Relativistic and QED corrections to the $g$ factor of Li-like ions

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Abstract

Calculations of various corrections to the $g$ factor of Li-like ions are presented, which result in a significant improvement of the theoretical accuracy in the region $Z = 6–92$. The configuration-interaction Dirac-Fock method is employed for the evaluation of the interelectronic-interaction correction of order $1=Z^2$ and higher. This correction is combined with the $1=Z$ interelectronic-interaction term derived within a rigorous QED approach. The one-electron QED corrections of first in $1=Z$ are calculated to all orders in the parameter $Z$. The screening of QED corrections is taken into account to the leading orders in $Z$ and $1=Z$.

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I. INTRODUCTION

Recent high-precision measurements of $g$ factors of H-like carbon \cite{1, 2} and oxygen \cite{3} have provided a possibility for studying binding QED effects in an external magnetic field in these systems. The experiments were performed on single H-like ions confined in a Penning ion trap at low temperatures. A relative accuracy of $5 \times 10^{-10}$ was obtained in Ref. \cite{2} for the ratio of the electronic Larmor precession frequency $\omega_L$ and the ion cyclotron frequency $\omega_c$, which is connected with the $g$-factor value by

$$\frac{\omega_L}{\omega_c} = \frac{g}{2} \frac{e \mu}{m} ;$$

\hspace{1cm} (1)

where $e$ is the elementary charge unit, $\mu$ is the charge of the ion, $m_{\text{ion}}$ is the ion mass, and $m$ is the electron mass. The experimental results are shown to be sensitive to one- and two-loop binding QED effects and to the nuclear-recoil corrections. Further progress is anticipated from the experimental side, as well as an extension of measurements to the ions with more than one electron.

New perspectives for testing QED effects in $g$ factors of highly charged ions motivated numerous theoretical investigations on this subject during the last years. We mention here numerical calculations of the one-loop self-energy correction to all orders in $Z$ \cite{4, 5, 6, 7, 8}, numerical \cite{5, 6} and analytical \cite{9, 10, 11} evaluations of the one-loop vacuum-polarization contribution, analytical results for the nuclear-size correction \cite{9, 12}, and calculations of the nuclear-recoil effects \cite{13, 14, 15, 16} and two-loop binding QED corrections \cite{17, 18, 19}. As a result of these studies, the present theoretical accuracy of the $g$-factor values is several times better than that of the experimental results. An important consequence of the investigations of the $g$ factor is the possibility to determine the electron mass from Eq. (1) by combining the theoretical $g$-factor value and the experimental result for $\omega_L/\omega_c$. We note that the 1998 CODATA value for the electron mass \cite{20} has an error of $2 \times 10^{-9}$, which is 4 times larger than the experimental uncertainty of the result for carbon \cite{2} and 3 times larger than the one for oxygen \cite{3}. A new determination of the electron mass presented in Refs. \cite{14, 15, 21} provided an improvement of the accuracy of the electron mass by a factor of 4. As a result, the 2002 CODATA value for the electron mass \cite{22} is derived mainly from the $g$ factor of H-like ions. It is expected that in the future an extension of experimental investigations towards higher-$Z$ ions could lead also to an independent determination of the fine structure constant \cite{18, 23}.

The accuracy of theoretical values for the $g$ factor of high-$Z$ H-like ions is presently limited by
nuclear effects [15, 24]. The uncertainty introduced by them in the high-$Z$ region is comparable with the binding QED correction of second order in $\lambda$. Since the nuclear effects do not allow an accurate theoretical description at present, this puts a serious obstacle on the way to improvement of theoretical predictions and to an identification of two-loop QED corrections in future experiments. However, it was recently shown [23, 26] that the uncertainty due to the nuclear effects can be significantly reduced in a specific combination of the $g$ factors of H- and Li-like ions with the same nucleus,

$$g^0 = g_{\text{H-like}}^0 \\ g_{\text{Li-like}}$$

(2)

where $g_{\text{H-like}}$ and $g_{\text{Li-like}}$ are the $g$ factors of H- and Li-like ions, respectively, and the parameter $\lambda$ is calculated numerically, as explained in Ref. [25]. Numerical calculations show that the influence of the nuclear effects on the difference $g^0$ is by two orders of magnitude smaller than that on the $g$-factor values $g_{\text{H-like}}$ and $g_{\text{Li-like}}$ separately. Therefore, the specific difference $g^0$ can be in principle studied up to much higher accuracy than the $g$ factor of an H-like or Li-like ion. In order to realize this project, one need to perform theoretical and experimental investigations of the $g$ factor of Li-like ions with an accuracy comparable to that for H-like ions.

Extending theoretical description from an H-like to a Li-like ion, one encounters a serious complication due to the presence of additional electrons. Moreover, all contributions to the $g$ value for an $ns$ state are of pure relativistic and QED origin, which makes the treatment of the electron correlation much more intricate than, e.g., in calculating the binding energies. A number of relativistic calculations of the $g$ factor of Li-like ions were carried out previously [27, 28, 29, 30, 31, 32]. However, in order to reach the accuracy comparable to the one for H-like ions, a systematic treatment of the QED corrections is required. In our previous publications [25, 26], we presented theoretical values for the $g$ factor of Li-like ions including all presently known QED, nuclear, and interelectronic-interaction corrections for a wide range of the nuclear-charge number $Z$. The goal of the present investigation is to improve these theoretical predictions by calculating several corrections that provide the leading uncertainty to the theoretical values.

For low-$Z$ ions, the uncertainty of the $g$-factor values [25, 26] was mainly determined by the error due to the interelectronic-interaction correction. A part of this correction that is of first order in $1=Z$ was evaluated in Ref. [25] within a rigorous QED approach, whereas the remainder (of order $1=Z^2$ and higher) was extracted from the variational calculations by Yan [30, 31] in case of low-$Z$ ions and from the many-body perturbation theory calculations by Lindroth and Ynnerman [29] for high-$Z$ ions. In the present work, we evaluate the interelectronic-interaction correction of
order $1=Z^2$ and higher by a large-scale configuration-interaction Dirac-Fock method.

