Many-electron QED corrections to the g factor of lithiumlike ions

A. V. Volotka,1,2 D. A. Glazov,2 V. M. Shabaev,2 I. I. Tupitsyn,2 and G. Plunien1
1 Institut für Theoretische Physik, Technische Universität Dresden,
Mommsenstraße 13, D-01062 Dresden, Germany
2 Department of Physics,
St. Petersburg State University, Oulianovskaya 1,
Petrodvorets, 198504 St. Petersburg, Russia

A rigorous QED evaluation of the two-photon exchange corrections to the g factor of lithiumlike ions is presented. The screened self-energy corrections are calculated for the intermediate-Z region and its accuracy for the high-Z region is essentially improved in comparison with that of previous calculations. As a result, the theoretical accuracy of the g factor of lithiumlike ions is significantly increased. The theoretical prediction obtained for the g factor of 28Si11+ gth = 2.000 889 892(8) is in an excellent agreement with the corresponding experimental value gexp = 2.000 889 889 9(21) [A. Wagner et al., Phys. Rev. Lett. 110, 033003 (2013)].

PACS numbers: 31.30.J-, 31.30.js, 31.15.ac

Highly charged ions provide not only a unique scenario for probing QED effects in the strongest electromagnetic fields but also give access to an accurate determination of fundamental physical constants and nuclear parameters. In recent years, amazing progress has been made in the experimental and theoretical investigations of the bound-electron g factor. High-precision measurements of the ground state g factor of H-like carbon [1] and oxygen [2] and the related theoretical calculations provided determination of the electron mass. Recently, due to the substantial progress in the experimental accuracy of the g factor of H-like carbon and silicon the mass of the electron is once again substantially increased [3]. So far H- and Li-like silicon ions represent the heaviest ions, where the g factor has been measured [4,6]. To date, these experiments provide the most stringent tests of the bound-state QED (BS-QED) corrections in the presence of a magnetic field. Accurate measurements of the g factor in few-electron ions, such as Li-like calcium and B-like argon [7], are already anticipated. The investigations of the few-electron ions unlike H-like ions provide also an access to the many-electron QED corrections, which are represented by a different facet of the QED diagrams.

The theoretical contributions to the g factor of Li-like ions can be separated into one-electron and many-electron parts. The one-electron terms are similar to the corresponding corrections to the g factor of H-like ions. The many-electron contributions, which define the main difference between the g factors of H- and Li-ions, were investigated in Refs. [8,13]. The many-electron contributions are mainly determined by the screened radiative and the interelectronic-interaction corrections. For low-Z ions, the screened radiative corrections were obtained employing the perturbation theory to the leading orders in αZ [9,10]. For intermediate-Z ions, the screening effect was evaluated by introducing the effective screening potential in the QED calculations to all orders in αZ [11]. For high-Z ions, the most accurate results for the screened radiative corrections were obtained rigorously within a systematic QED approach [12,13]. The one-photon exchange diagrams, which represent the interelectronic-interaction correction of the first order in 1/Z, were evaluated in the framework of QED in Ref. [13]. The second and higher-orders contributions of the interelectronic interaction were calculated by means of the large scale configuration-interaction Dirac-Fock-Sturm (CI-DFS) method in Ref. [10]. However, until now, for all values of Z the theoretical uncertainty was determined by the interelectronic-interaction corrections and for the intermediate-Z region also by the screened self-energy corrections. In the present Letter we report on the complete evaluation of the two-photon exchange and the screened self-energy corrections in the framework of a rigorous QED approach within an extended Furry picture.

In the extended Furry picture, to zeroth order we solve the Dirac equation with an effective spherically symmetric potential treating the interaction with the external Coulomb potential of the nucleus and the local screening potential exactly to all orders. This approach significantly accelerates the convergence of the perturbation expansion. We use different types of the screening potential. The simplest choice is the core-Hartree (CH) potential, which is created by the charge density distribution of the two core electrons in the 1s state. Other choices are the xα potentials: Kohn-Sham (KS), Dirac-Hartree (DH), and Dirac-Slater (DS), which were successfully employed in previous calculations of highly charged ions [14–19]. Moreover, we have also employed the Perdew-Zunger (PZ) potential [20] and the local Dirac-Fock (LDF) potential derived by inversion of the radial Dirac equation [21].

