g factor of high-*Z* lithiumlike ions

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The *g* factor of Li-like ions is evaluated in the range $Z=6-92$. The interelectronic-interaction correction of first order in $1/Z$ is calculated to all orders in αZ within a rigorous QED approach. The higher-order interelectronic-interaction, the one-electron QED, and the nuclear recoil corrections are evaluated to lowest orders in αZ. It is found that the uncertainty due to the nuclear size effect can be significantly reduced in a specific difference of the *g* factors of H- and Li-like ions.

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I. INTRODUCTION

Accurate measurements of the *g* factor of H-like carbon [1,2] stimulated theorists to calculate various contributions to this effect [3–15]. In particular, these investigations provided an independent determination of the electron mass [14]. The current accuracy of this determination is three times better than that of the accepted value for the electron mass [16]. An extension of these experiments to higher-*Z* systems, which is anticipated in the near future [17], would provide an independent determination of the fine structure constant [8,17], nuclear magnetic moments [17], and nuclear charge radii. They would also give a good possibility for a test of the magnetic sector of QED in a strong Coulomb field. However, as is known [6,18,19], investigations of the QED effects in high-*Z* hydrogenlike systems are strongly restricted by an uncertainty due to the nuclear size effect. In particular, the investigations of the hyperfine splitting in heavy ions [20] showed that the QED effects can be probed only at a specific difference of the hyperfine splitting values in H- and Li-like ions, where the nuclear structure effects can be significantly reduced. In the case of the bound-electron *g* factor the role of the nuclear structure effects is not so crucial as in the case of the hyperfine structure splitting. It is caused by the fact that, in contrast to the hyperfine splitting operator, the operator of the interaction of the atomic electron with a homogeneous magnetic field has a regular behavior at the nucleus. However, as can be seen from Table 3 of [15], for heavy H-like ions the uncertainty of the $1s$ *g* factor due to the finite nuclear size effect is comparable with the QED correction of second order in α and, therefore, restricts probing the QED effects on the *g* factor of H-like ions to first order in α. For this reason, investigations of the *g* factor of Li-like ions seem particularly important since one may expect that the uncertainty due to the nuclear size effect can be significantly reduced in a combination of the *g* factors of H- and Li-like ions. In addition, the investigations of the *g* factor of Li-like ions can serve as a very good test for various methods that are employed in relativistic calculations of many-electron systems [21–26], because all the contributions to the $g-2$ value for an *ns* state are of pure relativistic origin. We also expect that high-precision measurements of the *g* factor of Li-like ions combined with the related measurements for H-like ions and with the corresponding theoretical investigations will provide a more accurate determination of the electron mass.

In the present paper we calculate the *g* factor of Li-like ions with a spinless nucleus in a wide interval of the nuclear charge number *Z*. The interelectronic-interaction correction of first order in $1/Z$ is calculated to all orders in αZ within a rigorous QED approach. The higher-order interelectronic-interaction corrections, the one-electron QED, and the nuclear recoil corrections are evaluated to lowest orders in αZ. It is found that the uncertainty due to the nuclear size effect can be significantly reduced in a specific difference of the *g* factors of H- and Li-like ions.

Relativistic units ($\hbar=c=1$) and the Heaviside charge unit ($\alpha=e^2/4\pi, e<0$) are used in the paper.

II. BASIC FORMULAS AND CALCULATIONS

The ground-state *g* factor of a high-*Z* lithiumlike ion with a spinless nucleus can be written in the form

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

where

$$g_D=\frac{2[\sqrt{2+2\gamma}+1]}{3}=2-\frac{(\alpha Z)^2}{6}+\cdots \tag{2}$$

is the one-electron Dirac value for a point-charge nucleus, $\gamma=\sqrt{1-(\alpha Z)^2}$, $\Delta g_{\rm int}$ is the interelectronic-interaction correction, $\Delta g_{\rm QED}$ is the QED correction, $\Delta g_{\rm rec}$ is the nuclear recoil correction, and $\Delta g_{\rm NS}$ is the nuclear size correction. Below we evaluate all these corrections.