For middle- and high-Z ions, the main error of the theoretical values of Ref. [25] originated from the binding QED correction. In that work, it was evaluated to the leading order in $Z$ [namely, $(Z^2)$] and to the zeroth order in $1=Z$. In the present investigation, we employ the recent calculation of the self-energy term of the one-electron QED correction to all orders in $Z$ [8] and calculate the vacuum-polarization term. We also evaluate the screened QED correction to its leading orders in $Z$ and $1=Z$.

The relativistic units ($\sim c=1$) and the Heaviside charge unit ($e^2=(4\pi);e<0$) are used in the paper.

II. FORMULATION OF THE PROBLEM

The $g$ factor of an atom with a spinless nucleus is defined as

$$g = \frac{1}{0J} \frac{\partial E(H)}{\partial H} \bigg|_{H=0} = \frac{1}{0J} \frac{\partial}{\partial H} jH \frac{j}{H=0};$$

(3)

where $H$ is the Hamiltonian of the atom in magnetic field $H$, $H = jH$ and the $z$ axis is directed along $H$, $E(H)$ is the energy of the state with the maximal ($M_J = J$) projection of the angular momentum on the $z$ axis, and $\mu = j\varepsilon = (2m)$ is the Bohr magneton. If the perturbation theory of first order in $H$ is used to obtain the energy shift $E(H)$, Eq. (3) can be written as

$$g = \frac{1}{0J} \frac{E(H)}{H};$$

(4)

In what follows, we will use both definitions.

In the case of a high-Z Li-like ion, in the zeroth-order approximation one can neglect the interaction of the $2s$ electron with the closed $(1s)^2$ shell. We thus use the one-electron Dirac equation as the starting point in our evaluation of the $g$ factor. The corresponding Hamiltonian is

$$h = p + m + V + V^{\text{mag}};$$

(5)

where $V = Z=\varepsilon$ is the Coulomb potential induced by the nucleus and $V^{\text{mag}} = e \cdot A$ represents the interaction with the magnetic field. For the homogeneous magnetic field the vector potential is $A = 1=2 [H \cdot \varepsilon]$ and thus $V^{\text{mag}} = (e=2)H [\varepsilon \cdot \varepsilon]$.

Evaluating the energy shift as the expectation value of $V^{\text{mag}}$ with the Dirac wave functions, we obtain the lowest-order $g$-factor value for the $2s$ state,

$$g_0 = \frac{2}{3} \left( 1 + \frac{p}{2+2} \right) = 2 \left( \frac{Z^2}{6} \right) + \cdots;$$

(6)
where $p = \frac{1}{(Z^2)}$. Various corrections to $g_D$ arise due to the interelectronic interaction ($g_{\text{int}}$), one-electron QED effects ($g_{\text{QED}}$), the screened QED effects ($g_{\text{SQED}}$), and nuclear effects ($g_{\text{nuc}}$). We thus write the total theoretical value for the $g$ factor as

$$g = g_D + g_{\text{int}} + g_{\text{QED}} + g_{\text{SQED}} + g_{\text{nuc}};$$

(7)

with the corrections $g_{\text{int}}$, $g_{\text{QED}}$, $g_{\text{SQED}}$, and $g_{\text{nuc}}$ evaluated in Sections III, IV, V, and VI, respectively.

III. INTERELECTRONIC INTERACTION

To evaluate the interelectronic-interaction effects, we start with the relativistic Hamiltonian in the no-pair approximation,

$$H = \sum_j \hbar(j) + H_{\text{int}} + H_{\text{C}} + H_{\text{B}};$$

(8)

where $\hbar$ is the one-particle Dirac Hamiltonian $\mathfrak{h}$, the index $j = 1, \ldots, N$ numerates the electrons, $H_{\text{C}}$ is the Coulomb interaction, $H_{\text{B}}$ is the Breit interaction, and $+$ is the projector on the positive-energy states, which is the product of the one-electron projectors $+$ ($i$),

$$+ = + (1) \cdots (N);$$

(9)

Here,

$$+ (i) = \sum_n j \mathfrak{u}_n (i) \mathfrak{u}_n (i) j;$$

(10)

where $\mathfrak{u}_n (i)$ are the positive-energy eigenstates of an effective one-particle Hamiltonian $\mathfrak{h}_u$. Two different Hamiltonians $\mathfrak{h}$ and $\mathfrak{h}_{\text{HFD}}$ were considered as the operator $\mathfrak{h}_u$, where $\mathfrak{h}$ is the one-electron Dirac Hamiltonian $\mathfrak{h}$ and $\mathfrak{h}_{\text{HFD}}$ is the Hartree-Fock-Dirac operator without the Breit interaction but including the interaction with the external field [33, 34]. However, since $\mathfrak{h}_{\text{HFD}}$ corresponds to a better zero approximation and, therefore, provides much faster convergence, all the final results were obtained with this Hamiltonian. In both cases the functions $\mathfrak{u}_n$ and hence the projector $+$ depend on the external magnetic field. Therefore, the derivative with respect to $\mathfrak{h}$ in Eq. (3) contains not only the derivative of the one-electron part of the Hamiltonian $\mathfrak{h}$, but also the derivative of the projector $+$. The derivative of $+$ can be obtained explicitly and one can show that its contribution to the $g$ factor is equivalent to the contribution of the negative-energy states.
In our computational approach, we obtain the $g$-factor value by using Eq. (3) in the finite-difference approximation,
\[
g = \frac{1}{2} \frac{E(H)}{E(H)} + O[(H)^3];
\]
(11) since the Hellman-Feynman theorem is not exactly fulfilled for the approximate wave functions. The optimal choice of the finite difference $H$ was found to be $0.001 (a.u.)$. We checked that scaling this value by a factor of 2 does not influence our results for the $g$ factor.

