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Third-order Zeeman effect in highly charged ions

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ABSTRACT

The contribution of the third order in magnetic field to the Zeeman splitting of the ground state of hydrogenlike, lithiumlike, and boronlike ions in the range $Z = 6 - 82$ is investigated within the relativistic approach. Both perturbative and non-perturbative methods of calculation are employed and found to be in agreement. For lithiumlike and boronlike ions the interelectronic-interaction effects are taken into account within the approximation of the local screening potential. The contribution of the third-order effect in low- and medium-*Z* boronlike ions is found to be important for anticipated high-precision measurements.

1. Introduction

Recent experimental and theoretical studies of the bound-electron *g* factor in hydrogenlike and lithiumlike ions provided the most accurate up-to-date determination of the electron mass [1], the most stringent up-to-date test of the many-electron QED effects in the presence of magnetic field [2] and the first probe of the relativistic nuclear recoil effect in magnetic field [3]. The experimental precision have reached the level of 10^{-9}–10^{-11} [4–8,3]. Bound-state QED calculations have been accomplished for the one-photon and for some part of the two-photon diagrams (see e.g. Refs. [9,10] and references therein). Future high-precision investigations for hydrogenlike, lithiumlike and boronlike ions can lead to independent determination of the fine structure constant [11–13].

Spectroscopic measurement of the fine-structure transition in boronlike argon at MPI-K [14] was accurate enough to resolve the Zeeman sub-levels and to determine the *g* factors of the $2p_{1/2}$ and $2p_{3/2}$ states with an accuracy of 10^{-2} and 10^{-3}, respectively. The laser-microwave double-resonance spectroscopy will be implemented within the framework of the ARTEMIS experiment at GSI to provide the measurement of the Zeeman splitting of both ground and first excited states in boronlike argon with an accuracy at the ppb level [15]. First estimations of the non-linear effects in magnetic field show their importance in this case [15,16]. This is due to the mixing of the closely spaced $2p_j$ levels by the magnetic-field interaction. The second-order effect shifts equally the levels with the opposite sign of the total angular momentum projection M_j. Therefore, it affects only the Zeeman splitting of the $2p_{3/2}$ state and the $2p_{1/2}$–$2p_{3/2}$ optical transitions. The third-order effect is odd in M_j, and it affects the Zeeman splittings of both $2p_j$ states. It mimics a contribution of 3×10^{-9} to the *g* factor of the $2p_{1/2}$ state and a contribution of -3×10^{-9} to the *g* factor of the $2p_{3/2}$ state, assuming the magnetic field of 7 Tesla. Third-order Zeeman effect is present also in hydrogenlike and lithiumlike ions, however, there is no significant level mixing, and the contribution is much smaller.

In the present paper, we evaluate the third-order Zeeman effect for $1s$, $2s$, and $2p_{1/2}$ states. The case of the $2p_{3/2}$ state is more complicated and is presently under investigation. The many-electron effects in lithiumlike and boronlike ions are taken into account approximately with the use of the effective screening potential. In order to facilitate the treatment of the higher-order terms we employ the recursive scheme of the perturbation theory. We also

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perform an independent calculation by the numerical solution of the Dirac equation in the presence of magnetic field based on the dual-kinetic-balance approach [17]. The results in terms of the g-factor correction due to the third-order effect are presented for several hydrogenlike, lithiumlike and boronlike ions in the range $Z = 6 - 82$.

We use the relativistic units ($\hbar = 1, m_e = 1, c = 1$) and the Heaviside charge unit ($\alpha = e^2/(4\pi), e < 0$) throughout the paper.

