Radiative and interelectronic-interaction corrections to the hyperfine splitting in highly charged B-like ions

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Abstract

The ground-state hyperfine splitting values of high-$Z$ boronlike ions are calculated. Calculation of the interelectronic-interaction contribution is based on a combination of the $1/Z$ perturbation theory and the large-scale configuration-interaction Dirac-Fock-Sturm method. The screened QED corrections are evaluated utilizing an effective screening potential approach. Total hyperfine splitting energies are presented for several B-like ions of particular interest: $^{45}$Sc$^{16+}$, $^{57}$Fe$^{21+}$, $^{207}$Pb$^{77+}$, and $^{209}$Bi$^{78+}$. For lead and bismuth the experimental values of the $1s$ hyperfine splitting are employed to improve significantly the theoretical results by reducing the uncertainty due to the nuclear effects.

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I. INTRODUCTION

First accurate calculations [1, 2] of the hyperfine splitting in highly charged ions were stimulated by astronomical search in hot astrophysical plasma [3]. Later, high-precision measurements of the ground-state hyperfine splitting in heavy H-like ions were performed [4, 5, 6, 7, 8]. The main goal of such experiments was to probe quantum electrodynamics (QED) in the strong Coulomb field induced by a heavy nucleus. However, accurate theoretical calculations (see Ref. [9] and references therein) showed that the uncertainty of the theoretical results, which mainly originates from the nuclear magnetization distribution correction (the Bohr-Weisskopf effect), is comparable with the QED correction. For this reason, any identification of QED effects on the hyperfine splitting in heavy H-like ions turned out to be unfeasible. It was shown, however, that this uncertainty can be significantly reduced in a specific difference of the hyperfine splitting values of H- and Li-like ions with the same nucleus [10]. High-precision measurements of the hyperfine splitting in heavy Li-like ions are presently in preparation [11].

The motivation for accurate calculations of the hyperfine splitting in B-like ions is twofold. From one side, high-precision prediction of the hyperfine splitting of B-like Fe may be important for astronomical search [12]. From the other side, the study of the hyperfine splitting in heavy B-like ions can be used to reduce the uncertainty associated with the Bohr-Weisskopf effect in some specific difference of the hyperfine splitting values for B- and Li-like ions or B- and H-like ions. The origin of this reduction is essentially the same as for the related $g$-factor values [13] and can be easily seen from the approximate analytical expressions for the Bohr-Weisskopf correction given in Refs. [14, 15].

In this article we calculate the ground-state hyperfine splitting of B-like ions. The interelectronic-interaction correction of the first order in $1/Z$ is evaluated within the rigorous QED approach. The higher-order terms are calculated within the large-scale configuration-interaction Dirac-Fock-Sturm method. QED corrections are calculated using an effective potential approach in order to account for the effect of screening. The experimental values of the $1s$ hyperfine splitting in H-like $^{207}\text{Pb}^{81+}$ and $^{209}\text{Bi}^{82+}$ are employed to evaluate the Bohr-Weisskopf correction for the corresponding B-like ions. Due to the correlation between the values of this correction for $1s$ and $2p_{1/2}$ states mentioned above, the uncertainties of the theoretical values caused by the nuclear effects are strongly reduced.

Relativistic units ($\hbar = c = 1$) and the Heaviside charge unit ($\alpha = e^2/(4\pi)$, $e < 0$) are used.
II. BASIC FORMULAS AND CALCULATIONS

Within the point-dipole approximation, the hyperfine interaction is described by the Fermi-Breit operator

$$H_\mu = \frac{|e|}{4\pi} \frac{(\alpha \cdot [\mu \times r])}{r^3},$$

(1)

where the vector $\alpha$ incorporates the Dirac matrices and $\mu$ is the nuclear magnetic moment operator. The ground-state hyperfine splitting of a B-like ion can be written in the following form [15, 16]

$$\Delta E_\mu = \alpha (\alpha Z)^3 \frac{m \mu}{m_p \mu_N} \frac{2I + 1}{2I} mc^2 \times \left[A_\mu(\alpha Z)(1 - \delta)(1 - \varepsilon) + \frac{1}{Z} B_\mu(\alpha Z) + \frac{1}{Z^2} C_\mu(Z, \alpha Z) + x_{\text{rad}}\right],$$