In order to determine the space of one-electron functions $\ell_j^gM_j$, we employed the combined Dirac-Fock (DF) ($j = 1; \ldots; m$) and the Dirac-Fock-Sturm (DFS) ($j = m + 1; \ldots; M$) basis set. The index $j$ here enumerates different occupied and vacant one-electron states. The external magnetic field and the Breit interaction were not included in the DF and DFS operators, when the basis set was generated. For the occupied atomic shells, the orbitals $\ell_j^g$ were obtained by the restricted DF method, based on a numerical solution of the radial DF equations. The vacant orbitals $\ell_j^g (j = m + 1; \ldots; M)$ were obtained by solving the Dirac-Fock-Sturm equations
\[
h_{D F}^{\ell_j} \psi_j = \frac{1}{2} E(H) \psi_j, \quad j = m + 1; \ldots; M;
\]
(12) where $h_{D F}$ is the Dirac-Fock operator, $\psi_j$ is the one-electron energy of the occupied DF orbital $\ell_j^g$, and $\psi_j (r)$ is a constant-sign weight function. The parameter $\lambda$ in Eq. (12) can be considered as an eigenvalue of the Sturmian operator. If $\psi_j (r) \neq 0$ at $r = 1$, all Sturmian functions $\ell_j^g$ have the same asymptotics at $r = 1$. It is clear that for $\lambda = 0$ the Sturmian function coincides with the reference DF orbital $\ell_j^g$. The widely used choice of the weight function is $\psi_j (r) = 1 - r$, which leads to the well-known “charge quantization”. In the relativistic case this choice is not very successful. In our calculations we used the following weight function
\[
\psi_j (r) = \frac{1}{2} \exp \left[ \left( \frac{r}{r} \right)^2 \right];
\]
(13) which, unlike $1 - r$, is regular at the origin. It is well known that the Sturmian operator is Hermitian and, contrary to the Fock operator, does not have the continuum spectra. Therefore, the set of the Sturmian eigenfunctions including the negative-energy states forms the discrete and complete basis set in the space of one-electron wave functions. This basis set is orthogonal with the weight function $\psi_j (r)$.

To generate the one-electron wave functions $n$, we used the unrestricted DF method in the joined DF and DFS basis,
\[
n_j = \sum_{j} C_{j n} \ell_j^g:
\]
(14)
The coefficients \( C_{jn} \) were obtained by solving HFD matrix equations

\[
\hat{F} C_n = \hat{S} C_n; \tag{15}
\]

where \( \hat{F} \) is the Dirac-Fock matrix in the joined basis of DF and DFS orbitals of a free ion. The external magnetic field was included in the \( \hat{F} \) matrix, whereas the Breit interaction was not. The matrix \( \hat{S} \) in Eq. (15) is nonorthogonal, since the DFS orbitals are not orthogonal in the usual sense. The negative-energy DFS functions were included in the total basis set. Eq. (15) was used to generate the whole set of orthogonal one-electron wave functions \( n (n = 1; \ldots ; M) \), including all vacant states.

It should be noted that even if the external magnetic field \( H \) is equal to zero, the set of one-electron functions \( n \) differs from the set of basis functions ‘\( j \). For the occupied states, the unrestricted DF method accounts for the core-polarization effects (the spin polarization in our case), in contrast to the restricted DF method. For the vacant states, the difference is more significant, since the DF and DFS operators are essentially different.

The large-scale configuration-interaction Dirac-Fock (CI-DF) method was used to solve the Dirac-Coulomb-Breit equation in the external magnetic field

\[
H (M_J) = \mathcal{E} (M_J) (M_J) \tag{16}
\]

where \( H \) is the non-pair Hamiltonian (8). The many-electron wave function \( \Gamma (M_J) \) with quantum numbers and \( M_J \) was expanded in terms of a large number of the Slater determinants (SD) with the same projection \( M_J \) of the total angular momentum \( J \)

\[
\Gamma (M_J) = \sum \chi (M_J) \det (M_J) \tag{17}
\]

The configuration state functions (CSFs) with angular momentum \( J \) were not used in our calculations, since the Hamiltonian \( H \) contains the interaction with the external magnetic field and, therefore, does not commute with the operator \( J^2 \). The Slater determinants are constructed from the one-electron wave functions \( n \) (14). The same orbitals were used in Eq. (10) in order to construct the projector \( \hat{\mathcal{S}} \). The basis of one-electron functions used in our calculations was 12s 11p 10d 6f 4g 2h 1i. The set of the SD in expansion (17) was generated including all single, double, and triple excitations. The total number of SD was 552359. The results of the calculation are presented in Table I. The interelectronic-interaction correction \( g^{CI}_{int} DF \) is the difference of the result obtained by Eq. (11) for the point nuclear model and the Dirac \( g \)-factor value \( g_D \) (6).
The result for the $g_{\text{CI-DF}}^{\text{int}}$ correction obtained by the CI-DF method can be improved by employing a rigorous QED treatment of the part of this correction that is of order $1/Z$, which was presented in Ref. [25]. In order to combine two different treatments, we isolate the contribution of order $1/Z^2$ and higher from the $g_{\text{int}}^{\text{CI-DF}}$ correction by subtracting the value of the $1/Z$ term calculated in the Breit approximation. The resulting “higher-order” correction ($g_{\text{int}}^{(2+)}$) is listed in the third column of Table I. The numerical results for the interelectronic-interaction correction of first order in $1/Z$ ($g_{\text{int}}^{(1)}$) are taken from Ref. [25] and listed in the fourth column. This contribution was evaluated in framework of QED and utilizing the Fermi model for the nuclear-charge distribution. Total results $g_{\text{int}} = g_{\text{int}}^{(1)} + g_{\text{int}}^{(2+)}$ are presented in the last column. The error bars indicated represent a quadratical sum of a numerical error and an estimation of omitted terms, i.e., contributions beyond the Breit approximation to $g_{\text{int}}^{(2+)}$. They were estimated as $(Z)^2 g_{\text{int}}^{(2+)}$.

