Zeeman effect of the hyperfine structure levels in hydrogen-like ions

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Abstract

The fully relativistic theory of the Zeeman splitting of the 1s hyperfine structure levels in hydrogenlike ions 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. The results can be used for a precise determination of nuclear magnetic moments from $g$ factor experiments.

1 Introduction

Recent measurements of the $g$ factor of hydrogenlike carbon and oxygen have reached an accuracy of about $7 \cdot 10^{-10}$ [1–3]. Extensions of these measurements to ions with nonzero nuclear spin $I$ would provide the basis for new determinations of the nuclear magnetic moments [4] and the hyperfine structure (HFS) splitting in hydrogenlike ions. Experimental investigations in this direction are anticipated in the near future at GSI [5]. Corresponding values of the magnetic field are supposed to be in a range from 1 to 10 T.

For heavy ions with nonzero nuclear spin the ground state Zeeman splitting caused by the magnetic field in the range under consideration is much smaller than the hyperfine splitting and, therefore, the consideration can be conveniently reduced to the $g$ factor value [6]. However, for ions with the nuclear charge number $Z$ in the range $Z = 1 – 20$, which are being under current experimental investigations at Mainz University, the Zeeman splitting is comparable with the hyperfine splitting. This requires constructing the perturbation theory for quasidegenerate states. To a good accuracy, the solution of the problem is given by the well-known Breit – Rabi formula [7–9]. The aforesaid experimental precision has, however, shown the need for an improvement of the Breit – Rabi formula.

In the present paper, we improve the Breit – Rabi formula for the 1s hyperfine structure levels by calculating the second-order correction caused by the hyperfine interaction and the interaction with the external magnetic field. The obtained results are especially important for ions with $Z \leq 20$, where the 1s HFS splitting can be comparable with the Zeeman splitting if the magnitude of the homogeneous magnetic field does not exceed 10 T.

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

2 The Breit – Rabi formula

We consider a H-like ion with nonzero nuclear spin $I$ in a state with the total electron angular momentum $j = 1/2$. The ion is placed in a homogeneous magnetic field $\vec{B}$ directed along the $z$ axis. The magnetic splitting is linear with respect to $\vec{B}$ only if one of the following conditions is
fulfilled: either $\Delta E_{\text{mag}} \ll \Delta E_{\text{HFS}}$ or $\Delta E_{\text{mag}} \gg \Delta E_{\text{HFS}}$, where $\Delta E_{\text{HFS}} = E(F + 1) - E(F)$, $E(F) = E_{nk} + \varepsilon_{\text{hfs}}(F)$, $F = I \pm 1/2$ is the total atomic angular momentum, and $\varepsilon_{\text{hfs}}(F)$ is the hyperfine structure shift from the Dirac state with the energy

$$ E_{nk} = \frac{\gamma + n_r \nu}{N} m_e. \tag{1} $$

Here $n$ is the principal quantum number, $\kappa = (-1)^{j+2l+1}(j + \frac{1}{2})$, $l = j \pm \frac{1}{2}$ 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. It should be emphasized that in case the second inequality is fulfilled $\Delta E_{\text{mag}}$ must be much less than the distance to other Dirac’s levels. In the intermediate $\vec{B}$ case, $\Delta E_{\text{mag}} \sim \Delta E_{\text{HFS}}$, we must take into account mixing the HFS sublevels with the same $M_F$, where $M_F = -F, -F + 1, ..., F - 1, F$ is the $z$ projection of the total angular momentum. For the states with $j = 1/2$, there are only two HFS levels $F = I + 1/2$ and $F' = I + 1/2$ with the same $M_F = -I + 1/2, ..., I - 1/2$. This greatly simplifies the theory. Denoting

$$ \Delta E_{\text{mag}} = E - \frac{E(F) + E(F + 1)}{2}, $$

one can derive for the Zeeman splitting

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

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

$$ a_1 = -g_I', \tag{3} $$
$$ c_1 = g_j + g_I', \tag{4} $$
$$ c_2 = (g_j + g_I')^2, \tag{5} $$

g_j$ is the bound-electron $g$ factor,

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

g_D$ is the bound-electron $g$ factor derived from the Dirac equation [10],

$$ g_D = \frac{\kappa}{j(j + 1)} \left( \kappa \frac{E_{nk}}{m_e} - \frac{1}{2} \right), \tag{7} $$

$\Delta g_{\text{QED}}$ is the QED correction, $\Delta g_{\text{rec}}^{(e)}$ is the nuclear recoil correction to the bound-electron $g$ factor, $\Delta g_{\text{NS}}$ is the nuclear size correction, $\Delta g_{\text{NP}}$ 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, $\mu_z$ is the $z$ projection of the nuclear magnetic moment operator $\vec{\mu}$ acting in the space of nuclear wave

\footnote{In the present paper, the energy of a Zeeman sublevel $\Delta E_{\text{mag}}$ is counted with respect to the mean energy of the hyperfine structure doublet [9, 10]. If it is necessary to count $\Delta E_{\text{mag}}^{cg}$ from the center of gravity of the HFS doublet [7, 11], one should use the relation

$$ \Delta E_{\text{mag}}^{cg} = \Delta E_{\text{mag}} - \frac{\Delta E_{\text{HFS}}}{2(2I + 1)}. $$