(2)

where $m$ is the electron mass, $m_p$ is the proton mass, $\mu_N$ is the nuclear magneton, and $I$ is the nuclear spin. $A_\mu(\alpha Z)$ is the one-electron relativistic factor

$$A_\mu(\alpha Z) = \frac{6[2(1 + \gamma) - \sqrt{2(1 + \gamma)}]}{(1 + \gamma)^2 \gamma(4\gamma^2 - 1)},$$

(3)

where $\gamma = \sqrt{1 - (\alpha Z)^2}$, $\delta$ is the nuclear-charge-distribution correction, and $\varepsilon$ is the one-electron nuclear-magnetization-distribution correction (the Bohr-Weisskopf effect). The terms $B_\mu(\alpha Z)/Z$ and $C_\mu(Z, \alpha Z)/Z^2$ determine the interelectronic-interaction correction to the first and higher orders in $1/Z$, respectively. The $x_{\text{rad}}$ term stands for the QED correction.

Finite-nuclear-size correction $\delta$ can be calculated both analytically [14, 17] and numerically. In the present work, it is obtained numerically by solving the Dirac equation with the Fermi model for the nuclear charge distribution. The Bohr-Weisskopf correction $\varepsilon$ is calculated within the single-particle model as described in Refs. [1, 2, 18]. Apart from this direct evaluation, at the end of this section we also derive the $\varepsilon$ values for $^{207}\text{Pb}^{77+}$ and $^{209}\text{Bi}^{78+}$ using the experimental results for the $1s$ hyperfine splitting. The nuclear root-mean-square radii are taken from Ref. [19] and the nuclear magnetic moments are taken from Ref. [20].

The QED correction to the hyperfine splitting of the first order in $\alpha$ consists of two parts, self-energy correction and vacuum-polarization correction. The self-energy correction (Fig. II) is the sum of irreducible, reducible, and vertex parts,

$$\Delta E_{\text{SE}} = \sum_{M_1M'_{1m'}} \sum_{M_2M'_{2m'}} C^{FM}_1M_1jM_1j' C^{FM}_2M_2jM_2j' \chi_{IM_1}^+(M_{\text{irr}} + M_{\text{red}} + M_{\text{ver}}) \chi_{IM_2},$$

(4)
where \( C_{I M_{1} j m}^{F M} \) are the Clebsch-Gordan coefficients and \( \chi_{I M_{1}} \) is the nuclear wave function. The irreducible part is given by the expression

\[
M_{\text{irr}} = \sum_n \frac{\varepsilon_n \neq \varepsilon_a}{\varepsilon_a - \varepsilon_n} \langle a' | \left( \Sigma(\varepsilon_a) - \gamma^0 \delta m \right) | n \rangle \langle n | H_\mu | a \rangle.
\]

Here \(|a\rangle\) and \(|a'\rangle\) are the states of the valence electron with angular momentum projections \(m\) and \(m'\), respectively, \(\varepsilon_n\) is the energy of the state \(|n\rangle\) in the binding potential under consideration, \(H_\mu\) is the magnetic-dipole hyperfine-interaction operator, and \(\delta m\) is the mass counterterm. \(\Sigma(\varepsilon)\) denotes the unrenormalized self-energy operator defined as

