_{1} n_{2} | I(0) | v' c \rangle + \langle v | V_{B}^{(e)} | n_{1} \rangle \langle n_{1} c | I(0) | v' n_{2} \rangle \langle n_{2} | W | c \rangle \right. \\ &+ \langle v | W | n_{1} \rangle \langle c | V_{B}^{(e)} | n_{2} \rangle \langle n_{1} n_{2} | I(0) | v' c \rangle + \langle v | W | n_{1} \rangle \langle n_{1} c | I(0) | v' n_{2} \rangle \langle n_{2} | V_{B}^{(e)} | c \rangle] + \sum_{n_{1},n_{2}}^{(\varepsilon_{n_{1}} \neq \varepsilon_{c}, \varepsilon_{n_{2}} \neq \varepsilon_{c})} \frac{2}{(\varepsilon_{c} - \varepsilon_{n_{1}})(\varepsilon_{c} - \varepsilon_{n_{2}})} [\langle c | V_{B}^{(e)} | n_{1} \rangle \langle n_{1} c | I(0) | v' n_{2} \rangle \langle n_{2} | V_{B}^{(e)} | c \rangle] + \sum_{n_{1},n_{2}}^{(\varepsilon_{n_{1}} \neq \varepsilon_{c}, \varepsilon_{n_{2}} \neq \varepsilon_{c})} \frac{2}{(\varepsilon_{c} - \varepsilon_{n_{1}})(\varepsilon_{c} - \varepsilon_{n_{2}})} [\langle c | V_{B}^{(e)} | n_{1} \rangle \langle n_{1} c | I(0) | v' n_{2} \rangle \langle n_{2} | W | c \rangle + \langle c | W | n_{1} \rangle \langle n_{1} | V_{B}^{(e)} | n_{2} \rangle \langle n_{2} c | I(0) | c v' \rangle] \\ &- \sum_{\varepsilon_{c} = E_{1,-1}} \sum_{n}^{(\varepsilon_{n_{1}} \neq \varepsilon_{c})} \frac{2}{(\varepsilon_{c} - \varepsilon_{n_{1}})^{2}} [\langle c | V_{B}^{(e)} | n_{1} \rangle \langle n | W | \tilde{c} \rangle \langle \tilde{c} c | I(0) | c v' \rangle + \langle c | V_{B}^{(e)} | n_{1} \rangle \langle n | I(0) | \tilde{c} v' \rangle \langle \tilde{c} | W | c \rangle + \langle c | V_{B}^{(e)} | \tilde{c} \rangle \langle \tilde{c} | W | n \rangle \langle n | I(0) | c v' \rangle + \langle c | V_{B}^{(e)} | n_{1} \rangle \langle n_{1} c | I(0) | c v' \rangle \langle \tilde{c} | W | c \rangle + \langle c | V_{B}^{(e)} | \tilde{c} \rangle \langle \tilde{c} | W | n \rangle \langle n_{2} | V_{B}^{(e)} | n_{1} \rangle \langle n_{1} c | I(0) | c v' \rangle + \langle c | V_{B}^{(e)} | n_{1} \rangle \langle n_{1} c | I(0) | c v' \rangle \langle n_{2} c | V_{B}^{(e)} | n_{1} \rangle \langle n_{1} c | I(0) | c v' \rangle \langle n_{2} c | V_{B}^{(e)} | n_{2} c | V_{B}^{(e)} | n_{2} \rangle \langle n_{2} c | V_{B}^{(e)} | n_{2} c | V_{B}^{(e)} | n_{2} \rangle \langle n_{2} c | V_{$$