2}
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 $\Delta g^{(n)}_{\text{rec}}$ is the recoil correction to the bound-nucleus $g$ factor (see section 4). Eq. (2) is usually called the Breit–Rabi formula (see, e.g., Refs. [7, 9–11]). It covers Zeeman splitting from weak ($x \ll 1$) to strong ($x \gg 1$) fields including the intermediate region. For $F' = I + \frac{1}{2}$, $M_F = \pm (I + \frac{1}{2})$ the splitting is linear in the first order of perturbation theory under arbitrary magnetic induction,

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}} \left[ \frac{1}{2} \pm d_1 x \right],$$

(9)

where

$$d_1 = \frac{1}{2} g_j - I g'_I$$

(10)

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

For H-like ions with $I = 1/2$, $F = 0$ and $F' = 1$ and, therefore, the two mixed sublevels have $M_F = 0$. In this case the Breit–Rabi formula takes the form

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

(11)

and for $M_F = \pm 1$ the effect is described by Eq. (9) with $d_1 = \frac{1}{2}(g_j - g'_I)$.

It should be noted that in the original paper [7] the lowest-order nonrelativistic expression $g_j = (j + 1/2)/(l + 1/2)$ was used for the electronic $g$ factor, and the corrections depending on $\frac{m_{\text{el}}}{m_{\text{p}}} g_I$ were introduced later [9].

If the magnetic field is strong, $\Delta E_{\text{mag}} \gg \Delta E_{\text{HFS}}$, Eqs. (2), (9), and (11) convert into formulas for the anomalous Zeeman effect of the state with $j = 1/2$. On the contrary, assuming that the energy level shift (splitting) due to interaction with $\overline{B}$ is much smaller than the hyperfine-structure splitting, $\Delta E_{\text{mag}} \ll \Delta E_{\text{HFS}}$, we can express the linear-dependent part of this shift in terms of the atomic $g$ factor,

$$\Delta E_{\text{mag}} = g \mu_0 B M_F,$$

(12)

where, to the lowest-order approximation (see, e.g., Refs. [9, 11]),

$$g(F) = g_D Y_{\text{el}}(F) - \frac{m_e}{m_p} g_I Y_{\text{nuc}}^{(\mu)}(F),$$

(13)

$$Y_{\text{el}}(F) = \frac{F(F + 1) + 3/4 - I(I + 1)}{2F(F + 1)} = \begin{cases} \frac{1}{2F+1} & \text{for } F = I - \frac{1}{2}, \\ \frac{1}{2F+3} & \text{for } F = I + \frac{1}{2}, \end{cases}$$

(14)

$$Y_{\text{nuc}}^{(\mu)}(F) = \frac{F(F + 1) + I(I + 1) - 3/4}{2F(F + 1)} = \begin{cases} \frac{2(I+1)}{2F+2} & \text{for } F = I - \frac{1}{2}, \\ \frac{2I}{2F+3} & \text{for } F = I + \frac{1}{2}. \end{cases}$$

(15)

The total 1s $g$ factor value for a hydrogenlike ion with nonzero nuclear spin can be represented by

$$g_{\text{tot}}(F) = (g_D + \Delta g_{\text{QED}} + \Delta g^{(e)}_{\text{rec}} + \Delta g_{\text{NS}} + \Delta g_{\text{NP}}) Y_{\text{el}}(F) - \frac{m_e}{m_p} g_I Y_{\text{nuc}}^{(\mu)}(F) + \delta g_{\text{HFS}}^{(1s)}(F),$$

(16)

where the HFS correction $\delta g_{\text{HFS}}^{(1s)}(F) = \delta g_{\text{HFS}(\mu)}^{(1s)}(F) + \delta g_{\text{HFS}(Q)}^{(1s)}(F)$ was calculated in Ref. [6].
3 Corrections to the Breit – Rabi formula for the 1s state

The hamiltonian of a hydrogenlike ion can be written as

\[ H = H_0 + V, \]  

(17)

where \( H_0 \) is the Dirac hamiltonian and

\[ V = V_{\text{HFS}} + V_B. \]  

(18)

The hyperfine interaction operator is given by the sum

\[ V_{\text{HFS}} = V_{\text{HFS}}^{(\mu)} + V_{\text{HFS}}^{(Q)}, \]  

(19)

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

\[ V_{\text{HFS}}^{(\mu)} = \frac{|e|}{4\pi} \left( \vec{\alpha} \cdot [\vec{\mu} \times \vec{r}] \right), \]  

(20)

and, in the point-quadrupole approximation,

\[ V_{\text{HFS}}^{(Q)} = -\alpha \sum_{m=-2}^{m=2} Q_{2m} n_{2m}^* (\vec{n}). \]  

(21)

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, \( n_{2m} = C_{2m}(\vec{n})/r^3 \) 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 \( i \)-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 \( I > 1/2 \).