To compare our results with the corresponding Yan’s calculations [30, 31], which account for the lowest-order relativistic effects, we have isolated the $2^2$ contribution in our CI-DF calculation. It was done by four times increase of the velocity of light (in atomic units) and by an extrapolation of the obtained results (with the $2^2$ factor isolated) to the $c = 1$ limit. Table II, which presents the related comparison for $g_{2^2}$ values, shows that for $Z > 5$ the contribution of the higher-order relativistic effects is much larger than the difference between our $2^2$ results and those of Yan.

### IV. ONE-ELECTRON QED CORRECTIONS

To zeroth order in $1/Z$, the QED correction for the ground state of a Li-like ion is given by the one-electron QED contribution evaluated for the $2s$ Dirac state. This correction is represented by a perturbation expansion in the fine-structure constant $\alpha$,

$$ g_{\text{QED}} = g_{\text{QED}}^{(1)} + g_{\text{QED}}^{(2)} + \cdots; \quad (18) $$

where the superscript indicates the order in $\alpha$.

The first-order QED correction is given by the sum of the self-energy and vacuum-polarization contributions, $g_{\text{QED}}^{(1)} = g_{SE}^{(1)} + g_{VP}^{(1)}$. The self-energy correction for the $2s$ state was recently calculated to all orders in $Z$ in Ref. [18]. The corresponding results are listed in the second column of Table III. The vacuum-polarization correction consists of two parts that can be thought to originate from the first-order vacuum-polarization diagram with the magnetic interaction inserted into
the external electron line (the *electric-loop* contribution \( g_{\text{P}}^e \)), and into the vacuum-polarization loop (the *magnetic-loop* contribution \( g_{\text{P}}^m \)). The electric-loop contribution is calculated in the present work by utilizing the known expression for the Uehling potential and approximate formulas for the Wichmann-Kroll potential taken from Ref. [35]. The results of the calculation are presented in the third and fourth columns of Table III. The remaining magnetic-loop correction is known to vanish in the Uehling approximation, and its contribution is small as compared to the electric-loop part. This correction was calculated to all orders in \( Z \) only for the \( 1s \) state [5, 6]. Because of this, we employ the analytical result of Ref. [11] for its leading contribution in \( Z \), which reads (for an \( ns \) state),

\[
g_{\text{P}}^m = \frac{7}{216} \left( \frac{Z}{n^3} \right)^5 ;
\]

The corresponding results are listed in the fifth column of Table III. The uncertainty of the magnetic-loop contribution is estimated by comparison of the all-order numerical results of Ref. [6] for the \( 1s \) state with the lowest-order analytical result (19).

QED corrections of higher orders in have not been calculated to all orders in \( Z \) up to now. Two first terms of their \( Z \) expansion can be represented by the free-electron \( g_2 \) factor multiplied by a relativistic kinematical factor [17, 18, 25, 36]. The result yields (for an \( ns \) state)

\[
g_{\text{QED}}^{(i)} = 2 - \frac{i A^{(i)}}{6n^2} \left( 1 + \frac{(Z)^2}{6n^2} \right) ;
\]

where \( 2 ( = i A^{(i)} \) is the contribution of order \( ^i \) to the free-electron \( g \) factor. Its numerical values (see [37, 38] and references therein) are

\[
A^{(1)} = \frac{1}{2} ;
\]

\[
A^{(2)} = 0.328478965 \ldots ;
\]

\[
A^{(3)} = 1.181241456 \ldots ;
\]

\[
A^{(4)} = 1.7366(384) ;
\]

Recently, a part of the two-loop QED contribution of order \( 2 (Z)^4 \) was evaluated in Ref. [19] with the result

\[
g_{\text{QED}}^{(2)} (h \chi) = - \frac{2}{n^3} \left( \frac{Z}{56} \right) \ln \left( \frac{Z^2}{2} \right) + a_{40} ;
\]

where the numerical values of the coefficient term are \( a_{40}^{(2)} (1s) = 18477948664 (1) \) and \( a_{40}^{(2)} (2s) = 19781820939 (1) \). This expression accounts for the complete logarithmic dependence in this order and the dominant part of the constant term. We observe, however, that in the
one-loop case, inclusion of the term of the order \((Z)^4\) is meaningful for sufficiently small values of \(Z\) only. In the high-\(Z\) region, addition of this term makes the \(Z\)-expansion results deviate more from the “exact” numerical values. We thus include the contribution (25) for \(Z > 30\) only. The relative uncertainty of the two-loop binding QED correction for \(Z > 30\) was estimated as the ratio of the part of the one-loop QED correction that is of order \((Z)^5\) and higher to the part that is within the \((Z)^4\) approximation [19], multiplied by a factor of 4. For \(Z > 30\), we estimate the relative uncertainty by the ratio of the part of the one-loop QED correction that is of order \((Z)^4\) and higher to the part that is within the \((Z)^2\) approximation, multiplied by a factor of 2.

V. SCREENED QED CORRECTIONS

In this section we investigate the influence of the interelectronic interaction on the QED effects, known also as the “screening” of QED corrections. To derive the screened QED correction of first order in \(1/Z\), we apply an approximate method, which yields the complete result to the order \((Z)^2\). Following Hegstrom [39], we adopt the Hamiltonian

\[
H = \sum_j h(j) + \sum_j h^{rad}(j) + H^{int};
\]  

where \(h\) is defined by Eq. (5), \(H^{int}\) incorporates the interelectronic interaction within the Breit approximation [5], and \(h^{rad}\) accounts for the interaction of the anomalous magnetic moment of electron with the magnetic and electric fields,

\[
h^{rad} = \frac{g_{\text{free}}}{2} \frac{2}{0} [ (H)_{ij} (E)];
\]  