$$\begin{split} I_{\mu,Q,\vec{B}}^{(3d)} &= -f\sum_{\varepsilon_c = E_{1,-1}} \left(\sum_{n_1,n_2}^{(\varepsilon_{n_1} \neq \varepsilon_v, \varepsilon_{n_2} \neq \varepsilon_c)} \frac{2}{(\varepsilon_v - \varepsilon_{n_1})(\varepsilon_c - \varepsilon_{n_2})} [\langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle c|W|n_2\rangle\langle n_1n_2|I(\omega)|cv'\rangle + \langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1c|I(\omega)|n_2v'\rangle\langle n_2|W|c\rangle \right. \\ &+ \langle v|W|n_1\rangle\langle c|V_{\vec{B}}^{(e)}|n_2\rangle\langle n_1n_2|I(\omega)|cv'\rangle + \langle v|W|n_1\rangle\langle n_1c|I(\omega)|n_2v'\rangle\langle n_2|V_{\vec{B}}^{(e)}|c\rangle] + \sum_{n_1,n_2}^{(\varepsilon_{n_1} \neq \varepsilon_c, \varepsilon_{n_2} \neq \varepsilon_c)} \frac{2}{(\varepsilon_c - \varepsilon_{n_1})(\varepsilon_c - \varepsilon_{n_2})} [\langle c|V_{\vec{B}}^{(e)}| + \langle v|W|n_1\rangle\langle n_1v|V_{\vec{B}}^{(e)}|c\rangle] + \sum_{n_1,n_2}^{(\varepsilon_{n_1} \neq \varepsilon_c, \varepsilon_{n_2} \neq \varepsilon_c)} \frac{2}{(\varepsilon_c - \varepsilon_{n_1})(\varepsilon_c - \varepsilon_{n_2})} [\langle c|V_{\vec{B}}^{(e)}| + \langle v|W|n_1\rangle\langle n_1v|V_{\vec{B}}^{(e)}|c\rangle] \\ &+ \langle v|W|n_1\rangle\langle n_1|W|n_2\rangle\langle n_2v|I(\omega)|v'c\rangle + \langle c|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1v|I(\omega)|v'n_2\rangle\langle n_2|W|c\rangle + \langle c|W|n_1\rangle\langle n_1|V_{\vec{B}}^{(e)}|n_2\rangle\langle n_2v|I(\omega)|v'c\rangle] \\ &- \sum_{\varepsilon_c = E_{1,-1}} \sum_{n_1}^{(\varepsilon_n \neq \varepsilon_c)} \frac{2}{(\varepsilon_c - \varepsilon_n)^2} [\langle c|V_{\vec{B}}^{(e)}|n\rangle\langle n|W|\tilde{c}\rangle\langle \tilde{c}v|I(\omega)|v'c\rangle + \langle c|V_{\vec{B}}^{(e)}|n\rangle\langle nv|I(\omega)|v'\tilde{c}\rangle\langle \tilde{c}|W|c\rangle + \langle c|V_{\vec{B}}^{(e)}|\tilde{c}\rangle\langle \tilde{c}|W|n\rangle\langle nv|I(\omega)|v'\tilde{c}\rangle\langle \tilde{c$$

$$\times \langle nv|I'(\omega)|v'c\rangle] - \sum_{\varepsilon_{\widetilde{c}}=E_{1,-1}} \sum_{n}^{(\varepsilon_{n}\neq\varepsilon_{v})} \frac{2}{\varepsilon_{v}-\varepsilon_{n}} [\langle v|V_{B}^{(e)}|n\rangle\langle nc|I'(\omega)|\widetilde{c}v'\rangle\langle \widetilde{c}|W|c\rangle + \langle v|W|n\rangle\langle nc|I'(\omega)|\widetilde{c}v'\rangle\langle \widetilde{c}|V_{B}^{(e)}|c\rangle]$$

$$+ \sum_{\varepsilon_{\widetilde{v}}=\varepsilon_{v}} \sum_{n}^{(\varepsilon_{n}\neq\varepsilon_{c})} \frac{2}{\varepsilon_{c}-\varepsilon_{n}} [\langle v|V_{B}^{(e)}|\widetilde{v}\rangle\langle \widetilde{v}c|I'(\omega)|nv'\rangle\langle n|W|c\rangle + \langle v|W|\widetilde{v}\rangle\langle \widetilde{v}c|I'(\omega)|nv'\rangle\langle n|V_{B}^{(e)}|c\rangle] - \sum_{\varepsilon_{\widetilde{v}}=\varepsilon_{v}} \sum_{\varepsilon_{\widetilde{c}}=E_{1,-1}} [\langle v|V_{B}^{(e)}|\widetilde{v}\rangle + \langle v|W|\widetilde{v}\rangle\langle \widetilde{v}c|I'(\omega)|nv'\rangle\langle n|V_{B}^{(e)}|c\rangle] + \sum_{\varepsilon_{\widetilde{c}}=E_{1,-1}} \sum_{\varepsilon_{\widetilde{c}}=E_{1,-1}} \langle c|V_{B}^{(e)}|\widetilde{c}\rangle\langle \widetilde{c}v|I''(\omega)|v'\check{c}\rangle\langle \widetilde{c}|W|c\rangle \right).$$

