Many body study of $g$-factor in boron-like argon

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Highly accurate measurements of the $g$-factor of boron like Ar are currently implemented within the ARTEMIS experiment at GSI (Darmstadt, Germany) and within the ALPHATRAP experiment at the MPIK (Heidelberg, Germany). A comparison with the corresponding theoretical predictions will allow one to test the modern methods of bound-state QED. However, at least three different theoretical values of the $g$-factor have been published up to date. The systematic study of the $g$-factor value of Ar$^{13+}$ in the ground $|(1s)^2(2s)^2p|^2P_{1/2}$ and the first excited $|(1s)^2(2s)^2p|^2P_{3/2}$ states is performed within the high order coupled cluster and configuration interaction theories up to the full configuration interaction treatment. Correlation contributions are discussed and results are compared with previous studies.

INTRODUCTION

Experiments on few-electron ions of heavy atoms are of great importance to test bound-state quantum electrodynamics (QED) $^{1,2}$. Highly accurate results for $g$-factor $^3$ and hyperfine structure $^{10,11}$ have already been obtained for H-like and Li-like systems. In particular, the most accurate value of the electron mass (almost by two orders of magnitude more precise than the value from the independent measurements) has been obtained in the study of $g$-factor of highly charged ions $^8$. An independent determination of the fine structure constant $\alpha$ is expected from the $g$-factor measurements in few-electron ions $^{12,14}$. Combined experimental and theoretical studies of the $g$-factor and hyperfine structure can be used to obtain the values of the nuclear magnetic moments $^{15,18}$.

The ARTEMIS experiment $^{19,21}$ at GSI implements the laser-microwave double-resonance technique with the fine or hyperfine structure of highly charged ions. In particular, it can yield the Zeeman splitting in boron-like argon Ar$^{13+}$ ion in the ground $|(1s)^2(2s)^2p|^2P_{1/2}$ and excited $|(1s)^2(2s)^2p|^2P_{3/2}$ states at the ppb level of accuracy. Apart from the $g$-factor of these states, it will also provide the possibility to measure the nonlinear Zeeman effect $^{19,21}$. The ALPHATRAP experiment $^{22}$ at the Max-Planck-Institut f"{u}r Kernphysik (MPIK) aims at the high-precision $g$-factor determination using the Larmor and cyclotron frequency measurements following the earlier experiments performed at the Mainz University $^{3,6}$.

Previously several theoretical values of $g$-factor have been reported which are in a certain disagreement between each other: 0.663647(1) $^{23}$, 0.663728 $^{24}$ and 0.663899(2) $^{25}$. As noted in Ref. $^{25}$, the difference between these values is within the accuracy of the ARTEMIS experiment $^{19}$. This discrepancy can be explained by the different methods used in these works to obtain the electron-electron interaction contributions.

All the other terms such as nuclear recoil and high-order (beyond the free-electron part) QED contributions calculated in Refs. $^{23,26}$ are much smaller than the difference. Thus, an independent calculation of $g$-factor is of high importance.

It was shown that for such properties as $g$-factor $^{27}$, enhancement factors of the electron electric dipole moment, effective electric field, hyperfine structure $^{28,32}$ in atoms and molecules the coupled cluster theory gives very accurate results. It allows to efficiently sum perturbation theory series up to an infinite order. Even for these neutral (or weakly charged) atoms and molecules the main uncertainty of the results were due to neglect of approximate inclusion of the Breit interaction.

The present paper is focused on the theoretical study of the boron like Ar ion within the Dirac-Coulomb-Breit Hamiltonian with accounting effects of electron correlations in all orders of perturbation theory.

THEORY

The first order Zeeman shift of the $^2P_J$ state with the angular momentum projection $M_J$ is directly related to the $g$ factor:

$$\Delta E^{(1)} = gM_J\mu_0B,$$

where $\mu_0 = \frac{|e|\hbar}{2m}$ is the Bohr magneton. Thus the atomic magnetic moment (and $g$-factor) is determined by the first derivative of the energy with respect to the magnetic field $B$ at zero field.