Here

\[
g_{\text{free}} = 2 \sum_i \begin{pmatrix} 1 & i \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} A^{(i)};
\]  

is the free-electron \(g\) factor and \(A^{(i)} = \begin{pmatrix} 0 & 0 \end{pmatrix} A\). The magnetic field \(H^{(j)}\) acting on the \(j\)th electron in Eq. (27) includes the external homogeneous magnetic field \(H\) and the field induced by the other electrons

\[
H^{(j)} = H + \sum_{k \neq j} \frac{e}{4} \frac{k}{r_{jk}^3} r_{jk} ;
\]  

where \( r_{jk} = r_j - r_k \). The electric field \( E(j) \) includes the fields induced by nucleus and by the other electrons

\[
E(j) = \frac{\pm e r_j}{4} \frac{r_j^3}{r_j} + X \frac{e r_{jk}}{4} \frac{r_j^3}{r_{jk}^3} : (30)
\]

We divide the contribution arising from \( h^{rad} \) into three parts,

\[
H^{rad}_1 = \frac{g_{\text{free}}}{2} \frac{2}{0} \frac{X}{j} j(j) ; (31)
\]

\[
H^{rad}_2 = \frac{g_{\text{free}}}{2} \frac{2}{0} \frac{\pm e}{4} \frac{X}{j} j(j) \frac{r_j}{r_j^3} ; (32)
\]

\[
H^{rad}_3 = \frac{g_{\text{free}}}{2} \frac{2}{0} \frac{e}{4} \frac{X}{j \neq k} j(j) j(k) \frac{r_{jk}}{r_{jk}^3} i(j) j(k) ; (33)
\]

The matrices \( j, j, j \) here act on the spinor variables of the \( j \)th electron. To first order in \( 1/Z \), the screened QED correction to the \( g \) factor can be now derived by the standard Rayleigh-Schrödinger perturbation theory, separating corrections linear in the magnetic field \( H \), which are of first order in the parameter \( 1/Z \). The contributions of interest can be conventionally represented by the following combinations:

\[
E_1 H^{rad}_1 H^{int} + (\text{permutations}) ; (34)
\]

\[
E_2 H^{rad}_2 V^{mag} H^{int} + (\text{permutations}) ; (35)
\]

\[
E_3 H^{rad}_3 V^{mag} + (\text{permutations}) : (36)
\]

After angular integration, the summation over the complete Dirac-Coulomb spectrum was performed by the finite basis set method with basis functions constructed from \( B \) splines [40, 41].

The numerical results for the screened QED correction of first order in \( 1/Z \), \( g_{SQ,ED}^{(1)} \), are presented in Table [IV] in terms of the function \( R(Z) \), defined as

\[
g_{SQ,ED}^{(1)} = (g_{\text{free}}) (Z) \frac{2}{Z} R(Z) : (37)
\]

The terms \( R_i(Z) \) with \( i = 1, 2, 3 \) are induced by Eqs. (34)-(36), respectively.

The screened QED correction of higher orders in \( 1/Z \) should be accounted for when considering low-Z ions. We extract this correction from the recent evaluations by Yan [30, 31], which were
performed on nonrelativistic wave functions but with the interelectronic interaction taken into account to all orders in \( \frac{1}{Z} \). Yan’s results for the screened QED correction can be represented in the form

\[
g_{\text{SQED}}^\text{Yan} = (g_{\text{free}}^2) \left( \frac{1}{Z} R(0) + \frac{1}{Z^2} Q(0) + \cdots \right); \tag{38}
\]

where \( R(0) = 274/2187 \). The functions \( R, Q, \cdots \) here do not have any dependence on \( Z \) since Yan’s calculations are based on the nonrelativistic form of the Hamiltonian (26). We obtain the numerical value of \( Q(0) \) by fitting Yan’s results for \( Z = 3–12 \) to the form (38), which yields \( Q(0) = 0.071(1) \). With this value of \( Q(0) \), formula (38) was used to estimate the higher-order screened QED correction for \( Z > 12 \).

In Table V we present the results for the screened QED correction of first order in \( \frac{1}{Z} \) \( \left( g_{\text{SQED}}^{(1)} \right) \) and of higher orders in \( \frac{1}{Z} \) \( \left( g_{\text{SQED}}^{(2+)} \right) \). The error of the term \( g_{\text{SQED}}^{(1)} \) was estimated as the part of the one-electron QED correction that is beyond the \( (Z)^2 \) approximation, multiplied by a factor \( 3/Z \). The uncertainty ascribed to the \( g_{\text{SQED}}^{(2+)} \) contribution was evaluated as \( 3(Z)^2 g_{\text{SQED}}^{(2+)} \).

VI. NUCLEAR EFFECTS

In this section we briefly summarize the known results for the nuclear effects on the \( g \) factor of Li-like ions. The correction to the Dirac \( g \)-factor value due to the extended nuclear size is relatively simple. For high-\( Z \) ions, it is evaluated numerically by employing the Fermi model for the nuclear-charge distribution. The uncertainty is estimated by taking the difference of the results obtained for the Fermi and sphere nuclear models. For low-\( Z \) ions, to a good accuracy, this correction can be evaluated by a simple analytical formula obtained in Ref. [12],

\[
g_{\text{NS}} = \frac{1}{3} (Z)^4 m^2 \hbar^2 i \left[ 1 + (Z)^2 \right] \frac{35}{16} C \frac{\hbar^2 \ln(\frac{Z m r i}{\hbar^2 i})}{\hbar^2 i}; \tag{39}
\]

Here \( C = 0.5772156649 \) is the Euler constant and the expectation value has to be evaluated with the proper nuclear-charge density.

Systematic QED theory for the nuclear-recoil effect on the atomic \( g \) factor to the first order in \( m = M \) and to all orders in \( Z \) was developed in Ref. [13]. The one-electron recoil correction derived in that work is expressed as the sum of the lower-order and the higher-order term. The first
one can be calculated analytically to yield for the $2s$ state (cf. 13)
\[
g_{\text{recL}} = \frac{m}{M} \left( \frac{(Z)^2}{4} \right) \frac{1}{1 + \left( \frac{(Z)^2}{3(1 + 1)^2} \right)^2 + \frac{\mathcal{Z}}{2(1 + 1)^2}} ;
\]
where $\mathcal{Z} = \frac{\mathcal{P}}{1} (Z)^2$. The higher-order term $g_{\text{recH}}$ was calculated numerically in Ref. 15 for the $1s$ state only. These numerical results showed the $(Z)^5$ behaviour of this term at low $Z$.