\[
\langle a | \Sigma(\varepsilon) | b \rangle = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \sum_n \frac{\langle an | I(\omega) | nb \rangle}{\varepsilon - \omega - \varepsilon_n (1 - i0)}.
\]
where \( I(\omega, x_1, x_2) = e^2 \alpha^\mu \alpha^\nu D_{\mu\nu}(\omega, x_1 - x_2) \) with the Dirac matrices \( \alpha^\mu = (1, \alpha) \), and the photon propagator \( D_{\mu\nu} \). To separate the ultraviolet divergencies, the expression (5) is decomposed into zero-, one-, and many-potential terms. The zero-potential \( M^{(0)} \) and one-potential \( M^{(1)} \) terms are calculated in momentum space using the formulas from Ref. [21]. The residual part of \( M \), the so-called many-potential term \( M^{(2+)} \), is calculated in coordinate space. The expressions for the reducible and the vertex parts read

\[
M_{\text{red}} = \langle a'|H_\mu|a \rangle \langle a| \frac{1}{d\varepsilon} \Sigma(\varepsilon) |\varepsilon = \varepsilon_a \rangle |a \rangle, \tag{7}
\]

\[
M_{\text{ver}} = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \sum_{n_1, n_2} \frac{\langle a'| I(\omega) |n_1 a \rangle \langle n_1 | H_\mu | n_2 \rangle}{(\varepsilon_a - \omega - \varepsilon_{n_1}(1 - i0))(\varepsilon_a - \omega - \varepsilon_{n_2}(1 - i0))}. \tag{8}
\]

Both reducible and vertex parts are ultraviolet-divergent, whereas the sum \( M_v = M_{\text{red}} + M_{\text{ver}} \) is finite. Following Refs. [22, 23, 24, 25], we separate out zero-potential term \( M^{(0)} \) and evaluate it in momentum space. The remaining many-potential term \( M^{(1+)} \) is calculated in coordinate space as a point-by-point difference between the contributions with bound and free propagators in the self-energy loop.

The angular integration and the summation over intermediate angular projections in the many-potential terms \( M^{(2+)} \) and \( M^{(1+)} \) are carried out in a standard manner. The many-potential terms involve infinite summation over relativistic angular quantum number \( \kappa = \pm (j + 1/2) \). The summation is terminated at a maximum value \(|\kappa| = 10\), while the residual part of the sum is evaluated by the least-square inverse-polynomial fitting. For any given \( \kappa \) the summation over the Dirac spectrum is performed utilizing the dual-kinetic-balance (DKB) approach [26] involving basis functions constructed from B-splines. The finite distributions of the nuclear charge and the nuclear magnetic moment are taken into account.

The electric-loop part of the vacuum-polarization correction (parts (a) and (b) of Fig. 2) is evaluated within an effective screening potential employing the DKB method. Explicit formulas for the Uehling potential can be found, e.g., in Refs. [9, 27]. For the evaluation of the electric-loop Wichmann-Kroll potential we consult the approximate formulas derived in Ref. [28]. The magnetic-loop part (diagram in Fig. 2 (c)) in the Uehling approximation was considered in Ref. [29]. We evaluate this term in the presence of an effective screening potential with account for the finite distribution of the nuclear charge and the nuclear magnetic moment. The value of the magnetic-loop Wichmann-Kroll part is estimated to be rather small. It was obtained by analyzing its relative contribution for \( s \) states [30, 31]. However, in Table III we include its estimation to the total QED term for the case of \( ^{207}\text{Pb}^{77+} \) and \( ^{209}\text{Bi}^{78+} \) ions.
In the present work, the QED corrections are evaluated based on four different spherically symmetric binding potentials $V_{\text{eff}}(r)$ which account for the interelectronic interaction between the valence $2p_{1/2}$ electron and the core electrons of the closed $(1s)^2(2s)^2$ shells. The simplest choice of $V_{\text{eff}}$ is the core-Hartree (CH) potential

$$V_{\text{eff}}(r) = V_{\text{nuc}}(r) + \alpha \int_0^\infty dr' \frac{1}{r'} \rho_c(r'),$$

where $V_{\text{nuc}}$ is the nuclear potential and $\rho_c$ is the density of the core electrons. The screening potential derived from the density-functional theory reads

$$V_{\text{eff}}(r) = V_{\text{nuc}}(r) + \alpha \int_0^\infty dr' \frac{1}{r'} \rho_t(r') - x_a \frac{\alpha}{32\pi^2} r \rho_t(r) \left( \frac{81}{32\pi^2} r \rho_t(r) \right)^{1/3}.$$ 