The interaction of the ion with the magnetic field is represented as

\[ V_B = V_B^{(e)} + V_B^{(n)}. \]  

(22)

Here \( V_B^{(e)} \) describes the interaction of the electron with the homogeneous magnetic field,

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

(23)

where the vector \( \vec{\alpha} \) incorporates the Dirac \( \alpha \) matrices, and

\[ V_B^{(n)} = - (\vec{\mu} \cdot \vec{B}) \]  

(24)

describes the interaction of the nuclear magnetic moment \( \vec{\mu} \) with \( \vec{B} \).

We assume that the Zeeman splitting \( \Delta E_{\text{mag}} \) of the 1s HFS levels \( F = I - 1/2 \) and \( F' = I + 1/2 \) is much smaller than the distance to other levels but is comparable with \( \Delta E_{\text{HFS}}^{(1s)} \). The unperturbed eigenstates form a two-dimensional subspace \( \Omega = \{|1^{(0)}\rangle, |2^{(0)}\rangle\} \), where \( |1^{(0)}\rangle = |10\frac{1}{2}IFM_F\rangle, |2^{(0)}\rangle = |10\frac{1}{2}IF'M_{F'}\rangle \), and \( |nljIFM_F\rangle \) denotes the atomic wave function that corresponds to given values of \( F \) and \( M_F \),

\[ |nljIFM_F\rangle = \sum_{m_j,M_{I}} C_{F_{M_F}m_jM_{I}}^{F'M_{F'}} |nljm_j\rangle |IM_{I}\rangle. \]  

(25)
Here $C_{j m_l, I M_l}^{F M_F}$ are the Clebsch-Gordan coefficients, $|n l l m_j\rangle$ are the unperturbed electron wave functions, which are four-component eigenvectors of the Dirac equation for the Coulomb field, and $|I M_l\rangle$ are the nuclear wave functions.

Employing the perturbation theory for degenerate states [12] and keeping the three lowest-order terms only, we get the following equation for the perturbed energies

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

(26)

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

$$
h_0(k) = E(k)
$$

(27)
is the energy of the HFS level,

$$
h_1(k) = \frac{1}{B} \left( \langle k| V_B |k \rangle + 2 \sum_{i}^{(E_i \neq E_{i-1})} \frac{\langle k| V_B |i \rangle \langle i| V_{\text{HFS}} |k \rangle}{E_{i-1} - E_i} \right)
+ (\Delta g_{\text{QED}} + \Delta g_{\text{rec}}(e) + \Delta g_{\text{NS}} + \Delta g_{\text{NP}}) Y_0(k) \mu_0 M_F - \Delta g_{\text{rec}}^{(n)} Y_0(k) \mu_N M_F
$$

(28)

$$
= g_{\text{tot}}(k) \mu_0 M_F,
$$

$$
h_2(k) = \frac{1}{B^2} \sum_{i}^{(E_i \neq E_{i-1})} \frac{\langle k| V_B |i \rangle |^2}{E_{i-1} - E_i},
$$

(29)

$$
\tilde{h}_1(j, k) = \frac{1}{B} \left( \langle j| V_B |k \rangle + \sum_{i}^{(E_i \neq E_{i-1})} \frac{\langle j| V_B |i \rangle \langle i| V_{\text{HFS}} |k \rangle + \langle j| V_{\text{HFS}} |i \rangle \langle i| V_B |k \rangle}{E_{i-1} - E_i} \right)
+ (\Delta_{\text{QED}} + \Delta_{\text{rec}} + \Delta_{\text{NS}} + \Delta_{\text{NP}}) \mu_0
$$

(30)

$$
\tilde{h}_2(j, k) = \frac{1}{B^2} \sum_{i}^{(E_i \neq E_{i-1})} \frac{\langle j| V_B |i \rangle \langle i| V_B |k \rangle}{E_{i-1} - E_i},
$$

(31)

$\text{j, } k = F, F'$. $\Delta_{\text{QED}}$, $\Delta_{\text{rec}}$, $\Delta_{\text{NS}}$, and $\Delta_{\text{NP}}$ are the 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. It should be noted that we have neglected here terms describing virtual transitions into excited nuclear states via the direct interaction of the nucleus with the magnetic field. We assume that these terms are extremely small. The calculation of $h_1(k)$ was discussed in detail in Ref. [6]. Calculating the other matrix elements, we obtain

$$
h_2(k)B^2 = \frac{1}{(\alpha Z)^2} U(\alpha Z)(\mu_0 B)^2/(m_e c^2),
$$

(32)

$$
\tilde{h}_1(j, k)B = \frac{1}{2} \sqrt{(I + 1/2)^2 - M_F^2} \left[g_j + g_j'\right]
- \alpha^2 Z \left\{ \frac{1}{3} \left( g_j' S(\alpha Z) + (\alpha Z)^2 \frac{11}{90} Q \left( \frac{m_e c}{\hbar} \right)^2 \frac{2I + 3}{2I} T(\alpha Z) \right) \right\} \mu_0 B,
$$

(33)

