Nuclear recoil correction to the $g$ factor of boron-like argon

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Abstract. The nuclear recoil effect to the $g$ factor of boron-like ions is investigated. The one-photon-exchange correction to the nuclear recoil effect is calculated in the non-relativistic approximation for the nuclear recoil operator and in the Breit approximation for the interelectronic-interaction operator. The screening potential is employed to estimate the higher-order contributions. The updated $g$-factor values are presented for the ground $^2P_{1/2}$ and first excited $^2P_{3/2}$ states of B-like argon $^{40}$Ar$^{13+}$, which are presently being measured by the ARTEMIS group at GSI.

1. Introduction

During the last 15 years, the $g$-factor measurements in low-$Z$ ions have reached an accuracy of $10^{-10}$ [1, 2, 3, 4, 5] and motivated corresponding theoretical investigations. In particular, the most accurate value of the electron mass was obtained in these studies [6]. The case of Li-like silicon manifests presently the most accurate verification of the many-electron QED effects in magnetic field [5, 7]. Experimental and theoretical investigations of the $g$ factor of heavy few-electron ions will provide stringent tests of bound-state QED in strong nuclear field. Moreover, they will serve for an independent determination of the fine structure constant, provided simultaneous investigations of H-like and B-like heavy ions of the same isotope will be performed [8, 9].

First measurement of the $g$ factor of a B-like highly charged ion sensitive to the QED effects was performed in Ref. [10]. The ARTEMIS project presently implemented at GSI will use the laser-microwave double-resonance spectroscopy to measure with ppb accuracy the Zeeman splittings of both ground state and first excited state in B-like argon $^{40}$Ar$^{13+}$. Corresponding theoretical predictions for the $g$ factor and the non-linear effects in magnetic field have been reported in Ref. [12]. In this contribution we report on the recent progress for the nuclear recoil effect evaluated with more rigorous consideration of the screening correction. Namely, the contribution of the one-photon-exchange diagrams for the nuclear recoil effect has been calculated in the non-relativistic approximation. Total results for the $g$ factor of $^2P_{1/2}$ and $^2P_{3/2}$
states of B-like argon presented here also include more accurate values of the interelectronic-interaction correction of the order 1/Z^2 and higher.

The relativistic units (ħ = m = c = 1) and the Heaviside charge unit (α = e^2/(4π), e < 0) are used in the paper. Electron-to-nucleus mass ratio is written as m/M for clarity.

2. Nuclear recoil effect
The theory of the nuclear recoil effect for the atomic g factor to the leading orders in the parameter αZ was developed in a number of papers, see, e.g. Refs. [13, 14, 15, 16, 17, 18] and references therein. The rigorous QED theory valid to all orders in αZ and to first order in electron-to-nucleus mass ratio m/M was developed in Ref. [19]. In Ref. [20] the corresponding numerical results were presented for 1s state. Since the contributions of the second and higher orders in m/M are negligible at the present level of accuracy, we do not consider them in the present paper.

First, we introduce the one-electron and the many-electron parts of the nuclear recoil correction, and present the former as the sum of the low-order and the higher-order terms:

$$\Delta g_{\text{rec}} = \Delta g_{\text{rec}}^{1-\text{el,L}} + \Delta g_{\text{rec}}^{1-\text{el,H}} + \Delta g_{\text{rec}}^{m-\text{el}}. \quad (1)$$

The lower-order term is given by the expression [19]

$$\Delta g_{\text{rec}}^{1-\text{el,L}} = \frac{1}{M_J M} \left\{ -\langle a | [r \times (p - D(0))]_z | a \rangle \\
+ \sum_n \frac{\langle a | [r \times \alpha]_z | n \rangle \langle n | [p^2 - p \cdot D(0) - D(0) \cdot p] | a \rangle}{\varepsilon_n - \varepsilon_a} \right\}. \quad (2)$$

Here |a⟩ is the one-electron reference state, M_J is the z-projection of the total angular momentum, while the z-axis is directed along the external magnetic field, α stands for the vector of Dirac matrices, p = −i∇ is the momentum operator, and

$$D(\omega) = \frac{\exp(\omega r)}{r} + \nabla(\alpha \cdot \nabla) \frac{\exp(\omega r) - 1}{\omega^2 r}. \quad (3)$$

While Δg_{rec}^{1-\text{el,L}} gives the one-electron nuclear recoil correction complete in orders m/M(αZ)^0 and m/M(αZ)^2, the higher-order term Δg_{rec}^{1-\text{el,H}} contains contributions of the order m/M(αZ)^3 and higher. Numerical evaluation of this term to all orders in αZ was done in [20] for 1s state only. In this work, we estimate the uncertainty due to unknown value of Δg_{rec}^{1-\text{el,H}} as (αZ)^3Δg_{rec}^{1-\text{el,L}}.