Here $\rho_t$ is the total electron density, including $(1s)^2(2s)^2$ shells and $2p_{1/2}$ electron. The parameter $x_a$ is varied from 0 to 1. The cases of $x_a = 0$, $2/3$, and 1 correspond to the Dirac-Hartree (DH), the Kohn-Sham (KS), and the Dirac-Slater (DS) potentials, respectively. At large $r$ expression (10) should be replaced by

$$V_{\text{eff}}(r) = -\frac{\alpha(Z - 4)}{r}$$

(11)

to provide the proper asymptotic behavior. The self-consistent potential is generated by iterations.

The results obtained for the QED correction for the pure nuclear potential and the screening potentials are presented in Table I. The first column corresponds to the values of the QED correction for the nuclear potential $V_{\text{nuc}}$. The second column gives the values of the screened QED correction for the core-Hartree potential (9), the other columns present the values of the screened QED correction for the Dirac-Hartree potential (eq. (10), $x_a = 0$), the Kohn-Sham potential (eq. (10), $x_a = 2/3$), and the Dirac-Slater potential (eq. (10), $x_a = 1$), respectively. The results for the pure nuclear potential agree with those presented in Ref. [32].

In the calculations performed the effect of screening on QED correction is taken into account only in the local effective potential approximation. We estimate that for the $p_{1/2}$ valence state the uncertainty due to this approximation amounts to about 50% for $Z = 15$ and decreases rapidly as $Z$ increases. Evaluation of the screened QED correction within the rigorous QED approach is presently underway.

The interelectronic-interaction correction of the first order in $1/Z$ defined by the function $B_{\mu}(\alpha Z)$ can be calculated within the rigorous QED approach. Such calculations for the ground and first excited states of Li-like ions were performed in Refs. [16, 33, 34]. The formulas derived
Table I: The QED correction $x_{\text{rad}}$ for the pure nuclear potential $V_{\text{nuc}}$ and for the effective screening potentials (core-Hartree, Dirac-Hartree, Kohn-Sham and Dirac-Slater potentials, respectively).

| Z  | $V_{\text{nuc}}$ | CH   | DH   | KS   | DS   |
|----|----------------|------|------|------|------|
| 15 | 0.00047        | 0.00030 | 0.00027 | 0.00031 | 0.00033 |
| 21 | 0.00041        | 0.00032 | 0.00029 | 0.00032 | 0.00033 |
| 26 | 0.00035        | 0.00030 | 0.00028 | 0.00030 | 0.00032 |
| 37 | 0.00020        | 0.00020 | 0.00020 | 0.00020 | 0.00020 |
| 49 | −0.00005       | 0.00001 | 0.00002 | 0.00001 | −0.00000 |
| 57 | −0.00029       | −0.00018 | −0.00016 | −0.00019 | −0.00021 |
| 67 | −0.00073       | −0.00056 | −0.00053 | −0.00058 | −0.00060 |
| 75 | −0.0013        | −0.0010 | −0.0010 | −0.0011 | −0.0011 |
| 82 | −0.0020        | −0.0017 | −0.0017 | −0.0017 | −0.0019 |
| 83 | −0.0023        | −0.0018 | −0.0018 | −0.0019 | −0.0020 |

there can easily be adopted for B-like ions by regarding the closed (1s)$^2$ and (2s)$^2$ shells as belonging to the vacuum state [9]. The results of the numerical evaluation by these formulas are presented in Table II. The function $B_{\mu}^{(0)}(\alpha Z)$ indicates the values obtained for the point-nucleus case using the method of the generalized virial relations for the Dirac equation [35]. The function $B_{\mu}^{(\text{NS})}(\alpha Z)$ takes into account the nuclear charge distribution effect. Its numerical calculation is performed using the DKB approach. The function $B_{\mu}^{(\text{BW})}(\alpha Z)$ incorporates also the Bohr-Weisskopf effect.

