g factor of the $[(1s)^2(2s)^2 2p]\ ^2P_{3/2}$ state of middle-Z boronlike ions

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Abstract

Theoretical g-factor calculations for the first excited $^2P_{3/2}$ state of boronlike ions in the range Z=10–20 are presented and compared to the previously published values. The first-order interelectronic-interaction contribution is evaluated within the rigorous QED approach in the effective screening potential. The second-order contribution is considered within the Breit approximation. The QED and nuclear recoil corrections are also taken into account.

I. INTRODUCTION

Significant progress in the g-factor studies in highly charged ions has been achieved in the last two decades [1, 2]. Contemporary experiments have reached the precision of 10^{-9}–10^{-11} for hydrogenlike and lithiumlike ions [3–7]. One of the highlights in this field is the most accurate determination of the electron mass from the combined experimental and theoretical studies of the g factor of hydrogenlike ions [8]. Extension of these studies to lithiumlike ions has provided the stringent test of the many-electron QED effects [7, 9–11]. The high-precision g-factor measurement of the two isotopes of lithiumlike calcium [10] and the most elaborate evaluation of the nuclear recoil effect for this system [12] have demonstrated a possibility to study the bound-state QED effects beyond the Furry picture in the strong field regime [13]. It is expected that g-factor studies in few-electron ions will be able to provide an independent determination of the fine structure constant α [14–16].

The ALPHATRAP experiment at the Max-Planck-Institut für Kernphysik (MPIK) is capable of the ground-state g-factor measurements for wide range of few-electron ions, including boronlike ones [1]. The ARTEMIS project at GSI implements the laser-microwave double-resonance spectroscopy of the Zeeman splitting in both ground $[(1s)^2(2s)^2 2p]\ ^2P_{1/2}$ and first excited $[(1s)^2(2s)^2 2p]\ ^2P_{3/2}$ states of middle-Z boronlike ions [17, 18]. In particular, boronlike argon is chosen as the first candidate for these measurements. Theoretical investigations of the g factor of boronlike ions were performed recently in Refs. [19–24]. Various methods have been used in these works for evaluation of the interelectronic-interaction contribution, including the large-scale configuration-interaction approach in the basis of the Dirac-Fock-Sturm orbitals (CI-DFS) [19, 21], the GRASP2K [20] and MCDFGME [22] packages based on relativistic multi-configuration Dirac-Hartree-Fock (MCDHF) method, the second-order perturbation theory (PT) in effective screening potential [21, 23], and the high order coupled cluster (CC) method [24]. For the ground-state g factor of boronlike argon the results of the CI-DFS, PT, and CC approaches are in agreement, while the both MCDHF results reveal a deviation on the level of 10^{-4}. In the present work, we extend the second-order perturbation-theory calculations to the $^2P_{3/2}$ state. The QED and nuclear recoil corrections are also taken into account. The results for boronlike ions in the range Z=10–20 are presented and compared to the previously published values [19–22, 24]. We use the relativistic units ($\hbar = c = 1$) and the Heaviside charge unit ($\alpha = e^2/(4\pi)$, $e < 0$)

throughout the paper.

II. METHODS AND RESULTS

The total g-factor value of boronlike ion with zero nuclear spin can be written as

$$g = g_{\mathrm{D}} + \Delta g_{\mathrm{int}} + \Delta g_{\mathrm{QED}} + \Delta g_{\mathrm{rec}} + \Delta g_{\mathrm{NS}}\,, \tag{1}$$

where Δg_{int}, Δg_{QED}, Δg_{rec}, and Δg_{NS} are the interelectronic-interaction, QED, nuclear recoil, and nuclear size corrections, respectively. The Dirac value g_{D} for the $2p_{3/2}$ state is

$$g_{\mathrm{D}} = \frac{4}{15}\left[2\sqrt{4-(\alpha Z)^2}+1\right] = \frac{4}{3} - \frac{2}{15}(\alpha Z)^2 - \dots\,. \tag{2}$$