$$(67)$$

Here

$$f = \begin{cases} 1 & \text{for } W = V_{\text{HFS}}^{(\mu)} \text{ or } W = V_{\text{HFS}}^{(Q)}, \\ \frac{1}{2} & \text{for } W = V_{\vec{B}}^{(e)}, \end{cases}$$
(68)

$$\langle n_1 n_2 | I(\omega) | n_3 n_4 \rangle \equiv \int d\vec{x}_1 d\vec{x}_2 u_{n_1}^{\dagger}(\vec{x}_1) u_{n_2}^{\dagger}(\vec{x}_2) I(\omega) u_{n_3}(\vec{x}_1) u_{n_4}(\vec{x}_2),$$

(69)

$$I(\omega) = \alpha \frac{(1 - \vec{\alpha}_1 \cdot \vec{\alpha}_2)\cos(\omega r_{12})}{r_{12}},\tag{70}$$

$$I'(\omega) = \frac{dI(\omega)}{d\omega}, \quad I''(\omega) = \frac{d^2I(\omega)}{d\omega^2}, \tag{71}$$

 $\omega = \varepsilon_v - E_{1,-1}$, and $r_{12} = |\vec{x}_1 - \vec{x}_2|$. As in the case of evaluation of $\delta g_{\rm HFS}^{(2s)}$ considered above, the diagrams corresponding to Eq. (61) are presented in Fig. 1 and the ones corresponding to Eq. (62) are presented in Figs. 3–5. Separating the interelectronic-interaction corrections is carried out according to Fig. 2 just as it was done in Sec. III.

The calculation of $h_1(k)$ was discussed in detail in Ref. [35]. We found that

$$\begin{split} h_{1}(k)B \\ &= M_{F} \Bigg\{ g_{j} Y_{\text{el}}(k) - g_{j}' Y_{\text{nuc}}^{(\mu)}(k) + \alpha^{2} Z \frac{1}{12} \Bigg[g_{j}' Y_{\text{nuc}}^{(\mu)}(k) \\ &\times S_{2}^{(t)}(\alpha Z) \\ &+ (\alpha Z)^{2} \frac{23}{180} \mathcal{Q} \bigg(\frac{m_{e} c}{\hbar} \bigg)^{2} Y_{\text{nuc}}^{(\mathcal{Q})}(k) T_{2}^{(t)}(\alpha Z) \Bigg] \Bigg\} \mu_{0} B. \end{split} \tag{72}$$

Calculating the other matrix elements, we obtain

$$h_2(k)B^2 = \frac{14}{(\alpha Z)^2} U_2^{(t)}(\alpha Z) (\mu_0 B)^2 / (m_e c^2),$$
 (73)

$$\begin{split} \widetilde{h}_{1}(j,k)B &= \frac{1}{2} \frac{\sqrt{(I+1/2)^{2} - M_{F}^{2}}}{I+1/2} \bigg\{ g_{j} + g_{I}' - \alpha^{2} Z \frac{1}{12} \bigg[g_{I}' S_{2}^{(t)}(\alpha Z) \\ &+ (\alpha Z)^{2} \frac{23}{360} Q \bigg(\frac{m_{e}c}{\hbar} \bigg)^{2} \frac{2I+3}{2I} T_{2}^{(t)}(\alpha Z) \bigg] \bigg\} \mu_{0}B, \end{split}$$

$$(74)$$

$$\tilde{h}_2(j,k) = 0. \tag{75}$$

Here the total functions are

$$U_2^{(t)}(\alpha Z) = U_2(\alpha Z) + \frac{1}{Z} B_{\bar{B}}(\alpha Z) + \frac{1}{Z^2} C_{\bar{B}}(\alpha Z) + \cdots, (76)$$

$$S_2^{(t)}(\alpha Z) = S_2(\alpha Z) + \frac{1}{Z}B_{\mu}(\alpha Z) + \frac{1}{Z^2}C_{\mu}(\alpha Z) + \cdots, \quad (77)$$

$$T_2^{(t)}(\alpha Z) = T_2(\alpha Z) + \frac{1}{Z}B_Q(\alpha Z) + \frac{1}{Z^2}C_Q(\alpha Z) + \cdots$$
 (78)