A. Interelectronic-interaction correction

The interelectronic-interaction correction $\Delta g_{\rm int}$ can be written in the following form:

$$\Delta g_{\rm int}=2\left[\frac{(\alpha Z)^2}{Z}B(\alpha Z)+\frac{(\alpha Z)^2}{Z^2}C(\alpha Z)+\frac{(\alpha Z)^2}{Z^3}D(\alpha Z)+\cdots\right], \tag{3}$$

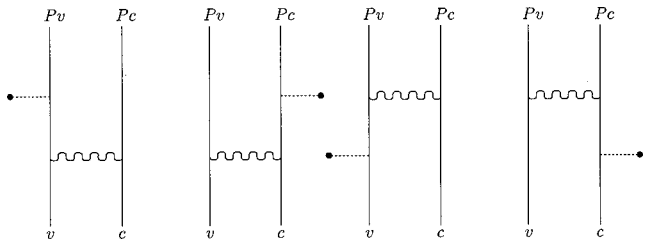

FIG. 1. The interelectronic-interaction corrections of first order in $1/Z$ to the g factor of Li-like ions.

where the functions $B(\alpha Z)$, $C(\alpha Z)$, and $D(\alpha Z)$ define the interelectronic-interaction corrections of first, second, and third orders in $1/Z$, respectively. The interelectronic-interaction correction of first order in $1/Z$ is defined by diagrams shown in Fig. 1, where the dashed line ended by a shaded circle indicates the interaction with the homogeneous magnetic field $\mathbf{A}_{\rm cl}(\mathbf{r})=[\mathcal{H}\times\mathbf{r}]/2$. In this figure, the label v denotes the valence electron while the label c denotes one of the core electrons. The formal expressions for the energy shift due to these diagrams can easily be derived by the two-time Green function method [19]. This derivation can even be simplified if one employs the representation in which the closed $(1s)^2$ shell is regarded as belonging to the vacuum. This derivation was considered in detail in [27] where the interelectronic-interaction corrections to the hyperfine splitting in Li-like ions were investigated. In the case under consideration, this derivation yields

$$
\begin{aligned}
\Delta E_{\rm int} &= \sum_{m_c}\left\{\sum_P (-1)^P \sum_n^{\varepsilon_n\neq\varepsilon_v} \frac{\langle Pv\,Pc|I(\Delta_{Pc})|nc\rangle\langle n|\delta V|v\rangle}{\varepsilon_v-\varepsilon_n}\right.\\
&+\sum_P (-1)^P \sum_n^{\varepsilon_n\neq\varepsilon_v} \frac{\langle v|\delta V|n\rangle\langle nc|I(\Delta_{Pc})|Pv\,Pc\rangle}{\varepsilon_v-\varepsilon_n}\\
&+\sum_P (-1)^P \sum_n^{\varepsilon_n\neq\varepsilon_c} \frac{\langle Pv\,Pc|I(\Delta_{Pv})|vn\rangle\langle n|\delta V|c\rangle}{\varepsilon_c-\varepsilon_n}\\
&+\sum_P (-1)^P \sum_n^{\varepsilon_n\neq\varepsilon_c} \frac{\langle c|\delta V|n\rangle\langle vn|I(\Delta_{Pv})|Pv\,Pc\rangle}{\varepsilon_c-\varepsilon_n}\\
&\left.-\langle cv|I'(\Delta_{vc})|vc\rangle(\langle v|\delta V|v\rangle-\langle c|\delta V|c\rangle)\right\}, \qquad (4)
\end{aligned}
$$

where v and c are the valence and core electron states, respectively, m_c denotes the angular momentum projection of the core electron, $\Delta_{ab}=\varepsilon_a-\varepsilon_b$, $\delta V(\mathbf{x})=-e\boldsymbol{\alpha}\cdot\mathbf{A}_{\rm cl}(\mathbf{x})$, $I(\omega)=e^2\alpha^\rho\alpha^\sigma D_{\rho\sigma}(\omega)$, $D_{\rho\sigma}(\omega,\mathbf{x}-\mathbf{y})$ is the photon propagator, which is given by

$$
D_{\rho\sigma}(\omega,\mathbf{x}-\mathbf{y})=g_{\rho\sigma}\frac{\exp(i|\omega||\mathbf{x}-\mathbf{y}|)}{4\pi|\mathbf{x}-\mathbf{y}|}
$$

in the Feynman gauge, and $I'(\omega)=dI(\omega)/d\omega$. The related contribution to the g factor is defined as $\Delta g_{\rm int}=\Delta E_{\rm int}/\mu_0\mathcal{H}m_v$, where $\mu_0=|e|/2m$ is the Bohr magneton, and m_v is the angular momentum projection of the valence electron. The numerical evaluation of the expression (4) was carried out similarly to our previous calculations of the corresponding correction to the hyperfine splitting [27,28]. After integration over angles, the finite basis set method was used to evaluate infinite summations over the electron spectrum. Basis functions were constructed from B splines by employing the procedure proposed in [29]. The results of the numerical evaluation, expressed in terms of the $B(\alpha Z)$ function defined by Eq. (3), are presented in Table I. The results for point- and extended-charge nuclei are listed in the third and fourth columns, respectively. In the extended nucleus case, the Fermi model was used to describe the nuclear charge distribution. The uncertainty of this calculation was estimated by taking the difference between the results obtained with the Fermi and uniform sphere models for the nuclear charge distribution. The root-mean-square nuclear radii were take from [30,31]. For comparison, the results of the related calculation performed in the framework of the Breit approximation for the point nucleus case are presented in the second column of the table. In that approximation, the operator $I(\omega)$ in Eq. (4) is replaced by I_C+I_B, where