The many-electron part of the nuclear recoil correction for an atom with one electron over closed shells can be found from Eqs. (73) and (92) of Ref. [19] employing the formalism of redefined vacuum [21]. In this way, we derive the following expression:

$$\Delta g_{\text{rec}}^{m-\text{el}} = \frac{2}{M_J M} \sum_c \left\{ \langle a | [r | c \rangle \times \langle c | [p - D(\Delta)] | a \rangle \rangle_z \\
- \sum_n \frac{\langle a | [r \times \alpha]_z | n \rangle \langle n | [p - D(\Delta)] \rangle \cdot \langle c | [p - D(\Delta)] | a \rangle}{\varepsilon_n - \varepsilon_a} \\
- \sum_n \frac{\langle c | [r \times \alpha]_z | n \rangle \langle n | [p - D(\Delta)] \rangle \cdot \langle a | [p - D(\Delta)] | c \rangle}{\varepsilon_n - \varepsilon_c} \\
+ \langle a | D'(\Delta) | c \rangle \cdot \langle c | [p - D(\Delta)] | a \rangle \left( \langle a | [r \times \alpha]_z | a \rangle - \langle c | [r \times \alpha]_z | c \rangle \right) \right\}. \quad (4)$$
Here the summation over $|c\rangle$ runs over all closed-shell electrons, $D'(\omega) = \partial D(\omega) / \partial \omega$, and 

$$\Delta = \varepsilon_a - \varepsilon_c.$$

We calculate the contributions $\Delta g_{\text{rec}}^{1-\text{el,L}}$ and $\Delta g_{\text{rec}}^{\text{el}}$ according to Eqs. (2) and (4) for $2P_{1/2}$ and $2P_{3/2}$ states. The numerical computation is performed employing the standard algebra for angular coefficients and the dual kinetic balance approach [22] to construct the finite basis set of the radial functions. Apart from the Coulomb potential (with account for the finite nuclear size), we use the core-Hartree and Kohn-Sham screening potentials. The explicit expressions for this potentials can be found e.g. in [23], while the examples of their numerical implementations and applications in various atomic structure calculations can be found, e.g. in Refs. [7, 24, 25, 26, 27]. The results for B-like argon are presented in the first and second lines of Table 1.

The next step in our consideration is to take into account the interelectronic-interaction beyond the screening-potential approximation, namely, to calculate the first-order correction to the nuclear recoil effect within the perturbation theory. In the non-relativistic limit Eqs. (2) and (4) yield together the well-known expression [13]

$$\Delta g_{\text{rec}}^{\text{non-rel}} = \frac{1}{M_J} \langle A | W_{\text{rec}} | A \rangle,$$

where $|A\rangle$ is the reference-state many-electron wave function in the non-interacting-electrons approximation, i.e. the Slater determinant for $(1s)^2 (2s)^2 2p_j$ configuration. We employ the approximation given by Eqs. (5), (6) to evaluate the first-order interelectronic-interaction correction to the nuclear recoil effect. The interaction operator is taken in the Breit approximation,

$$H_{\text{int}} = \sum_{j<k} \left( \frac{1}{r_{jk}} \frac{\alpha_j \cdot \alpha_k}{2} - \frac{1}{2} \left[ \left[ \alpha_j \cdot \nabla_j, \left[ \alpha_k \cdot \nabla_k, r_{jk} \right] \right] \right) \right).$$

The general expression for this contribution is

$$\Delta g_{\text{rec}}^{(1)} = \frac{2}{M_J} \sum_{E_N \neq E_A} \langle A | W_{\text{rec}} | N \rangle \langle N | H_{\text{int}} | A \rangle \frac{E_A - E_N}{E_A - E_N},$$

where the summation runs over the complete spectrum of the many-electron states $|N\rangle$, constructed as the Slater determinants from the one-electron solutions of the Dirac equation. Substitution of the two-electron operators $W_{\text{rec}}$ and $H_{\text{int}}$ leads to the rather lengthy formulae, which are not presented here, therefore. The structure of these formulae can be easily understood from the corresponding diagrams depicted in Fig. 1. The first diagram corresponds to the “one-electron” part of $W_{\text{rec}}$, i.e. to the case of $j = k$ in Eq. (6). Other diagrams correspond to the “two-electron” part of $W_{\text{rec}}$, i.e. to the case of $j \neq k$. We calculate $\Delta g_{\text{rec}}^{(1)}$ numerically for the pure Coulomb potential, as well as for the core-Hartree and Kohn-Sham screening potentials. When the screening potential is included in zeroth-order in the Dirac equation, the corresponding counter-term shall be taken into account for the first-order correction $\Delta g_{\text{rec}}^{(1)}$. It can be written as the following replacement in Eq. (8),

$$H_{\text{int}} \rightarrow H_{\text{int}} - \sum_j V_{\text{scr}}(r_j).$$

The diagrams for the counter-term are shown in Fig. 2.
Figure 1. Diagrams corresponding to $\Delta g_{\text{rec}}^{(1)}$ contribution to the $g$ factor, given by Eq. (8): the first-order interelectronic-interaction correction to the nuclear recoil effect. The dashed lines with the triangle and with the arrow correspond to the one-electron and many-electron parts of the non-relativistic recoil operator $W_{\text{rec}}$ (6).