2. Methods and results

The ground state of hydrogenlike, lithiumlike, or boronlike ion is described below as the valence bound electron in the $1s, 2s$, or $2p_{1/2}$ state, respectively. The many-electron effects are taken into account approximately via the effective screening potential $V_{\rm scr}(r)$ in the Dirac equation for the valence electron,

$$[\vec{\alpha}\cdot\vec{p} + \beta + V_{\rm nuc}(r) + V_{\rm scr}(r)]|a\rangle = \varepsilon_a|a\rangle, \tag{1}$$

where $\vec{\alpha}$ and β are the Dirac matrices, $V_{\rm nuc}(r)$ is the nuclear potential. We consider the screening potentials of two types: the core-Hartree potential and the Kohn-Sham potential derived from the local density approximation (see e.g. [18]). The effective potentials and the corresponding solutions of the Dirac equation are generated self-consistently within the dual-kinetic-balance approach [19].

The interaction with the external homogeneous magnetic field $\vec{B}$ directed along the z axis is represented by the operator,

$$V_{\rm m} = \lambda U, \qquad \lambda = \mu_{\rm B} B, \qquad U = [\vec{r}\times\vec{\alpha}]_z, \tag{2}$$

where $\mu_{\rm B} = |e|/2m_e$ is the Bohr magneton, the parameter λ and the B-independent operator U are introduced for convenience. We assume that $\lambda = (\mu_{\rm B}B)/(m_e c^2)$ in arbitrary units to ensure that it is dimensionless. The energy $\tilde{\varepsilon}_a$ and the wave function $|\tilde{a}\rangle$ in the presence of external magnetic field are found from the Dirac equation,

$$[\vec{\alpha}\cdot\vec{p} + \beta + V_{\rm nuc}(r) + V_{\rm scr}(r) + V_{\rm m}]|\tilde{a}\rangle = \tilde{\varepsilon}_a|\tilde{a}\rangle. \tag{3}$$

Perturbation theory yields for $\tilde{\varepsilon}_a$:

$$\tilde{\varepsilon}_a = \varepsilon_a + \Delta\varepsilon_a^{(1)} + \Delta\varepsilon_a^{(2)} + \Delta\varepsilon_a^{(3)} + \cdots \tag{4}$$

The first-order energy shift $\Delta\varepsilon_a^{(1)}$ is related to the g factor,

$$\Delta\varepsilon_a^{(1)} = \lambda g M_j, \tag{5}$$

$$g = \frac{1}{M_j}\langle a|U|a\rangle, \tag{6}$$

where M_j is the z projection of the total angular momentum $j = 1/2$. Various corrections to the Dirac g-factor value (6) due to the interelectronic-interaction, QED and nuclear effects were considered in numerous publications. We only refer here to the recent reviews on the topic [9,10].

The second-order term $\Delta\varepsilon_a^{(2)}$ according to Eqs. (3) and (4) is given by,

$$\Delta\varepsilon_a^{(2)} = \lambda^2 g^{(2)}(M_j), \tag{7}$$

$$g^{(2)}(M_j) = \sum_n{}' \frac{\langle a|U|n\rangle\langle n|U|a\rangle}{\varepsilon_a - \varepsilon_n}. \tag{8}$$

The summation here runs over the complete Dirac spectrum, excluding the reference state $|a\rangle$. Due to the symmetry relation $g^{(2)}(-M_j) = g^{(2)}(M_j)$ this term does not alter the Zeeman splitting for the levels with $j = 1/2$. As a consequence, it is not observable in the ground-state g-factor measurements in hydrogenlike and lithiumlike ions. Its importance for boronlike ions is twofold. Firstly, it shifts differently the levels with $M_j = \pm 1/2$ and $M_j = \pm 3/2$ and hence can be observed for the $2p_{3/2}$ state, which is accessible with the laser-microwave double-resonance spectroscopy [15]. Secondly, it provides a small correction to the fine-structure transition. It is negligible at the present level of accuracy [20] but may become observable in future high-precision measurements. In connection with the ARTEMIS experiment, the second-order effect has been estimated for boronlike argon in Refs. [15,16]. Recently, we have calculated the leading-order correlation and QED corrections to find $g^{(2)}$ with the 2% accuracy [21].