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

(34)
Here

\[ U(\alpha Z) = \frac{2}{9}(\alpha Z)^2[u_2(\alpha Z) + 2u_{-1}(\alpha Z)], \]

\[ u_{-1}(\alpha Z) = m^3_w \tilde{R}_{-1}, \]

\[ u_2(\alpha Z) = m^3_w \tilde{R}_2, \]

\[ \tilde{R}_{-1} = \sum_{n} \frac{1}{E_{1,1} - E_{n,1}} \int_{0}^{\infty} (g_{1,1}f_{n,1} + f_{1,1}g_{n,1})r^3 \, dr \int_{0}^{\infty} (g_{n,1}f_{1,1} + f_{n,1}g_{1,1})r^3 \, dr, \]

\[ \tilde{R}_2 = \sum_{n} \frac{1}{E_{1,1} - E_{n,2}} \int_{0}^{\infty} (g_{1,2}f_{n,2} + f_{1,2}g_{n,2})r^3 \, dr \int_{0}^{\infty} (g_{n,2}f_{1,1} + f_{n,2}g_{1,1})r^3 \, dr, \]

\[ S(\alpha Z) = \frac{2}{3\alpha Z}(R_2 + 2R_{-1}), \]

\[ R_{-1} = \sum_{n} \frac{1}{E_{1,1} - E_{n,1}} \int_{0}^{\infty} (g_{1,1}f_{n,1} + f_{1,1}g_{n,1})r^3 \, dr \int_{0}^{\infty} (g_{n,1}f_{1,1} + f_{n,1}g_{1,1}) \, dr, \]

\[ R_2 = \sum_{n} \frac{1}{E_{1,1} - E_{n,2}} \int_{0}^{\infty} (g_{1,2}f_{n,2} + f_{1,2}g_{n,2})r^3 \, dr \int_{0}^{\infty} (g_{n,2}f_{1,1} + f_{n,2}g_{1,1}) \, dr, \]

\[ T(\alpha Z) = -\frac{36}{11m_e(\alpha Z)^2}R_2, \]

\[ \mathcal{R}_2 = \sum_{n} \frac{1}{E_{1,1} - E_{n,2}} \int_{0}^{\infty} (g_{1,2}f_{n,2} + f_{1,2}g_{n,2})r^3 \, dr \int_{0}^{\infty} (g_{n,2}f_{1,1} + f_{n,2}g_{1,1}) \frac{1}{r} \, dr, \]

\( g_{n\kappa} \) and \( f_{n\kappa} \) are the upper and lower radial components of the Dirac wave function defined by

\[ \psi_{n\kappa}(\vec{r}) = \begin{pmatrix} g_{n\kappa}(r)\Omega_{\kappa\mu}(\vec{n}) \\ i f_{n\kappa}(r)\Omega_{-\kappa\mu}(\vec{n}) \end{pmatrix}, \]

and \( Q = 2 \langle II|Q_{20}|II \rangle \) is the electric-quadrupole moment of the nucleus. For the point-charge nucleus, the functions \( S(\alpha Z) \) and \( T(\alpha Z) \) are given by [6]

\[ S(\alpha Z) = \frac{2}{3} \left\{ \frac{2 + \gamma}{3(1 + \gamma)} + \frac{2}{\gamma(2\gamma - 1)}[1 - \frac{\gamma}{2} + (\alpha Z)^2] \right\} \]

\[ = 1 + \frac{97}{36}(\alpha Z)^2 + \frac{289}{72}(\alpha Z)^4 + ... \]

and

\[ T(\alpha Z) = \frac{12(35 + 20\gamma - 32(\alpha Z)^2)}{11\gamma(1 + \gamma)^2[15 - 16(\alpha Z)^2]} \]

\[ = 1 + \frac{43}{33}(\alpha Z)^2 + \frac{2405}{1584}(\alpha Z)^4 + ..., \]
where \( \gamma = \sqrt{1 - (\alpha Z)^2} \). Also the sum \( \tilde{R}_{-1} \) can be evaluated analytically, employing the method of generalized virial relations for the Dirac equation [13, 14]. For the \( 1s \) state, applying formulas from Ref. [6, 15], we find

\[
u_{-1}(\alpha Z) = (\gamma + 1) \left[ \frac{3}{4(\alpha Z)^2} - 1 \right]. \tag{48}\]

Numerical evaluation of \( u_{-1}(\alpha Z) \), \( u_2(\alpha Z) \), \( U(\alpha Z) \), \( S(\alpha Z) \), and \( T(\alpha Z) \) for extended-charge nuclei is considered in the next section.