It must be stressed that the contributions of order $1/Z^2$ and higher to these functions are not included in Eq. (54). Their evaluation would require consideration of some higher-order terms in operator (48). The expansions (77) and (78) are also included in Eqs. (26) and (27) for the hyperfine-interaction corrections. The function

$$U_2(\alpha Z) = \frac{(\alpha Z)^2 m_e c^2}{14(\mu_0 R)^2} \Delta E_{(B)}^{(2)}(F, F)$$
 (79)

determines the one-electron contribution. Calculations employing Eqs. (64)–(67) yield for the interelectronic-interaction corrections $B_{\vec{B}}(\alpha Z)$, $B_{\mu}(\alpha Z)$, and $B_{O}(\alpha Z)$,

$$B_{\vec{B}}(\alpha Z) = \frac{\alpha^2 Z^3 m_e c^2}{14(\mu_o R)^2} \Delta E_{(\vec{B})}^{(3)}(F, F), \tag{80}$$

$$B_{\mu}(\alpha Z) = \frac{12}{\alpha^2 \frac{m_e}{m_p} g_I Y_{\text{nuc}}^{(\mu)}(F)} \frac{\Delta E_{(\mu)}^{(3)}(F, F)}{\mu_0 B M_F}, \quad (81)$$

$$B_{Q}(\alpha Z) = \frac{2160}{23\alpha^{4}Z^{2}Q\left(\frac{m_{e}c}{\hbar}\right)^{2}Y_{\text{nuc}}^{(Q)}(F)} \frac{\Delta E_{(Q)}^{(3)}(F,F)}{\mu_{0}BM_{F}}.$$
 (82)

It must be noted that, because of the smallness of the contribution determined by $B_Q(\alpha Z)$, only $B_{\bar{B}}(\alpha Z)$ and $B_{\mu}(\alpha Z)$ were evaluated in the present paper. For checking purposes the calculation of these functions was performed in both Feynman and Coulomb gauges. The results of both calculations coincide with each other.

Solving Eq. (54), we can finally derive for $M_F = -I + 1/2, \dots, I - 1/2$,

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left(a_1 (1 + \epsilon_1) M_F x + \epsilon_2 \frac{\Delta E_{\text{HFS}}^{(2s)}}{m_e c^2} x^2 \right)$$

$$\pm \frac{1}{2} \sqrt{1 + \frac{4M_F}{2I + 1} c_1 (1 + \delta_1) x + c_2 (1 + \delta_2 + M_F^2 \delta_3) x^2},$$
(83)

where

$$\epsilon_{1} = -\frac{1}{2g'_{I}} \left[\delta g_{HFS}^{(2s)}(F) + \delta g_{HFS}^{(2s)}(F+1) \right] = -\alpha^{2} Z \frac{1}{12} \left[S_{2}^{(t)}(\alpha Z) - (\alpha Z)^{2} \frac{23Q}{120g'_{I}} \left(\frac{m_{e}c}{\hbar} \right)^{2} \frac{1}{I(2I-1)} T_{2}^{(t)}(\alpha Z) \right], \tag{84}$$

$$\epsilon_2 = \frac{14}{(\alpha Z)^2} U_2^{(t)}(\alpha Z), \tag{85}$$

$$\delta_{1} = \frac{2I+1}{2(g_{j}+g'_{I})} \left[\delta g_{\text{HFS}}^{(2s)}(F+1) - \delta g_{\text{HFS}}^{(2s)}(F) \right]$$

$$= -\alpha^{2} Z \frac{1}{12(g_{j}+g'_{I})} \left[g'_{I} S_{2}^{(t)}(\alpha Z) - (\alpha Z)^{2} \frac{23}{360} Q \left(\frac{m_{e} c}{\hbar} \right)^{2} \frac{4I^{2}+4I+3}{I(2I-1)} T_{2}^{(t)}(\alpha Z) \right], \quad (86)$$

$$\delta_{2} = -\alpha^{2} Z \frac{1}{6(g_{j} + g_{I}^{\prime})} \left[g_{I}^{\prime} S_{2}^{(t)}(\alpha Z) + (\alpha Z)^{2} \frac{23}{360} Q \left(\frac{m_{e} c}{\hbar} \right)^{2} \frac{2I + 3}{2I} T_{2}^{(t)}(\alpha Z) \right], \quad (87)$$

$$\delta_3 = \frac{1}{g_i + g_I'} \alpha^4 Z^3 \frac{23}{360} Q \left(\frac{m_e c}{\hbar}\right)^2 \frac{1}{I(2I - 1)} T_2^{(t)}(\alpha Z). \quad (88)$$