We estimate the relative uncertainty of the result (40) due to neglecting the higher-order term as the ratio $g_{\text{recH}} = g_{\text{recL}}$ for the $1s$ state, multiplied by a factor of 1.5.

The contribution of the two-electron recoil effect can be extracted from the results of Yan [30, 31]. For $Z = 3 \ldots 12$, it was evaluated as the difference of Yan’s result of order $^2m=M$ and the nonrelativistic limit of Eq. (40). Fitting this difference to the form
\[
g_{\text{two el}} = \frac{m}{M} \frac{(Z)^2}{4} \frac{1}{Z^C} + \frac{1}{Z^2 D} \cdots
\]
yields $C = 3B(Z)$. With this value of $C$, formula (41) was used to estimate the two-electron recoil correction for $Z > 12$.

Finally, we note that the nuclear polarization effect on the atomic $g$ factor was evaluated in Ref. 24.

VII. RESULTS AND DISCUSSION

In Table VI, we present the individual contributions to the $g$ factor of the ground state of Li-like ions. The Dirac point-nucleus value is obtained by Eq. (6). The finite nuclear size correction to this value is evaluated by Eq. (39) for low-$Z$ ions and by a direct numerical solution of the Dirac equation for high-$Z$ ions. The interelectronic-interaction correction $g_{\text{int}}$ is the sum of the part of first order in $1=Z$, $g_{\text{int}}^{(1)}$, obtained in framework of QED and of the higher-order part, $g_{\text{int}}^{(2+)}$, evaluated by the CI-DF method, as described in Section III. The QED correction of order 2 is the sum of the one-electron self-energy and vacuum-polarization terms presented in Table III. The QED correction of order 2 and higher incorporates the known terms of the $Z$ expansion, as explained in Section IV. The screened QED correction is discussed in Section V. The corresponding results are taken from Table V. The nuclear recoil correction is obtained as explained in Section VI. For lead and uranium, we include also the nuclear-polarization correction calculated in Ref. 24.
Table VI demonstrates a significant improvement achieved comparing to our previous evaluations [25, 26]. The uncertainty of the presented theoretical values for carbon and oxygen is 2 and 3 times better than those of Ref. [26], respectively; whereas for uranium the accuracy is improved by two orders of magnitude. Progress in the high-\(Z\) region is mainly due to the evaluation of the one-loop QED corrections to all order in \(Z\), while for low-\(Z\) ions it is largely due to the interelectronic-interaction correction and the screened QED correction.

The accuracy of the theoretical values in Table VI is several parts in \(10^{-8}\) for low-\(Z\) ions and a few parts in \(10^{-7}\) for middle-\(Z\) ions. It decreases further with \(Z\) increasing and reaches \(5 \times 10^{-6}\) for uranium. So, despite the achieved improvement, the accuracy for Li-like ions is still significantly lower than that for H-like ions [7, 15] and also than the precision that can be presently addressed in experiments [1, 2, 3]. In particular, the nearest aim of experimental investigations of the Mainz-GSI collaboration is the \(g\) factor of Li-like calcium. The anticipated experimental accuracy is at the ppb level, which can be compared with the relative theoretical error of \(10^{-7}\) from Table VI.

The uncertainty of the present theoretical values is mainly defined by the interelectronic-interaction correction and by the screened QED correction. An improvement in the theoretical description of the interelectronic-interaction effects can be achieved by a rigorous QED treatment of the part of order \(1/\langle Z^2\rangle\) and by calculating the remainder within the Breit approximation. Such a program has been carried out for the Lamb shift in Li-like ions [42, 43, 44, 45]. However, a similar calculation for the \(g\) factor is going to be significantly more difficult due to the presence of the external magnetic interaction and requires a further development of methods of calculational QED. As to the screened QED correction, in the present work it was calculated to its leading order in \(Z\) only. As a first step beyond this approximation, which can improve the results for this correction in the high-\(Z\) region, one may consider an evaluation of the one-loop QED corrections in an effective potential that partly accounts for the interelectronic-interaction effects [46, 47]. These two topics will be the subjects of our subsequent investigations.

In summary, we have presented calculations of the interelectronic-interaction, one-electron QED, and screened QED corrections to the \(g\) factor of the ground state of Li-like ions. This resulted in a significant improvement of theoretical predictions in a wide range of the nuclear-charge values \(Z\). We have analyzed also perspectives for further progress in the theoretical description of these systems and for probing the QED effects in future experiments.
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TABLE I: The interelectronic-interaction correction $g_{\text{int}} = g_{\text{int}}^{(1)} + g_{\text{int}}^{(2+)}$. The contributions $g_{\text{int}}^{CI}$ and $g_{\text{int}}^{(2+)}$ are calculated for the point nucleus, whereas the correction $g_{\text{int}}^{(1)}$ — for the Fermi model of the nuclear-charge distribution. All values shown in units of $10^{-6}$.