$$
I_C=\frac{\alpha}{r_{12}}, \qquad (5)
$$

TABLE I. The interelectronic-interaction correction of first order in $1/Z$ to the ground-state g factor of Li-like ions, expressed in terms of the function $B(\alpha Z)$ defined by Eq. (3). $B_{\rm p.n.}(\alpha Z)$ and $B_{\rm f.n.}(\alpha Z)$ denote the results of the rigorous QED calculation for point- and extended-charge nuclei, respectively. $B_{\rm Breit}(\alpha Z)$ indicates the results obtained within the Breit approximation.

Z	$B_{\rm Breit}(\alpha Z)$	$B_{\rm p.n.}(\alpha Z)$	$B_{\rm f.n.}(\alpha Z)$
3	0.214 937	0.214 942	
4	0.214 961	0.214 969	
5	0.214 992	0.215 005	
6	0.215 029	0.215 048	
8	0.215 125	0.215 159	
10	0.215 249	0.215 302	0.215 301
16	0.215 787	0.215 921	0.215 921
18	0.216 024	0.216 193	0.216 192
20	0.216 289	0.216 497	0.216 496
24	0.216 907	0.217 205	0.217 203
30	0.218 061	0.218 521	0.218 518
32	0.218 509	0.219 030	0.219 026
40	0.220 632	0.221 429	0.221 420
50	0.224 104	0.225 305	0.225 283
54	0.225 778	0.227 155	0.227 123
60	0.228 637	0.230 284	0.230 232
70	0.234 474	0.236 573	0.236 447
80	0.241 997	0.244 501	0.244 218(1)
82	0.243 753	0.246 327	0.245 991(1)
90	0.251 829	0.254 622	0.253 927(1)
92	0.254 155	0.256 984	0.256 152(2)
100	0.265 056	0.267 923	0.266 256(3)

$$I_B = -\alpha\left(\frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2}{r_{12}}+\frac{1}{2}[\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_1,[\boldsymbol{\alpha}_2\cdot\boldsymbol{\nabla}_2,r_{12}]]\right). \quad (6)$$

As one can see from the table, for low-Z systems the results of the rigorous QED calculation almost coincide with those derived from the Breit approximation.

To evaluate the interelectronic-interaction corrections of higher order in $1/Z$, we employed the results of [23], where the g factors of Li and Be^+ were calculated within the Breit approximation. Subtracting the $1/Z$ term from those results and fitting the rest to the form $2(\alpha Z)^2[C(0)/Z^2+D(0)/Z^3]$, we find $C(0)\approx -0.0445$ and $D(0)\approx -0.0497$. The uncertainty of this determination is estimated to be about 20%.

B. QED corrections

To zeroth order in $1/Z$, the QED correction is defined by the one-electron QED correction for the $2s$ state. According to [7,32,33], the one-electron QED correction accurate up to order $(\alpha Z)^2$ and exact in α/π can be derived by using the operator

$$H_{\rm rad}=\frac{|e|}{2m}\frac{g_{\rm free}-2}{2}[\beta(\boldsymbol{\sigma}\cdot\mathcal{H})-i\beta(\boldsymbol{\alpha}\cdot\mathcal{E})], \quad (7)$$

where

$$g_{\rm free}=2[1+(1/2)(\alpha/\pi)-0.328\,478...\times(\alpha/\pi)^2+\cdots] \quad (8)$$

is the g factor of the free electron and $\mathcal{E}=(|e|Z/4\pi)(\mathbf{r}/r^3)$. The expectation value of $H_{\rm rad}$ has to be evaluated with the Dirac wave function of the electron that accounts for the interaction with the homogeneous magnetic field to first order in $\mathcal{H}$. The first-order correction to the electron wave function due to the interaction with the magnetic field can be derived analytically by employing the method of generalized virial relations for the Dirac equation [34]. Using the explicit form for this correction presented in [12], we obtain in the case of an ns state

$$\Delta g_{\rm QED}=(g_{\rm free}-2)\left[1+\frac{(\alpha Z)^2}{6n^2}\right]. \quad (9)$$

For the $1s$ state, this formula coincides with the corresponding result obtained in [7,8,32]. To date, the complete αZ-dependence calculations of the one-electron QED correction of first order in α have been performed only for the $1s$ state [3–6]. These calculations indicate that the higher-order QED correction grows when Z increases and, at $Z=92$, amounts to about 25% of the total QED contribution. The error due to omitting the interelectronic-interaction effect on the QED correction (''the screened QED correction'') is estimated to be smaller by a factor α/π than the interelectronic-interaction correction discussed in the previous subsection.

