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Communication

g Factor of Few-Electron Highly Charged Ions

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Abstract: The current status of the theoretical investigation of the bound-electron g factor in lithium-like and boron-like highly charged ions is reported. Some tension between the several theoretical values and measurements is discussed. Then, prospects for future investigations are briefly reviewed.

Keywords: g factor, highly charged ions, quantum electrodynamics

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1. Introduction

High-precision g-factor measurements in highly charged H-like ions [1–5] provided an unprecedented test of the bound-state QED predictions, see, e.g., the reviews in references [6–8] and more recent works [9–12]. In assuming that the theory [13–20] at this level is correct, the most accurate up-to-date value of the electron mass was obtained [5,21–23]. The ultimate limit of the theoretical precision is set by the nuclear size and polarization effects. To overcome this limit, it was proposed that we consider the so-called specific differences of the g-factor values of different charge states of the same isotope [24–29]. Future progress in experiments and theory for these specific differences can provide independent determination of the fine structure constant α [25–27,29]. Rigorous tests of the bound-state QED, including the relativistic nuclear recoil effect [28,30–33] and searches for new physics [33–35], are also anticipated. These proposals motivate investigations into few-electron ions, in particular, Li- and B-like ones. Theoretical progress in this field was achieved by successful experiments with Li-like silicon [36,37], Li-like calcium [30], and B-like argon [38–40]. An agreement between the theory and the experiment for Li-like ions provided the most accurate up-to-date test of the many-electron QED theory, including the second-order contributions: two-photon exchange [36,37,41–44] and two-electron self-energy and vacuum-polarization [37,41,43,45–50]. Meanwhile, along with the better accuracy of the calculations, an apparent disagreement was established recently in references [42,50], motivating further investigations. In the case of B-like ions, there is some disagreement between the theoretical values [51–57]. Recent measurements for the ground [38] and first excited [39,40] states of B-like argon have confirmed the results obtained by the St. Petersburg group. Below, we focus on these cases where the bound-state QED predictions are put to the stringent test. The recent advances in theory, (dis)agreement with the experiments, and opportunities for the future are discussed.

2. Li-like Silicon and Calcium

A semi-relativistic g-factor theory for few-electron systems was developed, in particular, in references [58–60] (see also the references therein). Recently, the non-relativistic quantum electrodynamics (NRQED) approach has been applied to Li-like systems [50,61]. Within this approach, leading corrections for the g factor are represented by effective two-component operators, while the Schrödinger equation yields the many-electron wave

function. Inspired by the experimental and theoretical progress for H-like ions, and by the idea of the specific difference, systematic QED calculations for Li-like ions started about twenty years ago. They gradually covered the one-photon-exchange [24], one-electron QED [17,62–65], two-electron QED [41,43,45,46,50], two-photon-exchange [41–43], and nuclear recoil [31,32] corrections.

In 2013, the first high-precision measurement for Li-like ions was presented, with an experimental value $g_{\rm exp}[^{28}{\rm Si}^{11+}] = 2.000\,889\,889\,9\,(21)$ in excellent agreement with the theory $g_{\rm th}[^{28}{\rm Si}^{11+}] = 2.000\,889\,909\,(51)$ [36]. This theoretical value included the first rigorous evaluation of the two-photon-exchange diagrams ($\sim 1/Z^2$). Further improvements to be accomplished in reference [41] were the calculations of the two-electron self-energy diagrams and the inclusion of effective screening potentials.

In 2019, new experimental and theoretical values were published: $g_{\rm exp}[^{28}{\rm Si}^{11+}] = 2.000\,889\,888\,45\,(14)$ and $g_{\rm th}[^{28}{\rm Si}^{11+}] = 2.000\,889\,894\,4\,(34)$ [37]. The 15-fold improvement of $g_{\rm exp}$ was achieved through the phase-sensitive pulse and amplify (PnA) method used for the determination of the ion's cyclotron frequency and the electron mass value from reference [5]. The two-fold theoretical improvement came mainly from the accurate treatment of the higher-order interelectronic-interaction and many-electron QED contributions using recursive perturbation theory [66]. The theoretical uncertainty of $g_{\rm th}$ is largely dominated by the estimation of unknown non-trivial QED contributions, which was made based on the analysis of the lower-order results. So, the deviation of 1.7σ between $g_{\rm exp}$ and $g_{\rm th}$ was considered as a hint of the magnitude of these unknown contributions rather than as a potential problem.