Solving equation (26), we finally obtain for \( M_F = -I + 1/2, \ldots, I - 1/2 \)

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

\[
\pm \frac{1}{2} \sqrt{1 + \frac{4M_F}{2I + 1} \epsilon_1(1 + \delta_1)x + \epsilon_2(1 + \delta_2 + M_F^2 \delta_3)x^2} \tag{49}\]

Here

\[
\epsilon_1 = -\frac{1}{2g'_I} [\delta g_{\text{HFS}}^{(1s)}(F) + \delta g_{\text{HFS}}^{(1s)}(F + 1)]
\]

\[
= -\alpha^2 Z \frac{1}{3} \left[ S(\alpha Z) - (\alpha Z)^2 \frac{11Q}{30g'_I} \left( \frac{m_e c^2}{h} \right)^2 \frac{1}{I(2I - 1)} T(\alpha Z) \right], \tag{50}\]

\[
\epsilon_2 = \frac{1}{(\alpha Z)^2} U(\alpha Z), \tag{51}\]

\[
\delta_1 = \frac{2I + 1}{2(g_j + g'_I)} [\delta g_{\text{HFS}}^{(1s)}(F + 1) - \delta g_{\text{HFS}}^{(1s)}(F)]
\]

\[
= -\alpha^2 Z \frac{1}{3(g_j + g'_I)} \left[ g'_I S(\alpha Z) - (\alpha Z)^2 \frac{11}{90} Q \left( \frac{m_e c^2}{h} \right)^2 \frac{4I^2 + 4I + 3}{I(2I - 1)} T(\alpha Z) \right], \tag{52}\]

\[
\delta_2 = -\alpha^2 Z \frac{2}{3(g_j + g'_I)} \left[ g'_I S(\alpha Z) + (\alpha Z)^2 \frac{11}{90} Q \left( \frac{m_e c^2}{h} \right)^2 \frac{2I + 3}{2I} T(\alpha Z) \right], \tag{53}\]

\[
\delta_3 = \frac{1}{g_j + g'_I} \alpha^4 Z^3 \frac{22}{45} Q \left( \frac{m_e c^2}{h} \right)^2 \frac{1}{I(2I - 1)} T(\alpha Z). \tag{54}\]

For \( F' = I + \frac{1}{2}, \ M_F = \pm (I + \frac{1}{2}) \), in contrast to Eq. (39), we have

\[
\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(1s)} \left[ \frac{1}{2} \pm d_1(1 + \eta_1)x + \eta_2 \frac{\Delta E_{\text{HFS}}^{(1s)}}{m_e c^2} x^2 \right], \tag{55}\]

where

\[
\eta_1 = \alpha^2 Z \frac{2}{3(g_j - 2Ig'_I)} \left[ g'_I S(\alpha Z) + (\alpha Z)^2 \frac{11}{90} Q \left( \frac{m_e c^2}{h} \right)^2 T(\alpha Z) \right], \tag{56}\]

\[
\eta_2 = \epsilon_2 = \frac{1}{(\alpha Z)^2} U(\alpha Z), \tag{57}\]

and the “–” and “+” 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 \( M_F = 0 \):

\[
\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(1s)} \left[ \epsilon_2 \frac{\Delta E_{\text{HFS}}^{(1s)}}{m_e c^2} x^2 \pm \frac{1}{2} \sqrt{1 + c_2(1 + \delta_2)x^2} \right] \tag{58}\]
with
\[ \delta_2 = -\frac{2g'_I}{3(g_j + g'_I)} \alpha^2 Z S(\alpha Z). \] (59)

For \( I = 1/2, M_F = \pm 1 \), the effect is described by formula (55) with
\[ \eta_1 = \frac{g'_I}{3(g_j - g'_I)} \alpha^2 Z S(\alpha Z). \] (60)

4 Numerical results

In Table 1, we present the numerical results for the functions \( u_{-1}(\alpha Z), u_2(\alpha Z), U(\alpha Z), S(\alpha Z), \) and \( T(\alpha Z) \) (only for the isotopes with \( I > 1/2 \)) defined by Eqs. (36), (37), (35), (41), and (43), respectively. \( u_{-1}^{\text{point}}(\alpha Z), S^{\text{point}}(\alpha Z), \) and \( T^{\text{point}}(\alpha Z) \) are the point-nucleus values obtained by analytical formulas (18), (16), and (17), correspondingly. \( u_{13}^{\text{ext}}(\alpha Z), u_2^{\text{ext}}(\alpha Z), U^{\text{ext}}(\alpha Z), S^{\text{ext}}(\alpha Z), \) and \( T^{\text{ext}}(\alpha Z) \) are the values calculated for the extended nuclear charge distribution. The root-mean-square nuclear charge radii \( \langle r^2 \rangle^{1/2} \) were taken from Ref. [16]. The calculations were performed using the dual-kinetic-balance (DKB) basis set method [17] with the basis functions constructed from B-splines [18,19]. The uncertainties include the difference between the results obtained with the Fermi and the homogeneously-charged sphere model for the nuclear charge distribution as well as the error arising from the uncertainty of \( \langle r^2 \rangle^{1/2} \).