In the four-component Dirac theory Zeeman Hamiltonian can be written in the following form:

$$H_Z = \mu_0 \sum_i [r_i \times \alpha_i] \cdot B,$$

where $\alpha$ is the vector of the Dirac matrices.

Contribution of the QED to the atomic magnetic moment (and $g$-factor) outside the Breit approximation can
be approximately estimated as an expectation value of the following operator \( \Sigma \):

\[
m_{\mu} \frac{\lambda_{\mu}^{2} - 2}{2} \sum_{i} \beta_{i} \Sigma_{z,i},
\]

where \( \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \), \( \Sigma_{z} \) is the z-component of the vector operator \( \Sigma = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix} \), \( \sigma \) are Pauli matrices and \( \lambda_{\mu} = 2 \cdot 0023193 \ldots \) is the free-electron g-factor.

The frequency independent Breit interelectronic interaction is given by the following operator:

\[
H_{B} = -\frac{1}{2} \sum_{i<j} \left( \frac{\alpha_{i} \cdot \alpha_{j}}{r_{ij}} + \frac{(\alpha_{i} \cdot r_{ij})(\alpha_{j} \cdot r_{ij})}{r_{ij}^{3}} \right),
\]

where \( \alpha_{i} \) and \( \alpha_{j} \) act on variables of \( i \)-th and \( j \)-th electrons, correspondingly. This operator is the first QED correction to the Coulomb term and includes both of the magnetic interaction (Gaunt) and "retardation" effects. Note that due to the off-diagonal structure of \( \alpha \)-matrices \( H_{B} \) and \( H_{Z} \) couple large and small bispinor components. Therefore, negative energy states can be of great importance for accurate calculation of \( g \)-factor. Similar effect is well-known in the calculation of the shielding constants (see e.g. \( [37, 38] \)).

The coupled cluster (CC) approach \( [39-42] \) is one of the most successful methods to consider dynamic electron correlation effects. It is based on the exponential ansatz for the wavefunction \( \Psi \):

\[
\Psi_{CC} = e^{\hat{T}} \Phi_{0}.
\]

For the single-reference case \( \Phi_{0} \) is one-determinant wavefunction of a system obtained in some approximation, e.g. within the Dirac-Fock method. \( \hat{T} \) is the excitation cluster operator which expansion has terms of different excitation orders:

\[
\hat{T} = \sum_{k=1}^{n} \hat{T}_{k},
\]

where

\[
\hat{T}_{k} = \sum_{b_{1}<b_{2}<...<b_{k}} \hat{a}_{b_{1}}^{+} \hat{a}_{b_{2}}^{+} ... \hat{a}_{b_{k}}^{+} \hat{a}_{i_{1}} \hat{a}_{i_{2}} ... \hat{a}_{i_{k}},
\]

and indexes \( i_{k} \) correspond to occupied orbitals while \( b_{k} \) correspond to unoccupied ones. Truncation of the \( \hat{T} \) operator at \( \hat{T}_{2} \) leads to the coupled cluster with single and double cluster amplitudes, CCSD, etc. In the coupled cluster technique \( [39, 42] \) Schrödinger equation \( H \Psi_{CC} = E \Psi_{CC} \) is reduced to nonlinear equation system with unknown cluster amplitudes and energy and is solved iteratively. From the perturbation theory (PT) point of view even truncated CC methods includes some terms of PT (in interelectron interaction) up to an infinite order due to the exponential ansatz. For example, the coupled cluster with single, double, triple and quadruple cluster amplitudes, CCSDTQ, (or its approximation CCSDT(Q)) \( [43] \) which was used in the present paper (see below) includes all terms of PT up to order six and some terms up to an infinite order. The CCSDT theory (and its approximation CCSD(T)) includes all terms of PT of the fourth order (and some terms up to an infinite order). Contrary to the CC theory the configuration interaction (CI) method uses a linear anzatz instead of the exponential one in Eq. (5). If \( n \) in Eq. (5) equals to the number of electrons in the system the CC and CI methods will give the same exact (Full CI) wavefunction (within the given basis set, Hamiltonian and in no-pair approximation).