However, afterwards, Yerokhin et al. recalculated the two-electron self-energy and two-photon exchange diagrams to obtain the values $g_{\rm th}[^{28}{\rm Si}^{11+}] = 2.000\,889\,896\,3\,(15)$ [50] and $g_{\rm th}[^{28}{\rm Si}^{11+}] = 2.000\,889\,893\,7\,(17)$ [42]. These values are in stronger disagreement with the experimental one, 5.2σ and 3.1σ away, respectively, mostly due to the smaller uncertainty. It is estimated in a rather optimistic way, while the source is still the unknown part of the many-electron QED diagrams. The main difference between the calculation procedure is the zeroth approximation within the QED perturbation theory is that, in references [42,50], the Coulomb potential is used, while in references [37,41], various effective screening potentials are used.

Aiming to clarify this situation, extensive calculations of the interelectronic interaction, starting from the Coulomb and four different screening potentials, have been performed in reference [43]. The numerical uncertainty of the calculations has been significantly reduced, and the comparison of the results shows that the unknown higher-order terms for the Coulomb potential are definitely larger than the uncertainty proposed in references [42,50]. This is illustrated in Figure 1, where the results for this contribution are presented along with their uncertainty. For the Coulomb potential we give two values: the one colored pink with smaller uncertainty from reference [42] and the other colored yellow with larger uncertainty from reference [43]. Only the second one is consistent with the screening potential results.

Similar analysis has been done for many-electron QED contributions with the conclusion being similar. The two-electron self-energy and vacuum-polarization diagrams have been recalculated with different screening potentials [43] (see Figure 1). In this case, we have only one value from reference [50] for the Coulomb potential, which does not overlap with the screening potential results. It is interesting that the noticeable differences between the Coulomb and screening potential have opposite signs for the interelectronic interaction and for the many-electron QED, and that they largely cancel out in total. The final value of $g_{\rm th}[^{28}{\rm Si}^{11+}] = 2.000\,889\,892\,4\,(28)$ [43] differs from the experiment by 1.4σ.

The current situation for Li-like calcium is basically the same. In reference [30], the experimental results for two isotopes, $A = 40$ and $A = 48$, are presented, in agreement with the theory [30,41]. A recent evaluation of the two-electron self-energy and two-photon-exchange contributions starting from the Coulomb potential by Yerokhin et al. [42,50] has yielded a new value, 4.2σ away from the experiment. The calculations based on the

screening potentials give a result which differs from the experiment by only 0.6σ [43]. In Table 1, we present the recent theoretical and experimental values for both silicon and calcium discussed above.

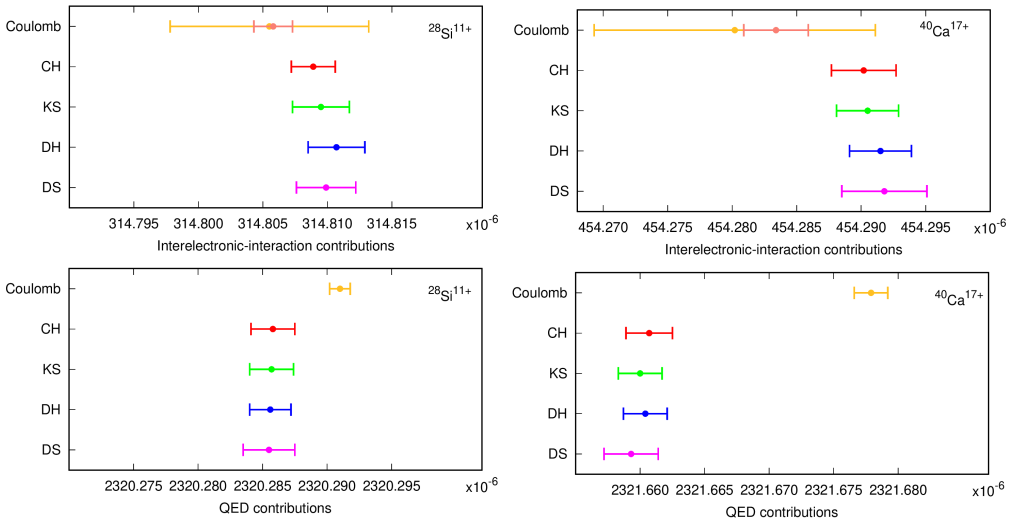

Figure 1. Interelectronic–interaction and QED contributions to the g factor of Li-like silicon and calcium calculated with different binding potentials: Coulomb, core–Hartree, Dirac–Hartree, Kohn–Sham, and Dirac–Slater (see reference [44] for definitions of the potentials).