Let us now turn to the evaluation of the two-photon exchange corrections to the g factor of Li-like ions. These corrections are defined by diagrams of third order in the QED perturbation theory. The corresponding diagrams are presented in Fig. 1. The electron propagators in the figure have to be treated in the effective potential (we indicate this diagrammatically via the triple electron line). In contrast to the case of the original Furry picture, in the extended Furry picture the additional counterterm diagrams appear. These diagrams are de-
FIG. 1: Feynman diagrams representing the second-order interelectronic-interaction corrections to the g factor in local effective potentials. The wavy line indicates the photon propagator and the triple lines describe the electron propagators in the effective potential. The dashed line terminated with the triangle denotes the interaction with the magnetic field. The counterterm diagrams are depicted in the second line. The symbol $\otimes$ represents the extra interaction term associated with the screening potential counterterm.

TABLE I: Interelectronic-interaction corrections to the ground-state g factor of Li-like $^{28}$Si$^{11+}$ ion in various starting potentials in units $10^{-6}$.

|             | Coulomb | CH  | PZ  | LDF  |
|-------------|---------|-----|-----|------|
| Zeroth order| 348.267 | 321.632 | 349.636 |      |
| First order | 321.592 | -33.549 | -5.990 | -33.846 |
| Second order| -6.876  | 0.137 | -0.866 | -0.976 |
| Higher orders| 0.085(22) | -0.046(6) | 0.034(6) | -0.005(6) |
| Total       | 314.801(22) | 314.809(6) | 314.810(6) | 314.808(6) |

In Table I the interelectronic-interaction corrections to the g factor of Li-like silicon are given. The results are obtained with four different starting potentials: Coulomb, core-Hartree, Perdew-Zunger, and local Dirac-Fock potentials. In the extended Furry picture, the interelectronic interaction contributes already in the zeroth order, due to the presence of the screening potential in the Dirac equation. The one-photon (first order) and two-photon (second order) exchange corrections have been evaluated to all orders in $\alpha Z$ in the framework of rigorous QED approach. The higher-order corrections have been extracted from the calculations performed by means of the large-scale configuration-interaction Dirac-Fock-Sturm method described in Refs. [10, 23]. As it was expected, the employment of the extended Furry picture increases the convergence of the perturbation expansion. This allows us to reduce the absolute uncertainty of the higher order interelectronic-interaction corrections. Finally, the rigorous evaluation of the two-photon exchange corrections and the improved calculations of the higher-order terms allow us to significantly increase the total accuracy of the interelectronic-interaction terms for all ions under consideration. E.g., in the case of $^{28}$Si$^{11+}$ ion the previous result was 0.000 314 903(74) [10], while the present calculation yields 0.000 314 809(6), and in the case of $^{208}$Pb$^{79+}$ ion instead of previous value 0.002 140 7(27) [10] we now receive 0.002 139 34(4).