**ELECTRONIC STRUCTURE CALCULATION DETAILS**

In all calculations we used Gaussian basis sets. For the main Dirac-Coulomb-Breit calculation the Dyall’s ACV4Z basis set \( [44] \) with excluded \( f- \) and \( g- \) type functions have been used. This basis set includes 25\( s- \), 15\( p- \) and 9\( d- \) functions for large component and in the following will be called the MBAs basis set. Additionally the correction on the basis set extension was considered within the Dirac-Coulomb approximation using the CCSDT method. The extended basis set, LBas, included 61\( s- \), 50\( p- \), 33\( d- \), 6\( f- \) and 4\( g- \) type functions. Finally, also the truncated version of the MBas basis set, SBas, was used which includes 25\( s- \), 15\( p- \) and 4\( d- \) functions. The Gauss finite nuclear model was used in all of the calculations.

For the Dirac-Fock-Gaunt calculations and Coulomb integral transformations we used the \textsc{dirac15} code \( [45] \). Relativistic correlation calculations were performed within the \textsc{mrcc} code \( [46, 47] \). The code to compute matrix elements of the Breit operator over one-electron bispinors including corresponding 4-index transformation from the original basis functions to the basis of bispinors has been developed in the present paper.

**RESULTS AND DISCUSSION**

Table I gives positive energy contribution to \( g \)-factor of the ground \(^2\text{P}_{1/2}\) and excited \(^2\text{P}_{3/2}\) states of \( \text{Ar}^{13+} \) via different methods within the Breit approximation. In this study the Dirac-Fock-Gaunt method (without retardation part of the Breit interaction) for the open-shell \(^2\text{P}_{1/2}\) state of \( \text{Ar}^{13+} \) has been used to obtain one-electron bispinors for subsequent correlation calculation. In this procedure negative/positive one-electron functions were updated at each iteration of the Dirac-Fock-Gaunt proce-
Correlation calculations were performed within the Breit approximation – retardation part was added to the Hamiltonian after the self-consistent stage. MP2(S) is the first order in the interelectron interaction (with respect to chosen zero-order approximation) contribution to \( g \)-factor. It can be seen from Table I that higher order terms of PT also contribute, however, their sum gives rather small contribution for the problem under consideration.

Table I also provides results for the \( g \)-factor of \( ^2P_{1/2} \) state within the multireference (MR) configuration interaction method, where the small active space includes only 2\( p_{1/2} \) bispinors. As can be seen in the present case of 5 correlated electrons the \( g \)-factor value converges very fast with respect to inclusion of the n-fold excitation, series with \( n=1,2,3,4 \) (note, that the convergence of the correlation energy is slower). Converged result coincides with the coupled cluster result. The Full CI treatment of correlation effects for positive energy spectrum, i.e. in the CISDTQP/CCSDTQ models was possible within the SBas basis set. As expected inclusion of pentaple excitations gave negligible contribution to \( g \)-factor.

Table II presents the final value of \( g \)-factor including the negative energy spectrum contribution which was calculated in the first order of the interelectronic interaction (within the MP2(S) method). For the positive energy spectrum the CCSDTQ result was taken as the most accurate one (it included 1.3 \( 10^8 \) cluster amplitudes). We also took into account basis set correction calculated within the Dirac-Coulomb Hamiltonian employing the CCSDT method [43]. This correction is totally included in the uncertainty of the final value.

### Table I. Positive energy contributions to \( g \)-factor of the ground \( ^2P_{1/2} \) and excited \( ^2P_{3/2} \) states of \( \text{Ar}^{13+} \).