Table 1. Theoretical and experimental values of the ground-state g factor of Li-like silicon and calcium ions.

	$^{28}Si^{11+}$	$^{40}Ca^{17+}$
g_{th} [Wagner et al. (2013) [36]]	2.000 889 909 (51)	
g_{th} [Volotka et al. (2014) [41]]	2.000 889 892 (8)	1.999 202 041 (13)
g_{th} [Köhler et al. (2016) [30]]		1.999 202 042 (13)
g_{th} [Glazov et al. (2019) [37]]	2.000 889 894 4 (34)	
g_{th} [Yerokhin et al. (2020) [50]]	2.000 889 896 3 (15)	
g_{th} [Yerokhin et al. (2021) [42]]	2.000 889 893 7 (17)	1.999 202 052 9 (27)
g_{th} [Kosheleva et al. (2022) [43]]	2.000 889 892 4 (28)	1.999 202 042 6 (29)
g_{exp} [Wagner et al. (2013) [36]]	2.000 889 889 9 (21)	
g_{exp} [Köhler et al. (2016) [30]]		1.999 202 040 5 (11)
g_{exp} [Glazov et al. (2019) [37]]	2.000 889 888 45 (14)	

In order to clarify the situation, we continue to improve and cross-check the calculation approach. First, in a joint effort by the two groups [67], we investigate the partial-wave convergence of the two-electron self-energy diagrams. We find that the high-l behaviour of this contribution is non-monotonic and that a larger number of calculated terms is needed to achieve a reliable estimation of the remainder, altogether with the careful choice of the extrapolation scheme. Second, the gauge invariance of the particular sets of diagrams can serve for the non-trivial check of both the formulas and numerical procedures. We have identified a number of gauge-invariant subsets for the two-electron self-energy diagrams and verified this by a comparison of the numerical results in the Feynman and Coulomb gauges [68].

We have also performed systematic calculations of the interelectronic interaction contributions to the g factor of Li-like ions in the range of Z = 14–82 [44]. The one- and two-photon-exchange terms are evaluated within the rigorous QED approach, while the third- and higher-order terms are treated within the Breit approximation using the recursive perturbation theory. This provides a solid theoretical background for the anticipated measurements with heavier ions. Further theoretical progress requires the rigorous evaluation of the third-order many-electron QED diagrams mentioned above.

3. B-like Argon

Following the success with Li-like ions, high-precision measurements of the g factor of B-like argon were performed. In reference [38], the value of $g_{\rm exp}[^{40}{\rm Ar}^{13+}] = 0.663\,648\,455\,32\,(93)$ was presented for the ground $2P_{1/2}$ state by the ALPHATRAP team from MPIK. Using a somewhat different technique, they obtained the value of $g_{\rm exp}[^{40}{\rm Ar}^{13+}] = 1.332\,14\,(15)$ for the excited $2P_{3/2}$ state [39]. Finally, the quantum logic measurement delivered the ratio of these g factors, from which $g_{\rm exp}[^{40}{\rm Ar}^{13+}, 2P_{3/2}] = 1.332\,289\,5\,(13)(56)$ was obtained [40] using the ground-state value from reference [38]. Meanwhile, the first theoretical calculations for boron-like ions encountered a serious discrepancy with each other [51–54]. In light of this, independent calculations of the g factor of B-like ions in the range $Z = 10$–20 were carried out, for the ground state in reference [55] and for the excited state in reference [57]. The result of reference [55] for the $2P_{1/2}$ state in argon is in excellent agreement with the previous results of the same group [51,53]. This was also confirmed by using the coupled-cluster calculation [56] and the CI-DFS calculations [49]. The experimental result by Arapoglou [38] conclusively approved this set of values. For the $2P_{3/2}$ state, the value from reference [57] was also confirmed by the experiment [39,40]. The systematic deviation of the MCDHF (GRASP2K) [52] and MCDF (MCDFGME) [54] values is presumably due to the incomplete treatment of the negative-spectrum contribution within these methods. The g-factor values for boron-like argon from the discussed works are presented in Table 2.