Let us now turn to the screened self-energy corrections to the g factor of Li-like ions. In Refs. [12, 13] these corrections have been rigorously evaluated only for the $^{208}$Pb$^{79+}$ and $^{238}$U$^{89+}$ ions. The reasons for this to are twofold. First is the large numerical cancellations which occur in the point-by-point difference. Second is the poor convergence of the partial-wave expansion. In order to overcome these problems, we have performed the calculations in the extended Furry pic-
tured and employed a special treatment of the many-potential terms. The Feynman diagrams in the extended Furry picture corresponding to the screened self-energy corrections to the g factor are presented in Fig. 2. The corresponding expressions derived in Refs. [12, 13] remain formally the same but keeping in mind that the Dirac spectrum is now generated by solving the Dirac equation with the effective potential. In the second line of Fig. 2 the additional counterterm diagrams are depicted. The derivation of the formal expressions for them is relatively simple and will be presented elsewhere. The employment of the extended Furry picture allows us to substantially reduce the numerical cancellations of different terms as well as to improve convergence of the partial-wave expansion. However, in order to improve the convergence even further, we have employed a specific treatment of some many-potential terms. The standard way to treat the vertex and reducible corrections is to separate terms (zero-potential contributions) in which bound-electron propagators are replaced by free propagators. The remaining many-potential terms being ultraviolet finite are generally calculated directly in coordinate space [24]. However, for gaining better control over the partial-wave summation we separate also the so-called one-potential contributions. In this way the one-potential terms are treated in the momentum space. Such treatment of the one-potential term was applied in previous calculations of the one-electron self-energy corrections to the g factor in Refs. [23, 29] and to the magnetic-dipole transition amplitude in Ref. [50]. Here, we extend this procedure to the evaluation of the screened self-energy corrections to the g factor. Performing the analysis of the convergence of the partial-wave expansion for different terms we have found, that such treatment should be applied to the terms (C1) Eq. (32), (H3) Eq. (38), (I1) Eq. (47), and (I3) Eq. (49) in Ref. [13]. The corresponding one-potential contributions are given by the expressions:

\[
\Delta E_{\text{SQUED}}^{(1)} = -4\pi i\alpha \sum_p (-1)^p \int \frac{d^3p \, d^3p' \, d^4k}{(2\pi)^{10}} \frac{1}{k^2} \frac{1}{\bar{\psi}_a(p)} \times \gamma_{\mu} S_F(p-k) \gamma_0 V_{\text{eff}}(q) S_F(p-k-q) \times T_0(p-p'-q) + T_0(q) S_F(p-k-q) V_{\text{eff}}(p-p'-q) \gamma_0 S_F(p-k) \gamma^\mu \bar{\psi}_{\gamma a P a P b}(p') + (a \leftrightarrow b),
\]

where \( p = (\varepsilon_a, p), p' = (\varepsilon_a, p'), q = (\varepsilon_a, q), \Delta = \varepsilon_a - \varepsilon_{P a} \), and the notation \((a \leftrightarrow b)\) stands for the contribution with interchanged labels \(a\) and \(b\); \( \gamma^\mu = (\gamma, \gamma) \) are the Dirac matrices, \( S_F(p) = (\gamma \cdot p - m)^{-1} \) is the free-electron propagator, the interelectronic-interaction operator \( I(\varepsilon) \) and its derivatives are defined in a similar way as in Ref. [13], and \( V_{\text{eff}} \) is the effective potential being the sum of the nuclear and screening potentials. \( T_0 \) is the operator of interaction with a constant magnetic field, which reads in the momentum space:

\[
T_0(p) = i\mu_0(2\pi)^3[\alpha \times \nabla_p \delta^3(p)] \cdot \mathbf{H},
\]

where \( \mu_0 = |e|/2 \) is the Bohr magneton and \( \mathbf{H} \) is the magnetic field directed along the \( z \) axis. The wave function \( |\eta_a\rangle \) is given by the expression:

\[
|\eta_a\rangle = \sum_p (-1)^p \left\{ |a\rangle \left[ \langle \xi_b | P a P b | T_0[a] \rangle + |\zeta_b | P a P b | T_0[a] \rangle \right] \right. + \langle a | b | I(\Delta) | P a P b \rangle \left[ |a| T_0[a] \left. - \frac{1}{2} |b| T_0[b] \right] \right] \right. \}

and the wave functions \( |\xi\rangle \) and \( |\zeta\rangle \) are defined similar as in Ref. [12].