The interelectronic-interaction correction is considered within the perturbation theory. The first-order term $\Delta g^{(1)}_{\mathrm{int}}$ (one-photon exchange) is calculated within the rigorous QED approach, i.e., to all orders in αZ. The second-order term $\Delta g^{(2)}_{\mathrm{int}}$ (two-photon exchange) is considered within the Breit approximation. The general formulae for this contribution can be found from the complete quantum electrodynamical formulae for the two-photon-exchange diagrams presented in Ref. [25]. Care should be taken to account properly for the contribution of the negative-energy states, since it is comparable in magnitude to the positive-energy counter-part.

We incorporate the effective screening potential in the zeroth-order approximation. This improves the convergence of the perturbation theory and provides a reliable estimation of the higher-order remainder. The corresponding counter-terms should be considered in calculations of the first- and second-order contributions. The difference between the g-factor values in the screening and pure Coulomb potentials is termed as the zeroth-order contribution $\Delta g^{(0)}_{\mathrm{int}}$. We use the following well-known screening potentials: core-Hartree (CH), Dirac-Hartree (DH), Kohn-Sham (KS), and Dirac-Slater (DS), see, e.g., Ref. [26] for more details.

In Table I we present the interelectronic-interaction contributions to the g-factor multiplied by 10^6. The total value of Δg_{int} is found as,

$$\Delta g_{\mathrm{int}} = \Delta g^{(0)}_{\mathrm{int}} + \Delta g^{(1)}_{\mathrm{int}} + \Delta g^{(2)}_{\mathrm{int}}\,, \tag{3}$$

where the first-order correction $\Delta g^{(1)}_{\mathrm{int}}$ is divided into the following three parts:

$$\Delta g^{(1)}_{\mathrm{int}} = \Delta g^{(1)}_{\mathrm{int}}[+] + \Delta g^{(1)}_{\mathrm{int}}[-] + \Delta g^{(1)}_{\mathrm{int}}[\mathrm{QED}]\,. \tag{4}$$

The positive-energy-states ($\Delta g^{(1)}_{\rm int}[+]$) and negative-energy-states ($\Delta g^{(1)}_{\rm int}[-]$) contributions are calculated in the Breit approximation. The QED contribution ($\Delta g^{(1)}_{\rm int}[{\rm QED}]$) is the difference between the rigorous QED and the Breit-approximation values.

As the final results for $\Delta g_{\rm int}$, we take the values calculated in the Kohn-Sham potential. The uncertainty due to unknown higher-order contributions can be estimated as the spread of the obtained results for different potentials. As one can see from the Table I, the maximal difference of the values of $\Delta g_{\rm int}$ varies between 1.8×10^{-6} for Z=10 and 0.8×10^{-6} for Z=20. Interelectronic-interaction corrections of the third and higher orders have been evaluated for lithiumlike ions within the CI-DFS [9] and CI [11] methods. The results obtained in these papers suggest that this estimation of the uncertainty is quite reliable.

The one-loop QED correction $\Delta g^{(1)}_{\rm QED}$ is given by the sum of the self-energy and vacuum-polarization contributions,

$$\Delta g^{(1)}_{\rm QED} = \Delta g_{\rm SE} + \Delta g_{\rm VP}\,. \tag{5}$$

The self-energy correction correction was calculated to all orders in αZ for both $2p_{1/2}$ and $2p_{3/2}$ states in the range Z=1–12 in Ref. [27]. This values can be extrapolated to a good accuracy by the following αZ-expansion [27, 28],

$$\Delta g_{\rm SE} = \frac{\alpha}{\pi}\left[b_{00} + \frac{(\alpha Z)^2}{4}\,b_{20} + \frac{(\alpha Z)^4}{8}\,\left\{\ln[(\alpha Z)^{-2}]b_{41} + b_{40}\right\}\right]\,. \tag{6}$$