In this paper, we focus our attention on the third-order contribution in magnetic field,

$$\Delta\varepsilon_a^{(3)} = \lambda^3 g^{(3)}(M_j). \tag{9}$$

The symmetry relation $g^{(3)}(-M_j) = -g^{(3)}(M_j)$ holds in this case, and therefore this term always alters the Zeeman splitting, whether in hydrogenlike, lithiumlike or boronlike ions. It can be represented also as a field-dependent correction to the g factor,

$$\delta g = \lambda^2 g^{(3)}(M_j)/M_j. \tag{10}$$

Due to the symmetry of $g^{(3)}(M_j)$ this correction doesn't depend on the sign of the projection M_j. We stress that strictly speaking δg is not a correction to the g factor, but only an effect observed in assumption that the energy shift is completely defined by Eq. (5). Still, it is a convenient quantity to estimate the importance of the third-order Zeeman effect, as it can be compared to the various g-factor contributions and to the theoretical or experimental accuracy. For this reason, we present the results for δg along with $g^{(3)}$.

According to the perturbation theory, the leading-order contribution to $g^{(3)}$ is given by,

$$g^{(3)}(M_j) = \sum_{n_1,n_2}{}' \frac{\langle a|U|n_1\rangle\langle n_1|U|n_2\rangle\langle n_2|U|a\rangle}{(\varepsilon_a - \varepsilon_{n_1})(\varepsilon_a - \varepsilon_{n_2})} - \sum_n{}' \frac{\langle a|U|n\rangle\langle n|U|a\rangle}{(\varepsilon_a - \varepsilon_n)^2}\langle a|U|a\rangle. \tag{11}$$

The summations here run over the complete Dirac spectrum, excluding the reference state $|a\rangle$. The terms with $|n_1\rangle = |n_2\rangle = |n\rangle = |2p_{3/2}\rangle$ yield the dominant contribution for the $2p_{1/2}$ state due to the small energy difference in the denominator. It makes $g^{(3)}$ for the $2p_{1/2}$ state much larger than for the $1s$ and $2s$ states. This expression can be computed employing the finite basis set constructed within the dual kinetic balance approach [19]. Eqs. (8) and (11) can be obtained also via the recursive system of equations, altogether with the corresponding wave-function corrections. Let the energy $\tilde{\varepsilon}_a$ and the wave function $|\tilde{a}\rangle$ be represented by the following perturbation-theory expansions,

$$\tilde{\varepsilon}_a = \sum_{k=0}^{\infty}\lambda^k\varepsilon_a^{(k)}, \tag{12}$$

$$|\tilde{a}\rangle = \sum_{k=0}^{\infty}\lambda^k|a^{(k)}\rangle = \sum_{k=0}^{\infty}\lambda^k\sum_n|n\rangle\langle n|a^{(k)}\rangle, \tag{13}$$

(according to Eq. (4), $\Delta\varepsilon_a^{(k)} = \lambda^k\varepsilon_a^{(k)}$). Given the values through the $(k-1)$th order, the energy corrections $\varepsilon_a^{(k)}$ and the coefficients $\langle n|a^{(k)}\rangle$ of the kth order can be found as,

$$\varepsilon_a^{(k)} = \sum_m\langle a|U|m\rangle\langle m|a^{(k-1)}\rangle - \sum_{j=1}^{k-1}\varepsilon_a^{(j)}\langle a|a^{(k-j)}\rangle, \tag{14}$$

$$\langle n|a^{(k)}\rangle\Big|_{n\neq a} = \frac{1}{\varepsilon_a - \varepsilon_n}\left[\sum_m\langle n|U|m\rangle\ \langle m|a^{(k-1)}\rangle - \sum_{j=1}^{k-1}\varepsilon_a^{(j)}\langle n|a^{(k-j)}\rangle\right], \tag{15}$$

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