The higher-order term $C_{\mu}(Z, \alpha Z)/Z^2$ is evaluated using the large-scale configuration-interaction Dirac-Fock-Sturm (CI-DFS) method [36, 37, 38]. The many-electron wave function $\Psi(\gamma J)$ with the total angular momentum $J$ and other quantum numbers $\gamma$ is expanded in terms of a large number of the configuration state functions (CSFs) with the same $J$,

$$\Psi(\gamma J) = \sum_{\alpha} c_\alpha \Phi_{\alpha}(J).$$

(12)

For each relativistic atomic configuration the CSFs $\Phi_{\alpha}(J)$ are eigenfunctions of $J^2$ and can be obtained as linear combinations of the Slater determinants corresponding to this configuration. The set of the CSFs in the expansion (12) was generated including all single, double and triple excitations. The Slater determinants are constructed from one-electron four-component Dirac spinors (orbitals). For the occupied shells these orbitals were obtained by the multiconfiguration
Table II: First-order interelectronic-interaction correction for the ground-state of B-like ions. $B^{(0)}_{\mu}(\alpha Z)$ and $B^{(NS)}_{\mu}(\alpha Z)$ correspond to the point and extended charge nucleus, respectively. $B^{(BW)}_{\mu}(\alpha Z)$ includes the BW correction.

| Z   | $B^{(0)}_{\mu}(\alpha Z)$ | $B^{(NS)}_{\mu}(\alpha Z)$ | $B^{(BW)}_{\mu}(\alpha Z)$ |
|-----|---------------------------|-----------------------------|----------------------------|
| 15  | −5.90979                  | −5.9097                     | −5.9097                    |
| 21  | −6.11189                  | −6.1117                     | −6.1116                    |
| 26  | −6.34230                  | −6.3417                     | −6.3413                    |
| 37  | −7.09270                  | −7.090                      | −7.090                     |
| 49  | −8.44727                  | −8.434                      | −8.431                     |
| 57  | −9.83459                  | −9.801                      | −9.798                     |
| 67  | −12.4859                  | −12.37                      | −12.35                     |
| 75  | −15.8639                  | −15.56                      | −15.51                     |
| 82  | −20.4837                  | −19.75                      | −19.51                     |
| 83  | −21.3367                  | −20.49                      | −20.42                     |

Dirac-Fock method.

The CI-DFS method allows us to calculate the interelectronic-interaction correction to all orders in $1/Z$ within the Breit approximation, whereas the $B_{\mu}(\alpha Z)/Z$ term is obtained within the rigorous QED approach as described above. In order to combine these approaches, we subtract the value of the $1/Z$ term calculated within the Breit approximation from the CI-DFS result. In this way we obtain the $C_{\mu}(Z, \alpha Z)/Z^2$ contribution.

Table III presents the individual contributions and the total theoretical results for the ground-state hyperfine splitting in B-like ions of particular interest. It can be seen that for heavy ions the uncertainties of the total theoretical values are completely determined by the Bohr-Weisskopf effect. These uncertainties can be strongly reduced employing the experimental values for the hyperfine splitting in the corresponding H-like ions. Following the works [10, 15] we use the experimental values for the ground state hyperfine splitting, $\Delta E^{(1s)}_{\text{exp}} = 1.2159(2)$ eV for H-like $^{207}\text{Pb}^{81+}$ [7] and $\Delta E^{(1s)}_{\text{exp}} = 5.0840(8)$ eV for H-like $^{209}\text{Bi}^{82+}$ [4], to extract the Bohr-Weisskopf corrections for the $1s$ state employing the theoretical values for all other contributions from Ref. [9]. Considering different models for the nuclear magnetization distribution, we have found that
Table III: Individual contributions to the ground-state hyperfine splitting of B-like ions, in meV. The total error bars indicated do not include the nuclear magnetic moment uncertainties [20].