The values $b_{00}(2p_{1/2}) = -1/3$ and $b_{00}(2p_{3/2}) = 1/3$ have long been known [29, 30]. The values $b_{20}(2p_{1/2}) = 0.48429$ and $b_{20}(2p_{3/2}) = 0.59214$ have been found in Ref. [28]. Our fitting procedure based on the least squares method reproduces these coefficients if they are taken as unknown, which serves as a check of its consistency. In this way we extrapolate the results of Ref. [27] up to Z=20. In addition, we estimate the screening correction for the $2p_{3/2}$ state employing the effective nuclear charge $Z_{\rm eff}$ instead of Z in Eq. (6). The effective nuclear charge $Z_{\rm eff}$ is found from our rigorous calculations of the self-energy correction for the $2p_{1/2}$ state with an effective screening potential [23]: Eq. (6) with $Z_{\rm eff}$ should reproduce the result obtained with the Kohn-Sham potential. The screening shift $Z - Z_{\rm eff}$ lies in the range 1.3–1.7 for the ions under consideration. We ascribe the 100% uncertainty to the screening correction obtained in this rather approximate way.

The dominant contribution of the vacuum polarization is given by the two-electron diagrams where the vacuum-polarization potential acts on the $1s$ and $2s$ electrons. This contribution was estimated as 5.5×10^{-9} for Z=18 in Ref. [19], which is much smaller than the total theoretical uncertainty. The two-loop contribution $\Delta g^{(2)}_{\rm QED}$ is represented by its zeroth-order term of the αZ-expansion [30].

The nuclear recoil effect in boronlike argon was calculated in Refs. [19, 21] within the Breit approximation to zeroth and first orders in $1/Z$. Systematic calculations of this effect for the $2p_{1/2}$ state in the range Z=10–20 were performed in Ref. [31]. Recently, these calculations have been extended to Z=20–92 including the leading-order QED contributions beyond the Breit approximation [32]. In the present paper, we evaluate this effect for the $2p_{3/2}$ state with the relativistic recoil operators to zeroth order in $1/Z$ with the Kohn-Sham effective screening potential. The leading-order term of the finite-nuclear-size correction can be written as [33]

$$\Delta g_{\rm NS} = \frac{(\alpha Z)^6}{720} m^4 \langle r^4 \rangle \,. \tag{7}$$

For Z=10–20 it gives the values of the order 10^{-18}–10^{-16} which is negligible at the present level of accuracy.

The individual contributions and the total g-factor values for the $2p_{3/2}$ state of boronlike ions in the range Z=10–20 are presented in Table I. The values of $\Delta g_{\rm int}$ calculated in the Kohn-Sham potential are used. Our results for argon are in agreement with the PT results from Refs. [19, 21] and with the CC results from Ref. [24]. The difference between the data from Ref. [20] and those of the present work ranges from 0.000 042 for Z=10 to 0.000 094 for Z=20. The difference between the data from Ref. [22] and those of the present work ranges from 0.000 067 for Z=14 to 0.000 102 for Z=20. The origin of this disagreement is not clear at present. We suppose that the negative-energy-states contribution was not taken into account completely in Refs. [20, 22].

Zeeman splitting of the $2p_j$ states acquires significant nonlinear contributions. In particular, the second- and third-order terms in magnetic field can be observed in forthcoming measurements for boronlike argon [17, 19]. Recently, the systematic calculations of these terms for the wide range of boronlike ions have been presented by our group [34]. The most important contribution for the $2p_{3/2}$ state is the shift of the levels with $m_j = \pm 1/2$ proportional to B^2. It can be represented as the m_j-dependent g-factor contribution varying from $\pm 1.52 \times 10^{-4}$ for Z=10 to $\pm 5.68 \times 10^{-6}$ for Z=20 at the field of 1 T (it scales linearly with B). For more detailed description of the second- and third-order contributions see Ref. [34].

