

Nuclear recoil effect on the g factor of highly charged Li-like ions

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The nuclear recoil effect on the g factor of highly charged Li-like ions is evaluated in the range $Z = 10\text{--}92$. The calculations are performed by using $1/Z$ perturbation theory. The one-electron recoil contribution is evaluated within the fully relativistic approach with the wave functions which account approximately for the screening effects. The two-electron recoil contributions of the first and higher orders in $1/Z$ are calculated within the Breit approximation by using a four-component approach.

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I. INTRODUCTION

Measurements of the g factor of low- and middle- Z H- and Li-like ions [1–8] have reached an accuracy of a few 10^{-10} . From the theoretical side, to get this accuracy we need to evaluate various contributions to the g -factor value [9–33]. The comparison of theory and experiment on the g factors of H- and Li-like silicon has provided the most stringent tests of bound-state quantum electrodynamics (QED) in the presence of a magnetic field, while the combination of the experimental and theoretical results on the g factor of H-like ions with $Z = 6, 8, 14$ lead to the most precise determination of the electron mass [7,28]. The measurement of the isotope shift of the g factor of Li-like ${}^A\text{Ca}^{17+}$ with $A = 40$ and $A = 48$ [8] has triggered a special interest in the calculations of the nuclear recoil contributions to the g factor.

The fully relativistic theory of the nuclear recoil effect to the first order in the electron-to-nucleus mass ratio m/M on the g factor of atoms and ions was formulated in Ref. [13], where it was used to derive closed formulas for the recoil effect on the g factor of H-like ions to all orders in αZ . These formulas also remain valid for an ion with one electron over closed shells (see, e.g., Ref. [18]), provided the electron propagators are redefined for the vacuum with the closed shells included. In that case, in addition to the one-electron contributions, one obtains two-electron recoil corrections of the zeroth order in $1/Z$ which can be used to derive effective four-component recoil operators within the Breit approximation [29]. The one-electron recoil contribution was evaluated numerically to all orders in αZ for the $1s$ and $2s$ states in Refs. [14] and [29], respectively. The calculations were performed for the point-nucleus case. For the ground state of Li-like ions, the two-electron recoil contribution vanishes to the zeroth order in $1/Z$. However, the effective recoil operator can be used to evaluate the recoil corrections of the first and higher orders in $1/Z$ within the framework of the Breit approximation. These calculations were carried out for $Z = 3\text{--}20$ in Ref. [29], where a large discrepancy between the obtained results and the previous Breit-approximation

calculations based on the two-component approach [34,35] was found. As was shown in Ref. [29], this discrepancy was caused by omitting some important terms in the calculation scheme formulated within the two-component approach for s states in Ref. [36]. Later [31], the four-component approach was also used to calculate the recoil effect within the Breit approximation for middle- Z B-like ions.

Special attention should be paid to probing the QED nuclear recoil effect in experiments with heavy ions, which are anticipated in the nearest future at the Max-Planck-Institut für Kernphysik in Heidelberg and at the HITRAP/FAIR facilities in Darmstadt. This would provide an opportunity for tests of QED in the strong-coupling regime beyond the Furry picture. To this end, in Ref. [30] the nuclear recoil effect on the g factor of H- and Li-like Pb and U was calculated, and it was shown that the QED recoil contribution can be probed on a few-percent level in a specific difference of the g factors of heavy H- and Li-like lead.

In the present paper we extend the calculations of the recoil effect on the g factor of Li-like ions performed in Refs. [29,30] to the range $Z = 10\text{--}92$. The one-electron recoil contribution is calculated in the framework of the rigorous QED approach with the wave functions which partly account for the screening of the Coulomb potential by the closed-shell electrons. As for the two-electron recoil contribution, it is evaluated within the Breit approximation to all orders in $1/Z$. All the calculations also partly account for the nuclear size corrections to the recoil effect.

Relativistic units ($\hbar = c = 1$) are used throughout the paper.