| Z  | $g_{\text{int}}^{CI}$ | $g_{\text{int}}^{(2+)}$ | $g_{\text{int}}^{(1)}$ | $g_{\text{int}}$   |
|----|----------------------|------------------------|---------------------|------------------|
| 3  | 61.591               | 7.082                  | 68.676              | 61.594 (10)      |
| 4  | 84.822               | 6.752                  | 91.591              | 84.839 (12)      |
| 5  | 107.806              | 6.679                  | 114.493             | 107.814 (14)     |
| 6  | 130.745              | 6.661                  | 137.419             | 130.758 (19)     |
| 8  | 176.627              | 6.662                  | 183.320             | 176.658 (30)     |
| 10 | 222.571              | 6.673                  | 229.301             | 222.628 (42)     |
| 12 | 268.604              | 6.682                  | 275.385             | 268.703 (55)     |
| 14 | 314.744              | 6.689                  | 321.592             | 314.903 (74)     |
| 16 | 361.011              | 6.695                  | 367.939             | 361.244 (94)     |
| 18 | 407.422              | 6.699                  | 414.451             | 407.75 (12)      |
| 20 | 453.994              | 6.702                  | 461.148             | 454.45 (14)      |
| 24 | 547.70               | 6.71                   | 555.18              | 548.48 (21)      |
| 32 | 737.93               | 6.71                   | 746.46              | 739.75 (37)      |
| 54 | 1291.39              | 6.81                   | 1306.22             | 1299.4 (1.1)     |
| 82 | 2120.76              | 7.64                   | 2148.29             | 2140.7 (2.7)     |
| 92 | 2481.67              | 8.48                   | 2509.84             | 2501.4 (3.8)     |
TABLE II: The comparison of the present CI-DF calculations of the $g$ factor and the values obtained by Yan [30, 31]. The second column presents our $g^2$ values, incorporating the effects of binding and electron correlation. The $g^2$ limit is shown in the third column. Yan’s contribution to the $g^2$ value of order $g^2$ is listed in third column. All numbers are in units of $10^{-6}$.

| Z  | $g$   | $g$ (CI-DF) | $g$ (CI-DF, $g^2$) | $g$ (Yan [30, 31]) |
|----|-------|-------------|---------------------|-------------------|
| 3  | -18.298 | -18.293     | -18.283             |
| 4  | -57.220 | -57.206     | -57.209             |
| 5  | -114.167 | -114.123   | -114.132            |
| 6  | -188.955 | -188.845   | -188.859            |
| 8  | -391.994 | -391.580   | -391.599            |
| 10 | -666.382 | -665.326   | -665.348            |
| 12 | -1012.504 | -1010.072  | -1010.096           |
TABLE III: One-electron self-energy and vacuum-polarization corrections of first order in $\gamma$. $\gamma^{\text{eff}}_{\gamma P}$ and $\gamma^{\text{eff}}_{\gamma P}^{K}$ are the Uehling and the Wichmann-Kroll part of the electric-loop vacuum-polarization contribution, respectively; $\gamma^{(1)}_{\gamma P} = \gamma^{\text{eff}}_{\gamma P} + \gamma^{\text{eff}}_{\gamma P}^{K} + \gamma^{m}_{\gamma P}$. All contributions are calculated with the point nuclear model. Units are $10^6$.

| Z  | $\gamma^{(1)}_{\text{SE}}$ | $\gamma^{\text{eff}}_{\gamma P}$ | $\gamma^{\text{eff}}_{\gamma P}^{K}$ | $\gamma^{m}_{\gamma P}$ | $\gamma^{(1)}_{\gamma P}$ | $\gamma^{(1)}_{\text{QED}}$ |
|----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 4  | 2322.905 1 (4)  | 0.000 215       | 0.000 000       | 0.000 001       | 0.000 214       | 2322.904 9 (4)  |
| 6  | 2323.018 3 (6)  | 0.001 070       | 0.000 000       | 0.000 005       | 0.001 065       | 2323.017 2 (6)  |
| 8  | 2323.185 1      | 0.003 326       | 0.000 002       | 0.000 020       | 0.003 304       | 2323.182 1      |
| 10 | 2323.413 2      | 0.008 00        | 0.000 01        | 0.000 06        | 0.007 93        | 2323.405 2      |
| 12 | 2323.707 2      | 0.016 35        | 0.000 02        | 0.000 15        | 0.016 18        | 2323.691 2      |
| 14 | 2324.074 3      | 0.029 92        | 0.000 06        | 0.000 33        | 0.029 53        | 2324.044 3      |
| 16 | 2324.520 3      | 0.050 48        | 0.000 12        | 0.000 64        | 0.049 71        | 2324.470 3      |
| 18 | 2325.052 5      | 0.080 06        | 0.000 25        | 0.001 16        | 0.078 66        | 2324.973 5      |
| 20 | 2325.674 5      | 0.121 0         | 0.000 5         | 0.002 0         | 0.118 6         | 2325.555 5      |
| 24 | 2327.225 5      | 0.247 5         | 0.001 3         | 0.004 9         | 0.241 3         | 2326.984 5      |
| 32 | 2331.726 6      | 0.772           | 0.007           | 0.021           | 0.745           | 2330.981 7      |
| 54 | 2358.184 9      | 6.652           | 0.138           | 0.28            | 6.23            | 2351.95 8       |
| 82 | 2456.245 9      | 48.266          | 1.886           | 2.3             | 44.1            | 2412.1 8        |
| 92 | 2532.207 9      | 93.309          | 4.260           | 4.0 (1.5)       | 85.0 (1.5)      | 2447.2 (1.5)    |
TABLE IV: Individual contributions to the screened QED correction of order $1=Z$ in terms of the function $R(Z)$ defined by Eq. (37). The terms $R_i$ with $i = 1; 2; 3$ are induced by Eqs. (34)-(36), respectively. The results in the last column are obtained for the extended-charge nucleus, whereas all the other results correspond to the point nuclear model.