III. CONCLUSION

In conclusion, the g factor of the $^2P_{3/2}$ state of boronlike ions in the range Z=10–20 has been evaluated with an uncertainty on the level of 10^{-6}. The leading interelectronic-interaction correction has been calculated to all orders in αZ. The higher-order interelectronic-interaction and nuclear-recoil effects have been taken into account within the Breit approximation. The one-loop self-energy correction has been found from extrapolation of the previously published high-precision results for Z=1–12 with an approximate account for screening.

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Table I: Interelectronic-interaction correction to the g factor of boronlike ions in the $^2P_{3/2}$ state. The terms of the zeroth ($\Delta g_{\rm int}^{(0)}$), first ($\Delta g_{\rm int}^{(1)}$), and second ($\Delta g_{\rm int}^{(2)}$) orders of perturbation theory obtained with the core-Hartree (CH), Dirac-Hartree (DH), Kohn-Sham (KS), and Dirac-Slater (DS) screening potentials. First-order term is split into the contributions of the positive-energy ($\Delta g_{\rm int}^{(1)}[+]$) and negative-energy ($\Delta g_{\rm int}^{(1)}[+]$) spectra calculated within the Breit approximation and the QED part ($\Delta g_{\rm int}^{(1)}[\rm QED]$). All numbers are in units of 10^{-6}.

	CH	DH	KS	DS
		$Z = 10$		
$\Delta g_{\rm int}^{(0)}$	302.983	376.227	312.152	276.157
$\Delta g_{\rm int}^{(1)}[+]$	−22.611	−117.851	−34.824	17.678
$\Delta g_{\rm int}^{(1)}[-]$	−22.371	−2.806	−19.623	−29.741
$\Delta g_{\rm int}^{(1)}[\rm QED]$	−0.141	−0.111	−0.141	−0.158
$\Delta g_{\rm int}^{(2)}$	6.256	6.889	6.580	−0.758
$\Delta g_{\rm int}$	264.116	262.348	264.143	263.178
		$Z = 12$		
$\Delta g_{\rm int}^{(0)}$	368.346	462.044	379.402	334.176
$\Delta g_{\rm int}^{(1)}[+]$	−27.393	−148.063	−41.786	22.005
$\Delta g_{\rm int}^{(1)}[-]$	−29.402	−4.746	−26.187	−38.614
$\Delta g_{\rm int}^{(1)}[\rm QED]$	−0.281	−0.233	−0.282	−0.308
$\Delta g_{\rm int}^{(2)}$	6.288	7.275	6.400	−0.441
$\Delta g_{\rm int}$	317.559	316.277	317.547	316.819
		$Z = 14$		
$\Delta g_{\rm int}^{(0)}$	433.852	547.842	446.756	392.322
$\Delta g_{\rm int}^{(1)}[+]$	−32.164	−178.105	−48.754	26.389
$\Delta g_{\rm int}^{(1)}[-]$	−36.370	−6.680	−32.691	−47.407
$\Delta g_{\rm int}^{(1)}[\rm QED]$	−0.489	−0.420	−0.492	−0.528
$\Delta g_{\rm int}^{(2)}$	6.306	7.516	6.289	−0.265
$\Delta g_{\rm int}$	371.135	370.154	371.108	370.511