C. Nuclear recoil correction

A systematic QED theory of the nuclear recoil effect on the atomic g factor to first order in m/M and to all orders in αZ was developed in [12]. In particular, there a complete αZ-dependence formula for the recoil correction to the g factor of a H-like ion was derived. This result was confirmed in [13] by a different method. To zeroth order in $1/Z$, this formula remains valid also for the case of a Li-like ion with one electron outside the closed $(1s)^2$ shell, if one replaces the electron propagators defined for the usual vacuum by those defined for the vacuum with the $(1s)^2$ shell included. In the case of an arbitrary valence state, this leads to the appearance of a two-electron contribution. However, for an ns valence state the two-electron contribution vanishes and, therefore, to zeroth order in $1/Z$, the recoil correction is completely defined by the one-electron contribution. According to [12], to lowest order in αZ, it is

$$\Delta g_{\rm rec}=\frac{m}{M}\frac{(\alpha Z)^2}{n^2}. \quad (10)$$

As for the higher-order recoil corrections, they can be evaluated by using the formulas derived in [12]. To date, such an evaluation has been performed only for the $1s$ state [15]. The results of [15] indicate that for high-Z systems the higher-order term may even exceed the lowest-order term.

D. Nuclear size correction

The calculation of the finite nuclear size correction can be performed numerically by a direct solution of the Dirac equation. For low-Z systems, in the case of an ns state, with a good accuracy, this correction is given by [11]

$$\Delta g_{\rm NS}=\frac{8}{3n^3}(\alpha Z)^4 m^2\langle r^2\rangle\left[1+(\alpha Z)^2\left(\frac{1}{4}+\frac{12n^2-n-9}{4n^2(n+1)}+2\Psi(3)-\Psi(n+2)-\frac{\langle r^2\ln(2\alpha Zmr/n)\rangle}{\langle r^2\rangle}\right)\right], \quad (11)$$

where $\Psi(x)=(d/dx)\ln\Gamma(x)$ and the expectation value has to be evaluated with the provided nuclear charge density.

III. RESULTS AND DISCUSSION

In Table II we present the individual contributions to the ground-state g factor for some Li-like ions in the range $Z=6-92$. The uncertainty of the finite nuclear size correction was estimated as the difference between the result obtained with the Fermi model of the nuclear charge distribution and with the homogeneously-charged-sphere model. The nuclear charge radii were taken from [30,31]. The QED correction was evaluated by formula (9). Its uncertainty includes the error resulting from the αZ expansion of the one-electron QED contribution as well as the error due to omitting the screened QED correction. The recoil correction was evaluated by formula (10). The error of this evaluation was assumed to be equal to the error of the corresponding evaluation for the $1s$ state [15]. The interelectronic-interaction corrections were calculated as described above. The higher-

TABLE II. The individual contributions to the ground-state g factor of Li-like ions.