The ultraviolet-finite one-potential terms given by Eqs. (1)-(4) have been evaluated in the momentum space. The corresponding expressions in the coordinate space have been subtracted from the related many-potential terms by means of point-by-point difference. The partial-wave expansion for the many-potential terms was terminated at \( n_{\text{max}} = 15 \), and the remainder of the sum was estimated by a least-square polynomial fitting and by the \( \epsilon \)-algorithm of the Padé approximation. As a result, we have significantly increased the accuracy of the screened self-energy correction. In the case of \( ^{28}\text{Si}^{11+} \) ion the previous result was \(-0.0000000000110 \) [10], while the present calculation yields \(-0.0000000000242(5) \), and in the case of \( ^{208}\text{Pb}^{79+} \) ion instead of previous value \(-0.0000033(2) \) [12, 13] we now receive \(-0.00000344(2) \).

In Table III the individual contributions and the total values of the g factor for Li-like silicon \( ^{28}\text{Si}^{11+} \), calcium \( ^{40}\text{Ca}^{17+} \),
lead $^{208}$Pb$^{79+}$ and uranium $^{238}$U$^{89+}$ are presented together with the previously reported theoretical results and the experimental value for the case of silicon. The screened self-energy and interelectronic-interaction corrections calculated in this Letter allow to substantially increase the theoretical accuracy for all ions under consideration. The other contributions to the g factor presented in Table II were considered in detail in our previous studies \[10\] - \[13\]. Comparison with the experimental value for Li-like silicon ion provides tests of relativistic in-
tron corrections for the high-$Z$ region. The techniques and numerical methods developed can also be extended for the g factor of B-like ions, where the corresponding studies can also lead to an independent determination of the fine-structure constant \[31\].

The work reported in this paper was supported by DFG (Grant No. VO 1707/1-2), RFBR (Grants No. 13-02-00630 and 14-02-31316), and Saint Petersburg State University (Grants No. 11.0.15.2010 and 11.38.269.2014). D.A.G. acknowledges financial support by the FAIR – Russia Research Center and by the “Dynasty” foundation.

[1] H. Höffner, T. Beier, N. Hermanspahn, H.-J. Kluge, W. Quint, S. Stahl, J. Verdú, and G. Werth, Phys. Rev. Lett. 85, 5308 (2000).

[2] J. Verdú, S. Djekić, S. Stahl, T. Valenzuela, M. Vogel, G. Werth, T. Beier, H.-J. Kluge, and W. Quint, Phys. Rev. Lett. 92, 093002 (2004).

[3] S. Sturm, F. Köhler, J. Zatorski, A. Wagner, Z. Harman, G. Werth, W. Quint, C. H. Keitel, and K. Blaum, Nature 506, 467 (2014).

[4] S. Sturm, A. Wagner, B. Schabinger, J. Zatorski, Z. Harman, W. Quint, G. Werth, C. H. Keitel, and K. Blaum, Phys. Rev. Lett. 107, 023002 (2011).

[5] S. Sturm, A. Wagner, M. Kretzschmar, W. Quint, G. Werth, and K. Blaum, Phys. Rev. A 87, 030501(R) (2013).

[6] A. Wagner, S. Sturm, F. Köhler, D. A. Glazov, A. V. Volotka, G. Plunien, W. Quint, G. Werth, V. M. Shabaev, and K. Blaum, Phys. Rev. Lett. 110, 033003 (2013).

[7] D. von Lindenfels, M. Wiesel, D. A. Glazov, A. V. Volotka, M. M. Sokolov, V. M. Shabaev, G. Plunien, W. Quint, G. Birkl, A. Martin, et al., Phys. Rev. A 87, 023412 (2013).

[8] V. M. Shabaev, D. A. Glazov, M. B. Shabaeva, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. A 65, 062104 (2002).

[9] Z.-C. Yan, J. Phys. B 35, 1885 (2002).

[10] D. A. Glazov, V. M. Shabaev, I. I. Tupitsyn, A. V. Volotka, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. A 70, 062104 (2004).

[11] D. A. Glazov, A. V. Volotka, V. M. Shabaev, I. I. Tupitsyn, and G. Plunien, Phys. Lett. A 357, 330 (2006).