For $F' = I + \frac{1}{2}$ and $M_F = \pm (I + \frac{1}{2})$, in contrast to Eq. (9), we have

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left(\frac{1}{2} \pm d_1 (1 + \eta_1) x + \eta_2 \frac{\Delta E_{\text{HFS}}^{(2s)}}{m_e c^2} x^2 \right), \tag{89}$$

where

$$\eta_{1} = \alpha^{2} Z \frac{1}{6(g_{j} - 2Ig'_{I})} \left[g'_{I} I S_{2}^{(t)}(\alpha Z) + (\alpha Z)^{2} \frac{23}{360} Q \left(\frac{m_{e} c}{\hbar} \right)^{2} \right. \\ \left. \times T_{2}^{(t)}(\alpha Z) \right], \tag{90}$$

$$\eta_2 = \epsilon_2 = \frac{14}{(\alpha Z)^2} U_2^{(t)}(\alpha Z),$$
(91)

and the minus and plus signs correspond to $M_F = -(I + \frac{1}{2})$ and $M_F = I + \frac{1}{2}$, respectively.

If I=1/2, the electrical quadrupole interaction vanishes and one can easily obtain for $M_E=0$,

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left(\epsilon_2 \frac{\Delta E_{\text{HFS}}^{(2s)}}{m_e c^2} x^2 \pm \frac{1}{2} \sqrt{1 + c_2 (1 + \delta_2) x^2} \right)$$
(92)

with

$$\delta_2 = -\frac{g_I'}{6(g_i + g_I')} \alpha^2 Z S_2^{(t)}(\alpha Z). \tag{93}$$

For I=1/2, $M_F=\pm 1$, the effect is described by Eq. (89) with

$$\eta_1 = \frac{g_I'}{12(g_I - g_I')} \alpha^2 Z S_2^{(t)}(\alpha Z). \tag{94}$$

V. NUMERICAL RESULTS

In Table I, we present the numerical results for the functions $U_2(\alpha Z)$, $B_{\bar{B}}(\alpha Z)$, $U_2^{(t)}(\alpha Z)$, $S_2(\alpha Z)$, $B_{\mu}(\alpha Z)$, $S_2^{(t)}(\alpha Z)$, and $T_2(\alpha Z)$ (only for the isotopes with I > 1/2) defined by Eqs. (79), (80), (76), (29), (81), (77), and (30), respectively, for the 2s state. All the values are calculated for the extended nuclear charge distribution. The root-mean-square nuclear charge radii $\langle r^2 \rangle^{1/2}$ were taken from Ref. [44]. For those elements for which no accurate experimental radii were available we employed the empirical expression [45]

$$\langle r^2 \rangle^{1/2} = 0.836A^{1/3} + 0.570(\pm 0.05) \text{ fm},$$
 (95)

where A is the nuclear mass expressed in a.m.u. The calculations were performed using the dual-kinetic-balance (DKB) basis set method [46] with the basis functions constructed from B-splines [47,48]. The uncertainties of $U_2(\alpha Z)$, $B_{\vec{B}}(\alpha Z)$, $S_2(\alpha Z)$, $B_{\mu}(\alpha Z)$, and $T_2(\alpha Z)$ were estimated by adding quadratically two errors, one obtained by varying $\langle r^2 \rangle^{1/2}$ within its uncertainty and the other obtained for Z=20-32 by changing the model of the nuclear-charge distribution from the Fermi to the homogeneously charged sphere model. The uncertainties of the total functions $U_2^{(t)}(\alpha Z)$ and $S_2^{(t)}(\alpha Z)$ due to uncalculated second- and higher-order terms were estimated as the first-order correction $[\sim B_{\vec{B}}(\alpha Z)/Z]$ and $\sim B_{\mu}(\alpha Z)/Z$, respectively] multiplied by the factor 2/Z. The uncertainty due to uncalculated first- and higher-order terms in Eq. (78) was estimated in a similar way.

In Table II, we present the individual contributions to the 2s g_i factor for some Li-like ions with $I \neq 0$ in the range Z

TABLE I. The numerical results for the extended-charge-nucleus values of functions $U_2^{(t)}(\alpha Z)$, $S_2^{(t)}(\alpha Z)$, and $T_2^{(t)}(\alpha Z)$ (for the ions with $I \neq 1/2$). The values of $\langle r^2 \rangle^{1/2}$ are taken from Ref. [44].