In Table 2, we present the individual contributions to the 1s \( g_j \) factor for some H-like ions with \( I \neq 0 \) in the range \( Z = 1 - 20 \). The error ascribed to the Dirac point-nucleus value results from the current uncertainty of the fine structure constant, \( 1/\alpha = 1/137.0359911(46) \) [20]. The QED correction includes the one-loop contribution to all orders in \( \alpha Z \) [21–23] and the existing \( \alpha Z \)-expansion QED terms of higher orders [24]. The recoil correction to the bound-electron \( g_j \) factor incorporates the recoil effect of first order in \( m/M \), calculated to all orders in \( \alpha Z \) in [25,26], and the existing \( \alpha Z \)-expansion terms of orders \( (m/M)^2 \) and \( \alpha (m/M) \) [27]. The nuclear-size correction was evaluated for the homogeneously-charged-sphere model. The nuclear polarization contribution to the 1s \( g_j \) factor of light H-like ions can be neglected [28]. The \( g_j \) factor values given in Table 2 are used for calculations of the coefficients in the Breit – Rabi formula, presented in Tables 3 and 4.

In Table 3, the numerical results for the coefficients in Eqs. (2), (13), (19), and (53) are listed for some isotopes with \( I \neq 1/2 \) in the interval \( Z = 1 - 20 \). The numerical values of the coefficients in Eqs. (3), (10), (33), and (55) for \( ^{13}\text{C}^+ (I = 1/2) \) are presented in Table 4. Since in all the cases under consideration the absolute value of the recoil correction to the bound-nucleus \( g_I \) factor is smaller than \( 10^{-11} \) [27], we actually have in Eq. (3): \( g'_I = \frac{m_e}{m_p} g_I \).

5 Discussion

The energy separation between the ground-state HFS components (\( F = I - 1/2 \) and \( F' = I + 1/2 \)) of a hydrogen-like ion can be written as [29]
\[ \Delta E_{\text{HFS}}^{(1s)} = \frac{4}{3} \alpha(\alpha Z)^3 \frac{\mu}{\mu_N} \frac{m_e}{m_p} \frac{2I + 1}{2I} m_e c^2 [A^{(1s)}(\alpha Z)(1 - \delta^{(1s)}(1 - \epsilon^{(1s)})) + x^{(1s)}_{\text{rad}}], \] (61)

where
\[ A^{(1s)}(\alpha Z) = \frac{1}{\gamma(2\gamma - 1)} = 1 + \frac{3}{2}(\alpha Z)^2 + \frac{17}{8}(\alpha Z)^4 + ... \] (62)
is the relativistic factor, $\delta^{(1s)}$ is the nuclear charge distribution correction, $\epsilon^{(1s)}$ is the nuclear magnetization distribution correction (the Bohr–Weisskopf effect), and $x^{(1s)}_{\text{rad}}$ is the QED correction. Therefore, the dimensionless variable $x = \mu_0 B/\Delta E^{(1s)}_{\text{HFS}}$ is of order of $x_0 \equiv \mu_0 B/[(\alpha Z)^3 m_e c^2]$. Table 5 shows the value $x_0$ for various $B$ and $Z$. The intervals of $B$ and $Z$, for which $x \sim 1$, are of special interest (in the original paper [7] the fields with $0.1 \leq x \leq 3$ were considered to be intermediate).

For the magnetic fields with the magnitude $B \sim 1 - 10 T$, that are generally used in this kind of experiments, H-like ions with $Z = 1 - 20$ meet the requirement $x \sim 1$. For this reason, only such ions are presented in Tables 2–4.

For ions with $Z \leq 20$, the electrical quadrupole corrections to the coefficients $a_1$, $c_1$, $c_2$, and $d_1$ are either by a factor $10^{-3} - 10^{-4}$ less than the magnetic dipole ones or equal to zero, if $I = 1/2$.

As one can see from Tables 3 and 4, the corrections $\epsilon_1$, $\delta_1$, $\delta_2$, $\delta_3$, and $\eta_1$ provide more precise determinations of the coefficients in the Breit–Rabi formula.

In the second-order approximation $\Delta E^{(1s)}_{\text{HFS}}$, formulas (2), (11), (49), and (58) do not contain $B$ to a power higher than two under the square root (because of $h_2(F) = h_2(F')$). For $B = 1 - 10 T$, an estimate of the terms of higher orders with respect to $B$ indicates that the contributions from these terms are negligibly small as compared with both magnetic dipole and electrical quadrupole corrections. However, it is very important to take into account $\epsilon_2 B^2$ and $\eta_2 B^2$ if $Z = 1 - 20$. This is due to the fact that these terms are comparable with the ones appearing from the corrections to the Breit–Rabi formula coefficients and the less $Z$ is, the more appreciable the contributions from $\epsilon_2 B^2$ and $\eta_2 B^2$ become.

The Breit–Rabi formula for the 1s state contains $\Delta E^{(1s)}_{\text{HFS}}$, and the coefficients in the formula and the corrections to them calculated above include the value of $\mu/\mu_N$. Therefore, one can determine both $\Delta E^{(1s)}_{\text{HFS}}$ and $\mu/\mu_N$ when carrying out the experiments on the Zeeman splitting.