| $Z$ | $R_1$ | $R_2$ | $R_3$ | $R(Z)$ | $R_{exp}(Z)$ |
|-----|-------|-------|-------|--------|-------------|
| 4   | 0.1134| 0.1139| 0.1253| 0.1258 | 0.1258      |
| 6   | 0.1135| 0.1144| 0.1254| 0.1264 | 0.1264      |
| 8   | 0.1135| 0.1153| 0.1254| 0.1272 | 0.1272      |
| 10  | 0.1136| 0.1163| 0.1255| 0.1283 | 0.1283      |
| 12  | 0.1136| 0.1176| 0.1256| 0.1296 | 0.1296      |
| 14  | 0.1137| 0.1192| 0.1258| 0.1312 | 0.1312      |
| 16  | 0.1138| 0.1210| 0.1259| 0.1331 | 0.1331      |
| 18  | 0.1140| 0.1231| 0.1261| 0.1352 | 0.1352      |
| 20  | 0.1141| 0.1255| 0.1263| 0.1377 | 0.1377      |
| 24  | 0.1144| 0.1311| 0.1268| 0.1435 | 0.1435      |
| 32  | 0.1152| 0.1465| 0.1280| 0.1593 | 0.1590      |
| 54  | 0.1188| 0.2324| 0.1336| 0.2473 | 0.2436      |
| 82  | 0.1274| 0.6196| 0.1491| 0.6412 | 0.5568      |
| 92  | 0.1324| 1.0501| 0.1588| 1.0765 | 0.8103      |
TABLE V: The total screened QED correction. $g_{SQ ED}^{(1)}$ and $g_{SQ ED}^{(2+)}$ are the screened QED contribution of first and of higher orders in $1/Z$, respectively. All numbers are in units of $10^{-6}$.

| Z   | $g_{SQ ED}^{(1)}$  | $g_{SQ ED}^{(2+)}$ | $g_{SQ ED}$     |
|-----|-------------------|-------------------|-----------------|
| 4   | 0.0621 (21)       | 0.00889 (2)       | 0.0532 (21)     |
| 6   | 0.0936 (60)       | 0.00879 (5)       | 0.0848 (60)     |
| 8   | 0.126 (12)        | 0.0088 (1)        | 0.117 (12)      |
| 10  | 0.158 (21)        | 0.0087 (1)        | 0.150 (21)      |
| 12  | 0.192 (32)        | 0.0087 (2)        | 0.183 (32)      |
| 14  | 0.227 (46)        | 0.0087 (3)        | 0.218 (46)      |
| 16  | 0.263 (62)        | 0.0087 (4)        | 0.254 (62)      |
| 18  | 0.301 (81)        | 0.0087 (5)        | 0.292 (81)      |
| 20  | 0.34 (10)         | 0.0087 (6)        | 0.33 (10)       |
| 24  | 0.43 (15)         | 0.009 (1)         | 0.42 (15)       |
| 32  | 0.63 (27)         | 0.009 (1)         | 0.62 (27)       |
| 54  | 1.6 (8)           | 0.009 (4)         | 1.6 (8)         |
| 82  | 5.6(2.0)          | 0.009 (9)         | 5.6(2.0)        |
| 92  | 9.2(2.6)          | 0.009 (12)        | 9.2(2.6)        |
TABLE VI: Individual contributions to the ground-state \( g \) factor of Li-like ions.

| Isotope        | \( ^{12}\text{C}\) | \( ^{16}\text{O}\) | \( ^{20}\text{Ne}\) | \( ^{24}\text{Mg}\) |
|----------------|-----------------|-----------------|-----------------|-----------------|
| Dirac value (point nucleus) | 1.999 680 300 | 1.999 431 380 | 1.999 110 996 | 1.998 718 893 |
| Finite nuclear size | 0.000 000 000 | 0.000 000 000 | 0.000 000 001 | 0.000 000 001 |
| Interelectronic interaction | 0.000 130 758 (19) | 0.000 176 658 (30) | 0.000 222 628 (42) | 0.000 268 703 (55) |
| QED, \( ^2\) | 0.000 003 516 (6) | 0.000 003 515 | 0.000 003 516 | 0.000 003 516 |
| Nuclear polarization | 0.000 000 010 | 0.000 000 017 | 0.000 000 025 | 0.000 000 032 |
| Total | 2.002 130 485 (19) | 2.001 927 604 (32) | 2.001 653 389 (47) | 2.001 307 619 (64) |

| Isotope        | \( ^{32}\text{Si}\) | \( ^{40}\text{Ar}\) | \( ^{40}\text{Ca}\) | \( ^{52}\text{Cr}\) |
|----------------|-----------------|-----------------|-----------------|-----------------|
| Dirac value (point nucleus) | 1.997 718 193 | 1.997 108 781 | 1.996 426 011 | 1.994 838 064 |
| Finite nuclear size | 0.000 000 005 | 0.000 000 009 | 0.000 000 014 | 0.000 000 035 |
| Interelectronic interaction | 0.000 361 24 (9) | 0.000 407 75 (12) | 0.000 454 45 (14) | 0.000 548 48 (21) |
| QED, \( ^2\) | 0.000 003 516 (1) | 0.000 003 517 (1) | 0.000 003 517 (2) | 0.000 003 518 (6) |
| Nuclear recoil | 0.000 000 046 (1) | 0.000 000 048 (1) | 0.000 000 061 (2) | 0.000 000 070 (4) |
| Total | 2.000 400 19 (11) | 1.999 837 75 (14) | 1.999 202 24 (17) | 1.997 709 70 (26) |

| Isotope        | \( ^{74}\text{Ge}\) | \( ^{132}\text{Xe}\) | \( ^{208}\text{Pb}\) | \( ^{238}\text{U}\) |
|----------------|-----------------|-----------------|-----------------|-----------------|
| Dirac value (point nucleus) | 1.999 572 307 | 1.972 750 205 | 1.932 002 904 | 1.910 722 624 (1) |
| Finite nuclear size | 0.000 000 162 | 0.000 003 37 (1) | 0.000 078 64 (16) | 0.000 241 83 (47) |
| Interelectronic interaction | 0.000 739 75 (37) | 0.001 299 4 (11) | 0.002 140 7 (27) | 0.002 501 4 (38) |
| QED, \( ^2\) | 0.000 330 981 (7) | 0.002 351 95 (8) | 0.002 412 1 (8) | 0.002 447 2 (15) |
| Nuclear polarization | 0.000 000 092 (9) | 0.000 000 16 (6) | 0.000 000 25 (35) | 0.000 000 28 (69) |
| Total | 1.993 819 14 (46) | 1.976 399 9 (14) | 1.936 625 3 (35) | 1.915 900 2 (50) |