Ion	¹³ C ³⁺	¹⁷ O ⁵⁺	²¹ Ne ⁷⁺	²⁵ Mg ⁹⁺	³³ S ¹³⁺	⁴³ Ca ¹⁷⁺	$^{53}Cr^{21+}$
Z	6	8	10	12	16	20	24
$\langle r^2 \rangle^{1/2}$ [fm]	2.461	2.695	2.967	3.028	3.251	3.493	3.659
$U_2(\alpha Z)$	0.998574	0.997464	0.996038	0.994295	0.989858	0.984153	0.977179
$\vec{B_B}(\alpha Z)$	2.47400	2.47359	2.47305	2.47240	2.47070	2.46848	2.46568
$U_2^{(t)}(\alpha Z)$	1.41(14)	1.31(8)	1.24(5)	1.20(3)	1.144(19)	1.108(12)	1.080(9)
$S_2(\alpha Z)$	1.00306	1.00545	1.00854	1.01235	1.02218	1.03513	1.05145
$B_{\mu}(\alpha Z)$	-1.60040	-1.60757	-1.61684	-1.62825	-1.65769(1)	-1.69639(1)	-1.74505(2)
$S_2^{(t)}(\alpha Z)$	0.74(9)	0.80(5)	0.85(3)	0.88(2)	0.919(13)	0.950(8)	0.979(6)
$T_2(\alpha Z)$		1.00448(2)	1.00710(2)	1.01051(3)	1.01927(4)	1.03083(7)	1.04531(10)
$T_2^{(t)}(\alpha Z)$		1.0(3)	1.0(2)	1.01(17)	1.02(13)	1.03(10)	1.05(9)
Ion		61 Ni $^{25+}$		$^{67}Zn^{27+}$		73 Ge ²⁹⁺	
Z		28		30		32	
$\langle r^2 \rangle^{1/2}$ [fm]		3.822		3.964		4.063	
$U_2(\alpha Z)$		0.968938		0.964342		0.959428	
$\vec{B_B}(\alpha Z)$		2.46226		2.46030		2.45817	
$U_2^{(t)}(\alpha Z)$		1.057(6)		1.046(5)		1.036(5)	
$S_2(\alpha Z)$		1.07146(1)		1.08296(1)		1.09555(2)	
$B_{\mu}(\alpha Z)$		-1.80458(3)		-1.83874(3)		-1.87609(4)	
$S_2^{(t)}(\alpha Z)$		1.007(5)		1.022(4)		1.037(4)	
$T_2(\alpha Z)$		1.06287(11)		1.07277(14)		1.08359(13)	
$T_2^{(t)}(\alpha Z)$		1.06(8)		1.07(7)		1.08(7)	

=6-32. The Dirac point-nucleus value is obtained by Eq. (7). The interelectronic-interaction ($\Delta g_{\rm int}$), QED ($\Delta g_{\rm QED}$), nuclear-recoil ($\Delta g_{\rm rec}^{(e)}$), and nuclear-size ($\Delta g_{\rm NS}$) corrections are obtained as described in Refs. [32,33]. The nuclear-size correction was evaluated for the homogeneously charged

sphere model if Z=6-16 and for the Fermi model if Z=20-32. The nuclear polarization contribution to the 2s g_j factor of light Li-like ions can be neglected [17]. The g_j -factor values given in Table II are used for calculations of the coefficients in the Breit-Rabi formula.

TABLE II. The individual contributions to the ground-state g_j factor of lithiumlike ions with nonzero nuclear spin and the nuclear charge in the range Z=6-32. The values of $\langle r^2 \rangle^{1/2}$ are the same as in Table I.

Ion	¹³ C ³⁺	¹⁷ O ⁵⁺	$^{33}S^{13+}$	⁴³ Ca ¹⁷⁺	
g_{D}	1.999680300	1.999431380	1.997718193	1.996426011	
$\Delta g_{ m int}$	0.000130758(19)	0.00017666(3)	0.00036124(9)	0.00045445(14)	
$\Delta g_{ m OED}$	0.002319417(6)	0.002319549(12)	0.00232070(6)	0.00232171(10)	
$\Delta g_{ m QED} \ \Delta g_{ m rec}^{(e)}$	0.00000009	0.000000016	0.000000045(1)	0.00000057(2)	
$\Delta g_{ m NS}$	0.0	0.0	0.000000005	0.000000014	
g_{j}	2.00213048(2)	2.00192760(3)	2.00040018(11)	1.99920224(17)	
on	$^{53}{ m Cr}^{21+}$		73 Ge $^{29+}$		
Ď	1.99483	8064	1.990752307		
g_{int}	0.00054	85(2)	0.0007397(4)		
$g_{ m QED}$	0.00232	304(15)	0.0023270(2)		
$\Delta g_{ m QED} \ \Delta g_{ m rec}^{(e)}$	0.00000	0069(4)	0.00000093(9)		
$\Delta g_{ m NS}$	0.00000	0035	0.00000160		
g_j	1.99770	97(3)	1.9938193(4)		