[12] A. V. Volotka, D. A. Glazov, V. M. Shabaev, I. I. Tupitsyn, and G. Plunien, Phys. Rev. Lett. 103, 033005 (2009).

[13] D. A. Glazov, A. V. Volotka, V. M. Shabaev, I. I. Tupitsyn, and G. Plunien, Phys. Rev. A 81, 062112 (2010).

[14] J. Sapirstein and K. T. Cheng, Phys. Rev. A 63, 032506 (2001).

[15] J. Sapirstein and K. T. Cheng, Phys. Rev. A 64, 022502 (2001).

[16] J. Sapirstein and K. T. Cheng, Phys. Rev. A 66, 042501 (2002).

[17] A. V. Volotka, D. A. Glazov, I. I. Tupitsyn, N. S. Oreshkina, G. Plunien, and V. M. Shabaev, Phys. Rev. A 78, 062507 (2008).

[18] Y. S. Kozhedub, A. V. Volotka, A. N. Artemyev, D. A. Glazov, G. Plunien, V. M. Shabaev, I. I. Tupitsyn, and T. Stöhlker, Phys. Rev. A 81, 042513 (2010).

[19] J. Sapirstein and K. T. Cheng, Phys. Rev. A 83, 012504 (2011).

[20] J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5084 (1981).

[21] V. M. Shabaev, I. I. Tupitsyn, K. Pachucki, G. Plunien, and V. A. Yerokhin, Phys. Rev. A 72, 062105 (2005).

[22] A. V. Volotka, D. A. Glazov, O. V. Andreev, V. M. Shabaev, I. I.
TABLE II: Individual contributions to the ground-state g factor of Li-like ions and comparison with the previously reported theoretical values as well as with the experimental result for the $^{28}$Si$^{11+}$ ion.

| Ion          | Dirac value (point nucleus) | Finite nuclear size | QED, $\sim\alpha$ | QED, $\sim\alpha^2$ | Interelectronic interaction | Screened self-energy | Screened vacuum-polarization | Nuclear recoil | Nuclear polarization | Total theory | Experiment |
|--------------|------------------------------|---------------------|------------------|---------------------|-----------------------------|---------------------|-----------------------------|---------------|-------------------|-------------|------------|
| $^{28}$Si$^{11+}$ | 1.998 254 751               | 0.002 324 044       | 0.000 003 517(1) | -0.000 003 502(2)  | 0.000 314 809(6)            | -0.000 000 242(5) | 0.000 000 006      | 0.000 003(1)  | -0.000 000 04(2)  | 2.000 889 892(8) | 2.000 889 899(51)$^a$ |
| $^{40}$Ca$^{17+}$ | 1.996 426 011               | 0.002 325 555(5)   | 0.000 003 520(2) | -0.000 003 520(2)  | 0.000 454 290(9)            | -0.000 000 387(7) | 0.000 000 017      | 0.000 000 61(2)  | -0.000 000 04(2)  | 1.999 202 041(13) | 1.999 202 24(17)$^b$  |
| $^{208}$Pb$^{79+}$ | 1.932 002 904               | 0.002 411 7(1)     | 0.000 003 6(5)   | -0.000 003 6(5)   | 0.002 139 34(4)             | -0.000 000 344(2) | 0.000 001 53(3)    | 0.000 000 25(35) | -0.000 000 04(2)  | 1.936 627 2(6)   | 1.936 628 7(28)$^c$  |
| $^{238}$U$^{89+}$ | 1.910 722 624               | 0.002 446 3(2)     | -0.000 003 6(8)  | 0.000 003 6(8)    | 0.002 500 05(6)             | -0.000 000 004(2) | 0.000 000 011(7)   | 0.000 000 25(35) | -0.000 000 04(2)  | 1.915 904 8(11) | 1.915 905 7(41)$^c$  |

$^a$Wagner et al. [6]; $^b$Glazov et al. [10]; $^c$Glazov et al. [13].