	$^{12}C^{3+}$	$^{16}O^{5+}$	$^{32}S^{13+}$	$^{40}Ar^{15+}$	$^{40}Ca^{17+}$
Dirac value (point nucleus)	1.999 680 30	1.999 431 38	1.997 718 19	1.997 108 78	1.996 426 01
Finite nuclear size	0.000 000 00	0.000 000 00	0.000 000 00	0.000 000 01	0.000 000 01
QED	0.002 319 49(34)	0.002 319 6(5)	0.002 320 6(29)	0.002 321(4)	0.002 321(6)
Recoil	0.000 000 02	0.000 000 03	0.000 000 06	0.000 000 06	0.000 000 07
Interelectronic interaction, order $1/Z$	0.000 137 42	0.000 183 32	0.000 367 94	0.000 414 45	0.000 461 15
Interelectronic interaction, higher orders	−0.000 005 6(11)	−0.000 005 4(11)	−0.000 005 1(10)	−0.000 005 0(10)	−0.000 005 0(10)
Total	2.002 131 6(11)	2.001 929 0(12)	2.000 401 7(30)	1.999 839(4)	1.999 204(6)
	$^{52}Cr^{21+}$	$^{74}Ge^{29+}$	$^{132}Xe^{51+}$	$^{208}Pb^{79+}$	$^{238}U^{89+}$
Dirac value (point nucleus)	1.994 838 06	1.990 752 31	1.972 750 21	1.932 002 90	1.910 722 62
Finite nuclear size	0.000 000 04	0.000 000 16	0.000 003 37(1)	0.000 078 64(16)	0.000 241 83(47)
QED	0.002 322(10)	0.002 325(25)	0.002 33(12)	0.002 35(40)	0.002 36(56)
Recoil	0.000 000 08	0.000 000 10(1)	0.000 000 16(3)	0.000 000 24(19)	0.000 000 26(36)
Interelectronic interaction, order $1/Z$	0.000 555 18	0.000 746 46	0.001 306 22	0.002 148 29(1)	0.002 509 84(2)
Interelectronic interaction, higher orders	−0.000 005 0(10)	−0.000 004 9(10)	−0.000 004 8(10)	−0.000 004 8(12)	−0.000 004 8(13)
Total	1.997 711(10)	1.993 819(25)	1.976 39(12)	1.936 6(4)	1.915 8(6)

order interelectronic-interaction correction includes the contributions of order $1/Z^2$ and higher.

From the table, we conclude that for low Z the theoretical uncertainty is mainly determined by the uncertainty of the interelectronic-interaction correction of second and higher orders in $1/Z$, while for high Z it results from the αZ expansion of the one-electron QED correction and from the finite nuclear size correction.

The one-loop QED and higher-order interelectronic-interaction corrections can be calculated to the required accuracy in the same way as was performed for the hyperfine splitting (see [19,20,35] and references therein). The recoil correction to the g factor of Li-like ions can be calculated to all orders in αZ by employing the methods developed in [12,15]. Taking into account recent progress in calculations of the QED correction of second order in α to the Lamb shift [36], we expect that, in the near future, the corresponding correction to the g factor will be evaluated as well. If all these corrections are calculated, the theoretical uncertainty of the g factor for heavy ions is completely determined by the error due to the nuclear size effect. For H- and Li-like uranium, this uncertainty amounts to about 3×10^{-6} and 5×10^{-7}, respectively, and strongly restricts investigations of the QED effects on the g factor. However, as in the case of the hyperfine splitting [20], this uncertainty can be significantly reduced in a specific difference of g factors of H- and Li-like ions. To demonstrate this fact, let us introduce the parameter ξ by

$$\xi = \Delta g_{\rm NS}^{[(1s)^2 2s]} / \Delta g_{\rm NS}^{[1s]}, \tag{12}$$

where $\Delta g_{\rm NS}^{[(1s)^2 2s]}$ denotes the total nuclear size correction to the g factor of a Li-like ion, including the nuclear size effect on the interelectronic-interaction correction, and $\Delta g_{\rm NS}^{[(1s)]}$ denotes the nuclear size correction to the g factor of the corresponding H-like ion. The numerical calculations performed for the Fermi and sphere models of the nuclear charge distribution indicate that the parameter ξ is rather stable with respect to a variation of the nuclear charge distribution parameters. For instance, for the Fermi model we obtain $\xi = 0.167\,026\,4$ for $Z=82$ and $\xi=0.183\,268\,4$ for $Z=92$ while for the sphere model we obtain $\xi=0.167\,028\,7$ for $Z=82$ and $\xi=0.183\,270\,9$ for $Z=92$. Comparing these values with the corresponding variations of the nuclear size corrections, which determine the uncertainty of this effect (see Table II of this paper for Li-like ions and Table 3 of [15] for H-like ions), we conclude that the parameter ξ is, at least, 100 times more stable with respect to a variation of the nuclear parameters than is the nuclear size correction. It follows that the nuclear size correction for a Li-like ion can be expressed, with high accuracy, in terms of the nuclear size correction for the corresponding H-like ion. As in the case of the hyperfine splitting [20], let us introduce the following difference:

$$g' = g_{(1s)^2 2s} - \xi g_{1s}, \tag{13}$$

where g_{1s} and $g_{(1s)^2 2s}$ are the g factors of H- and Li-like ions, respectively. According to the numerical results and the discussion presented above, we conclude that g' can be calculated to an accuracy of about 10^{-9} for $Z=82$ and about 3×10^{-9} for $Z=92$. This leads to good perspectives for a test of the QED effects on the g factor in heavy ions, provided the QED, interelectronic-interaction, and recoil corrections to g' are calculated to the desired accuracy. Such calculations are under way and will be published elsewhere.

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