TABLE III. The numerical values of the coefficients in Eqs. (2), (9), (11), (83), (89), and (92) for Li-like ions with Z=6-32. The values of μ/μ_N and Q are taken from Refs. [50,51], respectively.

Ion	$^{13}\text{C}^{3+}$	¹⁷ O ⁵⁺	$^{33}S^{13+}$	$^{43}\text{Ca}^{17+}$
	1/2	5/2	3/2	7/2
μ/μ_N	0.7024118(14)	-1.89379(9)	0.6438212(14)	-1.317643(7)
Q [barn]		-0.02558(22)	-0.0678(13)	-0.0408(8)
a_1		0.00041256(2)	-0.0002337573(5)	0.0002050317(11)
$\epsilon_{ m l}$		-0.0000284(18)	-0.0000653(9)	-0.0000843(7)
$a_1(1+\epsilon_1)$		0.00041254(2)	-0.0002337421(6)	0.0002050144(11)
$\epsilon_2(=\eta_2)$	$1.03(10) \times 10^4$	$5.4(3) \times 10^3$	$1.17(2) \times 10^3$	$7.28(8) \times 10^2$
c_1		2.00151505(4)	2.00063394(11)	1.99899721(17)
δ_1		0.0000000059(4)	-0.00000000763(11)	0.00000000864(7)
$c_1(1+\delta_1)$		2.00151506(4)	2.00063393(11)	1.99899722(17)
c_2	4.01159069(8)	4.00606248(15)	4.0025362(4)	3.9959898(7)
δ_2	-0.0000000151(18)	0.0000000117(7)	-0.0000000152(2)	0.0000001730(15)
δ_3		0.0	-0.00000000001	0.0
$c_2(1+\delta_2)$	4.01159062(8)	4.00606253(15)	4.0025361(4)	3.9959899(7)
$c_2\delta_3$		0.0	-0.00000000002(1)	0.0
d_1	1.000682697(10)	1.00199519(5)	0.99984946(5)	1.00031873(9)
η_1	0.000000075(9)	-0.0000000292(18)	0.0000000229(3)	-0.0000000605(5)
$d_1(1+\eta_1)$	1.000682704(10)	1.00199516(5)	0.99984948(5)	1.00031867(9)
1 11/	Ion	53(Cr^{21+}	73 Ge ²⁹⁺
	I	,	3/2	9/2
	μ / μ_N	-0.47	7454(3) -0.5	8794677(2)
	Q [barn]	-0.1	50(50)	-0.196
	a_1	0.00017	72295(11) 0.000	010643846(2)
	$oldsymbol{\epsilon}_1$	-0.000	01041(6) -0.0	0001472(6)
	$a_1(1+\epsilon_1)$	0.00017	72277(11) 0.000	10642279(7)
	$\epsilon_2(=\eta_2)$	4.93($4) \times 10^2$ 2.66	$60(13) \times 10^2$
	c_1	1.997	5374(3) 1.9	937129(4)
	δ_1	0.00000	000893(5) 0.000	000000776(3)
	$c_1(1+\delta_1)$	1.997	5374(3) 1.9	937129(4)
	c_2	3.990	1556(10) 3.9	748910(17)
	δ_2	0.000000	0.000	000001582(6)
	δ_3	-0.0000	0000004(2) -0.0	0000000001
	$c_2(1+\delta_2)$	3.990	1557(10) 3.9	748911(17)
	$c_2\delta_3$			0000000005
	d_1			973886(2)
	η_1			000000708(3)
	$d_1(1+\eta_1)$		` '	973886(2)

In Table III, the numerical results for the coefficients in Eqs. (2), (9), (11), (83), (89), and (92) are listed for some Li-like isotopes in the interval Z=6-32.