Recently, we extended the calculations to higher-Z B-like ions following the methods employed in references [55,57]. In Table 3, we present the results for B-like lead for both $2P_j$ states. The interelectronic interaction is accounted for by perturbation theory, the first-order term within the QED framework, and the second-order term in the Breit approximation. The one-loop QED correction is calculated in the effective screening potential. The two-loop QED contribution is presently known in the non-relativistic limit only [69]. The contribution of the nuclear recoil effect is taken from recent works [70,71]. The finite-nuclear-size effect is calculated directly using the Fermi model and the nuclear radius from reference [72]. The results from references [49,54] are given for comparison. Experimental and theoretical investigations for lead are capable of providing an independent determination of the fine structure constant α from the strong-field domain [25], which requires, of course, further theoretical developments along the same lines as for H- and Li-like ions. In particular, a rigorous evaluation of the two-photon-exchange and two-electron self-energy diagrams is necessary to achieve this goal.

Table 2. Theoretical and experimental values of the g factor of the ground and first excited states of B-like argon ion $^{40}{\rm Ar}^{13+}$.

	$2P_{1/2}$	$2P_{3/2}$
$g_{\rm th}$ [Glazov et al. (2013) [51]]	0.663 647 (1)	1.332 285 (3)
$g_{\rm th}$ [Verdebout et al. (2014) [52]]	0.663 728	1.332 365
$g_{\rm th}$ [Shchepetnov et al. (2015) [53]]	0.663 647 7 (7)	1.332 282 (3)
$g_{\rm th}$ [Marques et al. (2016) [54]]	0.663 899 (2)	1.332 372 (1)
$g_{\rm th}$ [Agababaev et al. (2018) [55]]	0.663 648 8 (12)	
$g_{\rm th}$ [Agababaev et al. (2019) [57]]		1.332 282 5 (14)
$g_{\rm th}$ [Maison et al. (2019) [56]]	0.663 652 (3)(6)	1.332 286 (3)(6)
$g_{\rm th}$ [Cakir et al. (2020) [49]]	0.663 648 1 (5)	
$g_{\rm exp}$ [Arapoglou et al. (2019) [38]]	0.663 648 454 63 (93)	
$g_{\rm exp}$ [Egl et al. (2019) [39]]		1.332 14 (15)
$g_{\rm exp}$ [Micke et al. (2020) [40]]		1.332 289 5 (13)(56)

Table 3. Contributions to the g factor of the ground and first excited states of B-like lead ion $^{208}_{82}Pb^{77+}$.

	$2P_{1/2}$	$2P_{3/2}$
Dirac value g_D	0.598 669 571	1.284 472 641
Interelectronic interaction Δg_{int}	0.003 639 3 (23)	0.002 501 7 (23)
One-loop QED $\Delta g^{(1)}_{QED}$	−0.000 501 6 (66)	0.000 945 3 (50)
Two-loop QED $\Delta g^{(2)}_{QED}$	0.000 001 2 (8)	−0.000 001 2 (8)
Nuclear recoil Δg_{rec}	−0.000 001 8	−0.000 000 7
Finite nuclear size Δg_{NS}	0.000 006 8	0.000 000 0
Total value g_{th}	0.601 813 5 (70)	1.287 917 7 (56)
g_{th} [Marques et al. (2016) [54]]	0.602 860 (33)	1.288 318 (24)
g_{th} [Cakir et al. (2020) [49]]	0.601 815 6 (18)	

4. Conclusions

In this paper, we have highlighted the recent advances of the g-factor investigations in Li- and B-like highly charged ions. The high-precision comparison between theory and experiment for Li-like silicon and calcium allows us to scrutinise the most elaborate QED calculations. The theoretical uncertainty is now determined by the unknown higher-order contributions of the many-electron two-loop diagrams whose calculation requires the development of new methods. For B-like argon, the g-factor calculations within the QED perturbation theory have been confirmed by high-precision measurements for both the ground state and the first excited states. To further improve the theoretical accuracy, rigorous calculations of higher-order QED and interelectronic interaction contributions are in demand. Modern experimental techniques are promising for the g-factors measurements of excited states in highly charged ions, which motivates appropriate theoretical calculations.

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