| Effect                          | \(^{45}\text{Sc}^{16+}\) | \(^{57}\text{Fe}^{21+}\) | \(^{207}\text{Pb}^{77+}\) | \(^{209}\text{Bi}^{78+}\) |
|---------------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
|                                 | \(\frac{\mu}{\mu_N} = 4.7565\) | \(\frac{\mu}{\mu_N} = 0.000623\) | \(\frac{\mu}{\mu_N} = 0.59258\) | \(\frac{\mu}{\mu_N} = 4.1106\) |
| Dirac value                     | 2.3126                    | 0.15010                   | 71.89                     | 296.35                    |
| Finite nuclear size             | -0.0001                   | -0.00001                  | -2.18(1)                  | -9.84(5)                  |
| Bohr-Weisskopf (direct calculation) | 0.0000                   | -0.00001                  | -0.84(8)                  | -0.97(34)                 |
| Interelectronic interaction, \(1/Z\) | -0.6424                  | -0.03406                  | -6.82                     | -28.17                    |
| Interelectronic interaction, \(1/Z^2\) and higher orders | 0.0408(9) | 0.00182(3) | 0.24(1) | 0.98(3) |
| QED                             | 0.0007                    | 0.00004                   | -0.06(1)                  | -0.26(3)                  |
| Total                           | 1.7116(9)                 | 0.11788(3)                | 62.23(8)                  | 258.09(35)                |
| Bohr-Weisskopf (from the \(1s\) experiment) |                    |                          |                          |                          |
| Total                           |                            |                          | 62.24(2)                  | 257.84(5)                 |

The ratio of the Bohr-Weisskopf corrections is rather stable, \(\varepsilon_{\text{Pb}}^{(2p)}/\varepsilon_{\text{Pb}}^{(1s)} = 0.287(2)\) for Pb and \(\varepsilon_{\text{Bi}}^{(2p)}/\varepsilon_{\text{Bi}}^{(1s)} = 0.295(2)\) for Bi. It allows us to deduce the following values for B-like ions: \(\varepsilon_{\text{Pb}}^{(2p)} = 0.0119(2)\) and \(\varepsilon_{\text{Bi}}^{(2p)} = 0.00437(15)\). The corresponding contributions to the hyperfine splittings are \(-0.83(1)\) meV and \(-1.25(4)\) meV, respectively. The total theoretical values, which include also the modification of the Bohr-Weisskopf effect to the interelectronic-interaction correction, amount to \(62.24(2)\) meV for \(^{207}\text{Pb}^{77+}\) and \(257.84(5)\) meV for \(^{209}\text{Bi}^{78+}\). It should be stressed that the uncertainty of these values is not equal to the sum of the uncertainties of the individual contributions. This is due to the fact, that the total hyperfine splitting value found in this way is sufficiently stable with respect to possible variations of the nuclear charge radius and the magnetic moment [15].
III. CONCLUSION

In this paper we have calculated the ground-state hyperfine splitting of high-$Z$ boronlike ions. The interelectronic-interaction correction is evaluated utilizing the $1/Z$ perturbation theory and the large-scale configuration-interaction Dirac-Fock-Sturm method. The radiative corrections are calculated in the presence of an effective potential that partly accounts for the screening effect. It is shown that the Bohr-Weisskopf effect for heavy boronlike ions can be calculated with a high precision utilizing the experimental value for the ground-state hyperfine splitting in the corresponding hydrogenlike ions. As a result, the most accurate theoretical predictions for the hyperfine splitting values of B-like Sc, Fe, Pb, and Bi are obtained.

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