II. BASIC FORMULAS

Let us consider a Li-like ion which is put into a homogeneous magnetic field $\mathbf{A}_c(\mathbf{r}) = [\mathcal{H} \times \mathbf{r}]/2$ with \mathcal{H} directed along the z axis. To zeroth order in $1/Z$, the m/M nuclear recoil contribution to the g factor is given by a sum of one- and two-electron contributions. In the case of the ground $(1s)^2 2s$ state the two-electron contribution of zeroth order in $1/Z$ is equal to zero and one has to consider the one-electron term

only. The one-electron recoil contribution to the g factor is given by [13]

$$\Delta g = \frac{1}{\mu_0 m_a} \frac{i}{2\pi M} \int_{-\infty}^{\infty} d\omega \left[\frac{\partial}{\partial \mathcal{H}} \langle \tilde{a} | [p^k - D^k(\omega) + eA_{\text{cl}}^k] \right. \\ \left. \times \tilde{G}(\omega + \varepsilon_a) [p^k - D^k(\omega) + eA_{\text{cl}}^k] | \tilde{a} \rangle \right]_{\mathcal{H}=0}. \quad (1)$$

Here a denotes the one-electron $2s$ state, μ_0 is the Bohr magneton, m_a is the angular-momentum projection of the state under consideration, M is the nuclear mass, $p^k = -i\nabla^k$ is the momentum operator, $D^k(\omega) = -4\pi\alpha Z\alpha^l D^{lk}(\omega)$,

$$D^{lk}(\omega, \mathbf{r}) = -\frac{1}{4\pi} \left\{ \frac{\exp(i|\omega|r)}{r} \delta_{lk} \right. \\ \left. + \nabla^l \nabla^k \frac{(\exp(i|\omega|r) - 1)}{\omega^2 r} \right\} \quad (2)$$

is the transverse part of the photon propagator in the Coulomb gauge, α is a vector incorporating the Dirac matrices, and summation over repeated indices is implied. The tilde sign means that the corresponding quantity [the wave function, the energy, and the Dirac-Coulomb Green's function $\tilde{G}(\omega) = \sum_{\tilde{n}} |\tilde{n}\rangle \langle \tilde{n}| [\omega - \varepsilon_n(1 - i0)]^{-1}$] must be calculated in presence of the magnetic field.

For practical calculations, the one-electron contribution is conveniently represented by a sum of low-order and higher-order terms, $\Delta g = \Delta g_L + \Delta g_H$, where

$$\Delta g_L = \frac{1}{\mu_0 \mathcal{H} m_a} \frac{1}{M} \langle \delta a | \left[\mathbf{p}^2 - \frac{\alpha Z}{r} \left(\alpha + \frac{(\alpha \cdot \mathbf{r}) \mathbf{r}}{r^2} \right) \cdot \mathbf{p} \right] | a \rangle \\ - \frac{1}{m_a} \frac{m}{M} \langle a | \left([\mathbf{r} \times \mathbf{p}]_z - \frac{\alpha Z}{2r} [\mathbf{r} \times \alpha]_z \right) | a \rangle, \quad (3)$$

$$\Delta g_H = \frac{1}{\mu_0 \mathcal{H} m_a} \frac{i}{2\pi M} \int_{-\infty}^{\infty} d\omega \left\{ \langle \delta a | \left(D^k(\omega) - \frac{[p^k, V]}{\omega + i0} \right) \right. \\ \times G(\omega + \varepsilon_a) \left(D^k(\omega) + \frac{[p^k, V]}{\omega + i0} \right) | a \rangle \\ + \langle a | \left(D^k(\omega) - \frac{[p^k, V]}{\omega + i0} \right) G(\omega + \varepsilon_a) \\ \times \left(D^k(\omega) + \frac{[p^k, V]}{\omega + i0} \right) | \delta a \rangle \\ \left. + \langle a | \left(D^k(\omega) - \frac{[p^k, V]}{\omega + i0} \right) G(\omega + \varepsilon_a) (\delta V - \delta \varepsilon_a) \right. \\ \left. \times G(\omega + \varepsilon_a) \left(D^k(\omega) + \frac{[p^k, V]}{\omega + i0} \right) | a \rangle \right\}. \quad (4)$$

Here $V(r)$ is the potential of the nucleus or an effective local potential which is the sum of the nuclear and screening potentials, $\delta V(\mathbf{r}) = -e\alpha \cdot \mathbf{A}_{\text{cl}}(\mathbf{r})$, $G(\omega) = \sum_n |n\rangle \langle n| [\omega - \varepsilon_n(1 - i0)]^{-1}$ is the Dirac-Coulomb Green's function, $\delta \varepsilon_a = \langle a | \delta V | a \rangle$, and $|\delta a\rangle = \sum_{n \neq a}^{\varepsilon_n \neq \varepsilon_a} |n\rangle \langle n | \delta V | a \rangle (\varepsilon_a - \varepsilon_n)^{-1}$. The low-order term corresponds to the Breit approximation, while the higher-order term defines the QED one-electron recoil contribution.