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Table 1: The numerical results for the functions $u_1(\alpha Z)$, $u_2(\alpha Z)$, $U(\alpha Z)$, $S(\alpha Z)$, and $T(\alpha Z)$ (for the ions with $I \neq 1/2$) defined by Eqs. (35), (37), (35), (40), and (43), accordingly. $u_{\text{point}}$, $S_{\text{point}}$, and $T_{\text{point}}$ are the point-charge-nucleus values obtained by formulas (48), (46), and (47), correspondingly. $u_{\text{ext}}$, $u_{\text{ext}}^2$, $U_{\text{ext}}$, $S_{\text{ext}}$, and $T_{\text{ext}}$ are the extended-charge-nucleus values. The values of $\langle r^2 \rangle_{1/2}$ are taken from Ref. [16].

| Ion       | $^1\text{H}$ | $^{13}\text{C}^{5+}$ | $^{17}\text{O}^{7+}$ | $^{33}\text{S}^{15+}$ | $^{43}\text{Ca}^{19+}$ | $^{55}\text{Cr}^{25+}$ | $^{73}\text{Ge}^{31+}$ |
|-----------|---------------|------------------------|-----------------------|------------------------|------------------------|------------------------|------------------------|
| $Z$       | 1             | 6                      | 8                     | 16                     | 20                     | 24                     | 32                     |
| $\langle r^2 \rangle_{1/2}$, fm | 0.879         | 2.461                  | 2.695                 | 3.251                  | 3.493                  | 3.659                  | 4.063                  |
| $u_{\text{point}}$ | 28165.9       | 780.079                | 437.756               | 107.663                | 68.0544                | 46.5408                | 25.1555                |
| $u_{\text{ext}}^1$ | 28167.0       | 781.203                | 438.880               | 108.783                | 69.1720                | 47.6550                | 26.2610                |
| $U_{\text{ext}}$ | 0.999929      | 0.997445               | 0.995459              | 0.981862               | 0.971691               | 0.959291               | 0.927886               |
| $S_{\text{point}}$ | 1.00014       | 1.00518                | 1.00922               | 1.03737(1)             | 1.05901                | 1.08609(1)             | 1.15830(3)             |
| $S_{\text{ext}}$ | 1.00014       | 1.00518                | 1.00922               | 1.03737(1)             | 1.05901                | 1.08609(1)             | 1.15830(3)             |
| $T_{\text{point}}$ | ———          | ———                   | 1.00446               | 1.01805                | 1.02846                | 1.04145                | 1.07586                |
| $T_{\text{ext}}$ | ———          | ———                   | 1.00357(2)            | 1.01577(4)             | 1.0253(1)              | 1.0373(1)              | 1.0687(1)              |

| Ion       | $^{129}\text{Xe}^{53+}$ | $^{131}\text{Xe}^{53+}$ | $^{207}\text{Pb}^{81+}$ | $^{209}\text{Bi}^{82+}$ | $^{235}\text{U}^{91+}$ |
|-----------|------------------------|------------------------|------------------------|------------------------|------------------------|
| $Z$       | 54                     | 54                     | 82                     | 83                     | 92                     |
| $\langle r^2 \rangle_{1/2}$, fm | 4.776       | 4.781                  | 5.494                  | 5.521                  | 5.829                  |
| $u_{\text{point}}^1$ | 7.35001       | 7.35001                | 1.97162                | 1.87551                | 1.15612                |
| $u_{\text{ext}}^1$ | 7.35130(1)       | 7.35130(1)             | 1.97598(1)             | 1.88008(1)             | 1.16343(1)             |
| $u_{\text{ext}}^2$ | 8.41758       | 8.41758                | 2.95636(1)             | 2.85645(1)             | 2.09992(2)             |
| $U_{\text{ext}}$ | 0.797806(1)   | 0.797806(1)            | 0.549690(2)            | 0.539399(2)            | 0.443386(4)            |
| $S_{\text{point}}$ | 1.54221       | 1.54221                | 2.99051                | 3.09142                | 4.37922                |
| $S_{\text{ext}}$ | 1.5249(2)       | 1.5249(2)              | 2.7193(14)             | 2.7907(16)             | 3.583(3)               |
| $T_{\text{point}}$ | ———          | ———                   | 1.24668                | 1.82424                | 2.20685                |
| $T_{\text{ext}}$ | ———          | ———                   | 1.2216(2)              | 1.6803(7)              | 1.933(1)               |

Table 2: The individual contributions to the 1s-electron $g_j$ factor of hydrogenlike ions with nonzero nuclear spin and the nuclear charge in the range $Z = 1 – 20$. The values of $\langle r^2 \rangle_{1/2}$ are the same as in Table 1.

| Ion       | $^{13}\text{C}^{5+}$ | $^{17}\text{O}^{7+}$ | $^{33}\text{S}^{15+}$ | $^{43}\text{Ca}^{19+}$ |
|-----------|------------------------|-----------------------|------------------------|------------------------|
| $g_D$     | 1.99872135439(1)       | 1.99776000306(2)      | 1.9908058242(6)        | 1.9857232037(1)        |
| $\Delta g_{QED}$ | 0.00232014777(3)       | 0.00232089878(11)     | 0.0023273918(32)       | 0.0023333328(100)      |
| $\Delta g_{\text{rec}}$ | 0.00000008087           | 0.00000011001         | 0.00000022876          | 0.00000012761          |
| $\Delta g_{\text{NS}}$ | 0.00000000040           | 0.00000000155(1)      | 0.0000000386(12)       | 0.0000001141(1)        |
| $g_j$     | 2.00104158344(3)       | 2.0004701337(11)      | 1.993208242(3)         | 1.988056927(10)        |
Table 3: The numerical values of the coefficients in Eqs. (2), (9), (49), and (55) for H-like ions with $I \neq 1/2$ and $Z = 1 - 20$. The values of $\mu/\mu_N$ and $Q$ are taken from Refs. [30] and [31], respectively.