VI. DISCUSSION

The energy difference between the ground-state hyperfine splitting components in a lithiumlike ion can be written as [49]

$$\Delta E_{\rm HFS}^{(2s)} = \frac{1}{6} \alpha (\alpha Z)^3 \frac{\mu}{\mu_N} \frac{m_e}{m_p} \frac{2I+1}{2I} m_e c^2 \left(\left[A^{(2s)} (\alpha Z) (1-\delta^{(2s)}) (1-\delta^{(2s)}) (1-\delta^{(2s)}) + x_{\rm rad}^{(2s)} \right] + \frac{1}{Z} B^{(2s)} (\alpha Z) + \frac{1}{Z^2} C^{(2s)} (\alpha Z) + \cdots \right),$$
(96)

where

$$A^{(2s)}(\alpha Z) = \frac{2[2(1+\gamma)+\sqrt{2(1+\gamma)}]}{(1+\gamma)^2\gamma(4\gamma^2-1)} = 1 + \frac{17}{8}(\alpha Z)^2 + \frac{449}{128}(\alpha Z)^4 + \cdots$$
(97)

is the one-electron relativistic factor, $\delta^{(2s)}$ is the nuclear charge distribution correction, $\epsilon^{(2s)}$ is the nuclear magnetization distribution correction (the Bohr-Weisskopf effect), $x_{\rm rad}^{(2s)}$ is the QED correction, $B^{(2s)}(\alpha Z)$ and $C^{(2s)}(\alpha Z)$ determine the interelectronic-interaction corrections to the hyperfine structure. Therefore, the dimensionless variable $|x| = \mu_0 B/|\Delta E_{\rm HFS}^{(2s)}|$ is of the order of $6\mu_0 B/[\alpha(\alpha Z)^3(m_e/m_p)m_ec^2]$. For the magnetic fields with $B \sim 1-10$ T Li-like ions with Z=6-32 are of special interest, since they meet the requirement $|x| \sim 1$. For this reason, only such ions are presented in Tables I–III.

For ions with $Z \le 32$, the electric-quadrupole corrections to the coefficients a_1 , c_1 , c_2 , and d_1 are either equal to zero, if I=1/2, as in the case of $^{13}C^{3+}$, or by a factor of $10^{-3}-10^{-4}$ smaller than the magnetic-dipole ones. This is due to an additional factor $(\alpha Z)^2$ in the electric-quadrupole contributions compared to the magnetic-dipole ones in the equations for the hyperfine-structure corrections to the Breit-Rabi formula coefficients and small values of Q for low-Z ions.

As one can see from Table III, the corrections ϵ_1 , δ_1 , δ_2 , δ_3 , and η_1 for Li-like ions are several times smaller as compared to the corresponding ones for the 1s state of the same H-like isotopes [21]. However, they provide more precise determinations of the coefficients in the Breit-Rabi formula.

For $B=1-10\,$ T, an estimate of the terms of the third and higher orders with respect to B in Eq. (54) shows that these

terms are negligibly small as compared to both magnetic-dipole and electric-quadrupole corrections calculated above. However, taking into account $\epsilon_2 B^2$ and $\eta_2 B^2$ is very important in case Z=6-32. This is due to the fact that these terms are comparable with the other corrections to the Breit-Rabi formula considered and the less Z is, the more appreciable the contributions from $\epsilon_2 B^2$ and $\eta_2 B^2$ become. One can see that for Li-like ions these terms are $10-10^3$ times larger as compared to the case of the 1s state of the same H-like isotopes [21]. In the second-order approximation (54) with respect to B, formulas (2), (11), (83), and (92) do not contain B to a power higher than 2 under the square root. This is due to the facts that $h_2(F)=h_2(F')$ and $\tilde{h}_2=0$.

The Breit-Rabi formula for the 2s state includes $\Delta E_{\rm HFS}^{(2s)}$. The value of μ/μ_N is contained in the coefficients of the formula and the corrections to them calculated above. The uncertainties of the nuclear magnetic moments indicated in Table III, as a rule, do not include errors due to unknown chemical shifts which, in some cases, can contribute on the level of a few tenths of a percent. Thus, carrying out the experiments on the Zeeman splitting with the aforesaid accuracy could provide the most precise determination of both $\Delta E_{\rm HFS}^{(2s)}$ and μ/μ_N . The corrections to the Breit-Rabi formula evaluated in this paper will be important for this determination.

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