The recoil contributions of the first and higher orders in $1/Z$ can be evaluated within the Breit approximation with

the use of the four-component recoil operators [29]. The total Breit-approximation recoil contribution can be represented as a sum of two terms. The first term is obtained as a combined interaction due to δV and the effective recoil Hamiltonian (see Ref. [37] and references therein):

$$H_M = \frac{1}{2M} \sum_{i,k} \left[\mathbf{p}_i \cdot \mathbf{p}_k - \frac{\alpha Z}{r_i} \left(\alpha_i + \frac{(\alpha_i \cdot \mathbf{r}_i) \mathbf{r}_i}{r_i^2} \right) \cdot \mathbf{p}_k \right]. \quad (5)$$

The second term is defined by the magnetic recoil operator:

$$H_M^{\text{magn}} = -\mu_0 \frac{m}{M} \mathcal{H} \cdot \sum_{i,k} \left\{ [\mathbf{r}_i \times \mathbf{p}_k] \right. \\ \left. - \frac{\alpha Z}{2r_k} \left[\mathbf{r}_i \times \left(\alpha_k + \frac{(\alpha_k \cdot \mathbf{r}_k) \mathbf{r}_k}{r_k^2} \right) \right] \right\}. \quad (6)$$

To zeroth order in $1/Z$, the one-electron parts of the operators (5) and (6) lead to the low-order contribution defined by Eq. (3).

Thus, within the four-component Breit-approximation approach, the m/M recoil effect on the g factor can be evaluated by adding the operators (5) and (6) to the Dirac-Coulomb-Breit Hamiltonian, which includes the interaction with the external magnetic field.

III. NUMERICAL CALCULATIONS

Let us consider first the calculations within the Breit approximation. For these calculations we use the operators (5), (6), and the standard Dirac-Coulomb-Breit Hamiltonian:

$$H^{\text{DCB}} = \Lambda^{(+)} \left[\sum_i h_i^{\text{D}} + \sum_{i < k} V_{ik} \right] \Lambda^{(+)}, \quad (7)$$

where the indices i and k enumerate the atomic electrons, $\Lambda^{(+)}$ is the projector on the positive-energy states, calculated by including the interaction with external magnetic field δV , h_i^{D} is the one-electron Dirac Hamiltonian including δV , and

$$V_{ik} = V_{ik}^{\text{C}} + V_{ik}^{\text{B}} \\ = \frac{\alpha}{r_{ik}} - \alpha \left[\frac{\alpha_i \cdot \alpha_k}{r_{ik}} + \frac{1}{2} (\alpha_i \cdot \nabla_i) (\alpha_k \cdot \nabla_k) r_{ik} \right] \quad (8)$$

is the electron-electron interaction operator within the Breit approximation. The numerical calculations have been performed by using the approach based on the recursive representation of the perturbation theory [38]. The key advantages of the recursive perturbation approach over the standard one are the universality and the computational efficiency. In Refs. [39,40], this method was applied to find the higher-order contributions to the Zeeman and Stark shifts in H- and B-like atoms. The perfect agreement of the obtained results with the calculations by other methods was demonstrated. In Refs. [38,41], the recursive method was used to calculate the higher-order contributions of the interelectronic interaction in few-electron ions.

The total Breit-approximation recoil contribution for the state under consideration can be expressed as

$$\Delta g_{\text{Breit}} = \frac{m}{M}(\alpha Z)^2 \left[A(\alpha Z) + \frac{1}{Z}B(\alpha Z) + \frac{1}{Z^2}C(\alpha Z, Z) \right], \quad (9)$$

where the coefficients $A(\alpha Z)$ and $B(\alpha Z)$ define the recoil contributions of the zeroth and first orders in $1/Z$, respectively, while $C(\alpha Z, Z)$ incorporates the recoil corrections of the second and higher orders in $1/Z$. In this work, in the calculation of $C(\alpha Z, Z)$ we have taken into account the terms of orders $1/Z^2$, $1/Z^3$, and $1/Z^4$. The contribution of terms of higher order is much smaller than the present numerical uncertainty.