| Method          | \(^2P_{1/2}\) | \(^2P_{3/2}\) |
|-----------------|---------------|---------------|
| Dirac-Fock-Gaunt| 0.664797      | 1.331708      |
| MP2(S)          | 0.664762      | 1.331609      |
| CCS             | 0.691488      | 1.330430      |
| MP2(SD)         | 0.665117      | 1.331589      |
| CCSD            | 0.664962      | 1.330711      |
| CCSD(T)         | 0.664732      | 1.331075      |
| CCSDT           | 0.664762      | 1.331602      |
| CCSDT(Q)        | 0.664762      | 1.331603      |
| CCSDTQ          | 0.664762      | 1.331603      |
| FullCI – CCSDTQ | 0.000000      | 0.000000      |
| MR-CIS          | 0.664637      |                |
| MR-CISD         | 0.664763      |                |
| MR-CISDT        | 0.664762      |                |
| MR-CISDTP       | 0.664762      |                |

Contribution of the QED has been estimated as an expectation value of the operator given by Eq. (3) which has also been employed in Refs. [24, 27]. Obtained values of the contribution to \( g \)-factor, are in reasonable agreement with rigorous one-loop QED calculation (-0.0007699(5) for the \(^2P_{1/2} \) state and 0.0007796(8) for the \(^2P_{3/2} \) state) in Ref. [23]. We add this contribution to our final value of \( g \)-factor obtained in the Breit approximation to be able to compare with previous results in some of which individual QED contribution was not given. However, rigorous corrections on the QED and nuclear recoil effects obtained in Refs. [23, 26] should be used for the final results.

It can be seen that the correlation part of the \( g \)-factor within the Breit approximation almost coincides with the corresponding values from Ref. [23]. Is should be stressed that in the present paper the completely different approach has been used: different nuclear model, different type of basis set (Gaussian functions), different zero-order approximation and different method to treat electron correlation (CC theory up to Full CC).

Taking into account the data from Table I one should note that a delicate check of the \( g \)-factor value is required in case when electron correlation effects are taken into account approximately. For example, in case of the \(^2P_{1/2} \) state the simplest MP2(S) model gives the same results as Full-CI method, where all correlation effects are treated. At the same time the CCSD(T) method which includes all terms of the fourth order of perturbation theory with respect to the interelectron interaction gives results which are in more poor agreement with the Full-CI results.

### Table II. Calculated \( g \)-factor of the ground \(^2P_{1/2} \) and excited \(^2P_{3/2} \) states of \( \text{Ar}^{13+} \) in comparison with previous studies.

| Method                                      | \(^2P_{1/2}\)  | \(^2P_{3/2}\)  |
|---------------------------------------------|----------------|----------------|
| Positive, CCSDTQ                           | 0.664762       | 1.331603       |
| Negative, (MP2(S))                         | -0.000335      | -0.000089      |
| Basis set correction (Coulomb)             | -0.000001      | -0.000002      |
| Total (no QED)                              | 0.664426(3)    | 1.331512(3)    |
| Glazov et al. [23]                         | 0.664427       | 1.331513       |
| (PT+CI-DFS, no QED/Recoil)                 |                |                |
| QED estimation                             | -0.000774      | 0.000773       |
| Total (with QED estimation)*               | 0.663652       | 1.332286       |
| Glazov et al. [23]                         | 0.663647(1)    | 1.332285(3)    |
| (PT+CI-DFS, with QED and Recoil)           |                |                |
| Marques et al. [25] (MCDF, with QED)       | 0.663899(2)    | 1.332372(1)    |
| Verdebou et al. [24] (MRCI, with QED)      | 0.663728       | 1.332365       |

* These values include estimation of QED correction (see text) to compare with previous theoretical results.

### CONCLUSION

The correlation treatment of \( g \)-factors of the ground and excited states of B-like Ar ion within the Dirac-Coulomb-Breit Hamiltonian has been performed. Uncertainty of the result have been tested by performing the Full CI calculation (i.e. full inclusion of correlation effects) and considering different basis sets. Obtained \( g \)-
factors of the ground $^2P_{1/2}$ and excited $^2P_{3/2}$ states coincide within the uncertainty with one of three previous theoretical results $[23]$ and thus can be considered as its independent confirmation. It is shown that high-order correlation effects give non-negligible individual contributions to the value of $g$-factor, however, their sum is small for the problem under consideration.

In the study the code to compute matrix elements of the Breit interaction has been developed. It does not use atomic symmetry and can be modified to study heavy electron systems.

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