	CH	DH	KS	DS
		$Z = 16$		
$\Delta g^{(0)}_{\rm int}$	499.514	633.710	514.250	450.613
$\Delta g^{(1)}_{\rm int}[+]$	-36.888	-208.003	-55.691	30.839
$\Delta g^{(1)}_{\rm int}[-]$	-43.298	-8.610	-39.151	-56.142
$\Delta g^{(1)}_{\rm int}[\mathrm{QED}]$	-0.780	-0.686	-0.783	-0.833
$\Delta g^{(2)}_{\rm int}$	6.315	7.682	6.204	-0.166
$\Delta g_{\rm int}$	424.863	424.092	424.828	424.311
		$Z = 18$		
$\Delta g^{(0)}_{\rm int}$	565.355	719.702	581.912	509.070
$\Delta g^{(1)}_{\rm int}[+]$	-41.544	-237.766	-62.572	35.370
$\Delta g^{(1)}_{\rm int}[-]$	-50.195	-10.541	-45.575	-64.829
$\Delta g^{(1)}_{\rm int}[\mathrm{QED}]$	-1.167	-1.043	-1.171	-1.235
$\Delta g^{(2)}_{\rm int}$	6.316	7.804	6.132	-0.116
$\Delta g_{\rm int}$	478.765	478.155	478.726	478.259
		$Z = 20$		
$\Delta g^{(0)}_{\rm int}$	631.397	805.864	532.824	567.713
$\Delta g^{(1)}_{\rm int}[+]$	-46.116	-267.395	-69.382	39.996
$\Delta g^{(1)}_{\rm int}[-]$	-57.065	-12.472	-51.964	-73.472
$\Delta g^{(1)}_{\rm int}[\mathrm{QED}]$	-1.661	-1.507	-1.668	-1.747
$\Delta g^{(2)}_{\rm int}$	6.311	7.896	6.065	-0.101
$\Delta g_{\rm int}$	532.866	532.386	532.824	532.134

Table II: Individual contributions to the g factor of the $^2P_{3/2}$ state of boronlike ions in the range Z=10–20. The values obtained with the Kohn-Sham potential are used for the interelectronic-interaction correction $\Delta g_{\rm int}$ (see Table I). The g-factor values from Refs. [20–22, 24] are given for comparison.

	$^{20}_{10}$Ne^{5+}	$^{24}_{12}$Mg^{7+}
Dirac value $g_{\rm D}$	1.332 623 079	1.332 310 417
Interelectronic interaction $\Delta g_{\rm int}$	0.000 264 1 (18)	0.000 317 5 (13)
One-loop QED $\Delta g^{(1)}_{\rm QED}$	0.000 775 7 (5)	0.000 776 3 (7)
Two-loop QED $\Delta g^{(2)}_{\rm QED}$	−0.000 001 2	−0.000 001 2
Nuclear recoil $\Delta g_{\rm rec}$	−0.000 008 9 (15)	−0.000 007 8 (11)
Total value g	1.333 652 8 (23)	1.333 394 1 (17)
g from Ref. [20]	1.333 695	1.333 448

	$^{28}_{14}$Si^{9+}	$^{32}_{16}$S^{11+}
Dirac value $g_{\rm D}$	1.331 940 789	1.331 514 136
Interelectronic interaction $\Delta g_{\rm int}$	0.000 371 1 (10)	0.000 424 8 (8)
One-loop QED $\Delta g^{(1)}_{\rm QED}$	0.000 777 2 (9)	0.000 778 2 (10)
Two-loop QED $\Delta g^{(2)}_{\rm QED}$	−0.000 001 2	−0.000 001 2
Nuclear recoil $\Delta g_{\rm rec}$	−0.000 006 8 (8)	−0.000 006 1 (6)
Total value g	1.333 081 1 (16)	1.332 709 8 (14)
g from Ref. [20]	1.333 143	1.332 783
g from Ref. [22]	1.333 148 (7)	1.332 788 (8)

	$^{40}_{18}Ar^{13+}$	$^{40}_{20}Ca^{15+}$
Dirac value g_D	1.331 030 389	1.330 489 471
Interelectronic interaction Δg_{int}	0.000 478 7 (6)	0.000 532 8 (7)
One-loop QED $\Delta g^{(1)}_{QED}$	0.000 779 5 (12)	0.000 780 9 (13)
Two-loop QED $\Delta g^{(2)}_{QED}$	−0.000 001 2 (1)	−0.000 001 2 (1)
Nuclear recoil Δg_{rec}	−0.000 004 9 (4)	−0.000 004 9 (4)
Total value g	1.332 282 5 (14)	1.331 797 1 (15)
g from Ref. [20]	1.332 365	1.331 891
g from Ref. [22]	1.332 372 (1)	1.331 899 (7)
g from Ref. [21]	1.332 282 (3)	
g from Ref. [24]	1.332 286	