For the point-nucleus case, the coefficient $A(\alpha Z)$, which is determined by the one-electron low-order term (3), can be evaluated analytically [13]. In case of the $2s$ state it is given by

$$A(\alpha Z) = \frac{1}{4} \frac{8(2\gamma + 1)}{3(1 + \gamma)[2\gamma + \sqrt{2(1 + \gamma)}]}, \quad (10)$$

where $\gamma = [1 - (\alpha Z)^2]^{1/2}$. To leading orders in αZ , it leads to

$$A(\alpha Z) = \frac{1}{4} + \frac{11}{192}(\alpha Z)^2 + \dots \quad (11)$$

The calculations to all orders in $1/Z$ have been performed with the point-nucleus recoil operators defined by Eqs. (5) and (6) but with the wave functions evaluated for extended nuclei. This corresponds to a partial treatment of the nuclear size corrections to the recoil effect. The Fermi model of the nuclear charge distribution was used and the nuclear charge radii were taken from Ref. [42]. The results of the calculations are presented in Table I. The indicated uncertainties are due to the numerical computation errors.

For the point-nucleus case, the higher-order one-electron contribution (4) was calculated for the $1s$ and $2s$ states over a wide range of nuclear charge number in Refs. [14,29]. In the present paper we perform the calculations for extended nuclei and effective potentials which partly account for the electron-electron interaction effects. Our first results for $Z = 82, 92$ were presented in Ref. [30], where they were used to search for a possibility to test QED beyond the Furry picture. In the present paper we extend these calculations to the range $Z = 10\text{--}92$. Since the inclusion of the screening potential into the zeroth-order Hamiltonian allows one to account for the interelectronic-interaction effects only partly, we perform the calculations with several different effective potentials to keep better control of the uncertainty of the corresponding contribution. The calculations have been performed for the core-Hartree (CH), local Dirac-Fock (LDF), and Perdew-Zunger (PZ) effective potentials. The CH screening potential is derived from the radial charge density of two $1s$ electrons,

$$V_{\text{CH}}(r) = \alpha \int_0^\infty dr' \frac{1}{r_>} \rho_{\text{CH}}(r'), \quad (12)$$

where $r_> = \max(r, r')$,

$$\rho_{\text{CH}}(r) = 2[G_{1s}^2(r) + F_{1s}^2(r)], \quad \int_0^\infty dr \rho_{\text{CH}}(r) = 2, \quad (13)$$

TABLE I. The Breit-approximation recoil contributions to the g factor of the $(1s)^2 2s$ state of Li-like ions expressed in terms of the coefficients $A(\alpha Z)$, $B(\alpha Z)$, and $C(\alpha Z, Z)$ defined by Eq. (9).

Z	$A(\alpha Z)$	$B(\alpha Z)$	$C(\alpha Z, Z)$
10	0.2503	-0.5172	-0.236(4)
12	0.2504	-0.5179	-0.243(3)
14	0.2506	-0.5187	-0.245(3)
16	0.2508	-0.5197	-0.248(3)
18	0.2510	-0.5207	-0.250(2)
20	0.2512	-0.5219	-0.250(2)
24	0.2517	-0.5247	-0.250(1)
28	0.2524	-0.5279	-0.247(1)
30	0.2527	-0.5297	-0.245(1)
32	0.2531	-0.5315	-0.243
40	0.2548	-0.5402	-0.228
48	0.2567	-0.5504	-0.205
50	0.2572	-0.5531	-0.198
56	0.2588	-0.5618	-0.177
60	0.2599	-0.5677	-0.160
64	0.2607	-0.5734	-0.141
70	0.2616	-0.5813	-0.105
72	0.2617	-0.5836	-0.092
80	0.2606	-0.5886	-0.037
82	0.2597	-0.5881	-0.019
90	0.2510	-0.5721	0.051
92	0.2471	-0.5629	0.065

and G/r and F/r are the large and small components of the radial Dirac wave function. The LDF potential is constructed by inversion of the radial Dirac equation with the radial wave functions obtained in the Dirac-Fock approximation. The corresponding procedure is described in detail in Ref. [43]. The last potential applied in our work is the Perdew-Zunger potential [44], which was widely employed in molecular and cluster calculations.