Table 1. Individual contributions to the nuclear recoil correction to the $g$ factor of B-like argon $^{40}\text{Ar}^{13+} \quad (m/M = 13.7308 \cdot 10^{-6})$ for $^2P_{1/2}$ and $^2P_{3/2}$ states. The units are $10^{-6}$.

|                | $^2P_{1/2}$                  |                | $^2P_{3/2}$                  |
|----------------|------------------------------|----------------|------------------------------|
|                | Coulomb core-Hartree Kohn-Sham | Coulomb core-Hartree Kohn-Sham | Coulomb core-Hartree Kohn-Sham |
| $\Delta g_{\text{rec}}^{1-\text{el,L}}$ |              | $-18.208$ | $-9.099$ | $-9.109$ | $-9.108$ |
| $\Delta g_{\text{rec}}^{\text{m-el}}$    | $7.548$    | $8.332$    | $3.698$    | $4.064$    | $4.119$    |
| $\Delta g_{\text{rec}}^{(1)}$            | $1.434$    | $0.790$    | $0.704$    | $0.459$    | $0.387$    |
| sum           | $-9.226$   | $-9.076$   | $-9.099$   | $-4.697$   | $-4.586$   | $-4.602$   |
| $\Delta g_{\text{rec}}$                  | $-9.10(13)$ | $-9.10(13)$ | $-4.60(9)$ |

In Table 1 the terms $\Delta g_{\text{rec}}^{1-\text{el,L}}$, $\Delta g_{\text{rec}}^{\text{m-el}}$, and $\Delta g_{\text{rec}}^{(1)}$ are presented for the case of B-like argon $^{40}\text{Ar}^{13+}$ for Coulomb, core-Hartree and Kohn-Sham potentials. The Kohn-Sham value is taken for the final result, while the uncertainty is estimated as the difference between the values for Coulomb and Kohn-Sham potentials. This rather conservative estimation, i.e. 100% of the contribution of higher orders, is based on the observation, that the effect of the screening potential for $\Delta g_{\text{rec}}^{1-\text{el,L}}$ and $\Delta g_{\text{rec}}^{\text{m-el}}$ constitutes only 50% of the total interelectronic-interaction correction obtained. Another minor uncertainty is related to $\Delta g_{\text{rec}}^{1-\text{el,H}}$, its estimation $((\alpha Z)^3 \Delta g_{\text{rec}}^{1-\text{el,L}})$ amounts to 0.041 and 0.021 for $^2P_{1/2}$ and $^2P_{3/2}$ states, respectively. In comparison to the previously published values [12], the obtained accuracy of the nuclear recoil effect is 2 times better for $^2P_{1/2}$ state and 4 times better for $^2P_{3/2}$ state.

3. $g$ factor of boron-like argon

Table 2 represents the individual contributions to the $g$ factors of B-like argon for the ground $[(1s)^2 (2s)^2 2p]^2^P_{1/2}$ and first excited $[(1s)^2 (2s)^2 2p]^2^P_{3/2}$ states. As compared to the previous
Table 2. Individual contributions to the \( g \) factor of boron-like argon for \( 2P_{1/2} \) and \( 2P_{3/2} \) states.

|                 | \( 2P_{1/2} \)          | \( 2P_{3/2} \)          |
|-----------------|-------------------------|-------------------------|
| Dirac value     | 0.663 775 447           | 1.331 030 389           |
| Finite nuclear size | 0.000 000 000         | 0.000 000 000           |
| One-photon exchange | \( \sim 1/Z \)        | 0.000 657 525           |
| Many-photon exchange | \( \sim 1/Z^{2+} \)   | -0.000 007 5 (4)        |
| One-loop QED     | \( \sim \alpha \)      | -0.000 769 9 (5)        |
| Higher-order QED  | \( \sim \alpha^{2+} \)  | 0.000 001 2 (1)         |
| Nuclear recoil   | -0.000 009 1 (2)        | -0.000 004 6 (1)        |
| Total            | 0.663 647 7 (7)         | 1.332 282 (3)           |

compilation [12], two terms are improved: the interelectronic interaction of the second and higher orders (\( 1/Z^{2+} \)) and the nuclear recoil effect. Evaluation of the latter has been presented in the previous section. The higher-order interelectronic-interaction correction was calculated in [12] for the ground state within the Breit approximation employing the large-scale configuration interaction method with the Dirac-Fock and Dirac-Fock-Sturm basis functions (CI-DFS). The 10% uncertainty was ascribed to it due to the moderate basis employed in the calculations and relatively poor convergence of the result with respect to the basis size. Recently we have performed calculations with larger basis and found justification for 2 times smaller uncertainty of the result. It is supported by the independent calculation of the \( 1/Z^{2} \)-term performed within the perturbation theory. The corresponding calculation for the \( 2P_{3/2} \) state yields the new value for this contribution, while the all-order CI-DFS result is still in demand. The details on this calculation will be published elsewhere. In total, we have an improvement by a factor of 1.5 for the \( g \) factor of the \( 2P_{1/2} \) state.

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