| Ion           | $^{17}\text{O}^{7+}$ | $^{33}\text{S}^{15+}$ | $^{43}\text{Ca}^{19+}$ |
|---------------|----------------------|-----------------------|------------------------|
| $I$           | 5/2                  | 3/2                   | 7/2                    |
| $\mu/\mu_N$  | -1.89379(9)          | 0.6438212(14)         | -1.317643(7)           |
| $Q$, barn     | -0.02558(22)         | -0.0678(13)           | -0.0408(8)             |
| $\alpha_1$   | 0.00041256(2)        | -0.0002337573(5)      | 0.000205032(1)         |
| $\epsilon_1$ | -0.0001433           | -0.0002947            | -0.0003759             |
| $\alpha_1(1 + \epsilon_1)$ | 0.00041250(2) | -0.0002336884(5)      | 0.000204955(1)         |
| $\epsilon_2(=\eta_2)$ | 292.087         | 72.0242               | 45.6181                |
| $c_1$         | 1.99963441(2)        | 1.993442046(4)        | 1.98785187(2)          |
| $\delta_1$   | 0.00000002957        | -0.00000003461        | 0.00000003874          |
| $c_1(1 + \delta_1)$ | 1.99963447(2) | 1.993441977(4)        | 1.98785194(2)          |
| $c_2$         | 3.98853778(8)        | 3.97381119(2)         | 3.95155504(6)          |
| $\delta_2$   | 0.00000005914        | -0.00000006905        | 0.00000007759          |
| $\delta_3$   | 0.0                  | -0.00000000004        | -0.00000000001         |
| $c_2(1 + \delta_2)$ | 3.98853802(8) | 3.97381092(2)         | 3.95155535(6)          |
| $c_2\delta_3$ | 0.0                  | -0.00000000017        | -0.00000000003         |
| $d_1$         | 1.00105487(5)        | 0.996253509(3)        | 0.99474606(1)          |
| $\eta_1$     | -0.0000001477        | 0.0000001037          | -0.0000002712          |
| $d_1(1 + \eta_1)$ | 1.00105473(5) | 0.996253612(3)        | 0.99474579(1)          |

Table 4: The numerical values of the coefficients in Eqs. (11) and (58) for $^{13}\text{C}^{5+}$ ($I = 1/2$). $\mu/\mu_N$ is taken from [30].

| Ion        | $^{13}\text{C}^{5+}$ |
|------------|----------------------|
| $\mu/\mu_N$ | 0.7024118(14)       |
| $\epsilon_2(=\eta_2)$ | 520.302             |
| $c_2$      | 4.007230231(6)      |
| $\delta_2$ | -0.00000008183      |
| $c_2(1 + \delta_2)$ | 4.007229903(6)     |
| $d_1$      | 1.0001382800(8)     |
| $\eta_1$  | 0.00000004095       |
| $d_1(1 + \eta_1)$ | 1.0001383209(8)    |
Table 5: The values $x_0 = \mu_0 B/[(\alpha \alpha Z)^3 m_e m_e c^2]$ for various $B$ and $Z$.

| $B, T$ | $Z = 1$ | 3 | 7 | 15 | 20 | 30 | 80 |
|--------|--------|---|---|----|----|----|----|
| 0.5    | 3.7 · 10 | 7.3 · 10 | 3.7 · 10² | 7.3 · 10² | 3.7 · 10³ | 7.3 · 10³ |
| 1      | 5.7 · 10⁻¹ | 1.1 | 5.7 | 1.1 · 10 | 1.1 · 10 | 1.1 · 10² |
| 10     | 1.1 · 10⁻⁴ | 2.1 · 10⁻¹ | 1.1 | 2.1 | 1.1 · 10 | 2.1 · 10 |
| 50     | 1.1 · 10⁻³ | 2.2 · 10⁻² | 1.1 · 10⁻¹ | 2.2 · 10⁻¹ | 1.1 | 2.2 |
| 100    | 4.6 · 10⁻⁵ | 9.2 · 10⁻³ | 4.6 · 10⁻² | 9.2 · 10⁻² | 4.6 · 10⁻¹ | 9.2 · 10⁻¹ |
| 60     | 1.4 · 10⁻³ | 2.7 · 10⁻³ | 1.4 · 10⁻² | 2.7 · 10⁻² | 1.4 · 10⁻¹ | 2.7 · 10⁻¹ |
| 80     | 7.2 · 10⁻⁹ | 1.4 · 10⁻⁴ | 7.2 · 10⁻⁴ | 1.4 · 10⁻³ | 7.2 · 10⁻³ | 1.4 · 10⁻² |