In Eq. (4), the summation over the intermediate electron states was performed by employing the finite-basis-set method. The basis functions were constructed from B splines [45] within the framework of the dual-kinetic-balance approach [46]. The integration over ω was carried out analytically for the ‘‘Coulomb’’ contribution (the term without the \mathbf{D} vector) and numerically for the ‘‘one-transverse’’ and ‘‘two-transverse’’ photon contributions (the terms with one and two \mathbf{D} vectors, respectively) by using Wick’s rotation. The total QED recoil contribution, Δg_{H} , for the $2s$ state is conveniently expressed in terms of the function $P^{(2s)}(\alpha Z)$:

$$\Delta g_{\text{H}}^{(2s)} = \frac{m}{M} \frac{(\alpha Z)^5}{8} P^{(2s)}(\alpha Z). \quad (14)$$

The numerical results are presented in Table II. For comparison, in the second column we list the point-nucleus results which were partly presented in Ref. [29].

In Table III, we present the total values of the recoil corrections to the g factor of the ground $(1s)^2 2s$ state of Li-like ions. They are expressed in terms of the function $F(\alpha Z)$, which is defined by

$$\Delta g = \frac{m}{M} (\alpha Z)^2 F(\alpha Z). \quad (15)$$

TABLE II. The higher-order (QED) recoil contribution to the $2s$ g factor expressed in terms of the function $P^{(2s)}(\alpha Z)$ defined by Eq. (14). The indices Coul, CH, LDF, and PZ refer to the Coulomb and various screening potentials (see text). The indices p.n. and f.n. correspond to the point-like and finite-size nuclear models.

Z	$P_{\text{Coul}}^{(\text{p.n.})}(\alpha Z)$	$P_{\text{Coul}}^{(\text{f.n.})}(\alpha Z)$	$P_{\text{CH}}(\alpha Z)$	$P_{\text{LDF}}(\alpha Z)$	$P_{\text{PZ}}(\alpha Z)$
10	8.8762(1)	8.9145	6.2670	6.1840	6.6098
12	8.1943(1)	8.2333	6.1987	6.1326	6.4787
14	7.6447(1)	7.6847	6.0614	6.0069	6.2955
16	7.1911(1)	7.2325	5.8998	5.8539	6.0995
18	6.8101(1)	6.8539	5.7349	5.6953	5.9081
20	6.4860(1)	6.5309	5.5740	5.5395	5.7264
24	5.9670(1)	6.0151	5.2844	5.2571	5.4065
28	5.5753(1)	5.6267	5.0429	5.0205	5.1446
30	5.4160(1)	5.4703	4.9412	4.9208	5.0351
32	5.2771(1)	5.3341	4.8509	4.8322	4.9382
40	4.8840(1)	4.9487	4.5900	4.5760	4.6588
48	4.6937(1)	4.7686	4.4789	4.4680	4.5375
50	4.6727(1)	4.7499	4.4723	4.4619	4.5290
56	4.6697(1)	4.7530	4.5028	4.4940	4.5557
60	4.7182(1)	4.8035	4.5658	4.5578	4.6171
64	4.8098(2)	4.8958	4.6670	4.6596	4.7173
70	5.039(1)	5.1144	4.8928	4.8865	4.9429
72	5.144(1)	5.2114	4.9908	4.9847	5.0411
80	5.753(3)	5.7437	5.5200	5.5152	5.5728
82	5.965(3)	5.9188	5.6926	5.6881	5.7464
90	7.19(2)	6.8284	6.5850	6.5818	6.6449
92	7.64(2)	7.1187	6.8689	6.8662	6.9309

The Breit-approximation recoil contributions are obtained from Eq. (9) with the coefficients given in Table I. The uncertainties include both the error bars presented in Table I and the uncertainties due to the approximate treatment of the nuclear size correction to the recoil effect. We have assumed that the relative value of the latter uncertainty is equal to the related contribution to the binding energy which was evaluated within the Breit approximation in Ref. [47]. For the QED recoil contribution we use the LDF values from Table II. The uncertainty of this term is estimated as a sum of two contributions. The first one is due to the approximate treatment of the electron-electron interaction effect on the QED recoil contribution. This uncertainty was estimated by performing the calculations of the low-order (non-QED) one-electron recoil contribution with the LDF potential and comparing the obtained result with the total Breit recoil value evaluated above. The ratio of the difference obtained to the non-QED LDF result was chosen as the relative uncertainty of the corresponding correction to the QED recoil contribution. Note that this uncertainty exceeds the difference between the results obtained for the different screening potentials presented in Table II. The second contribution to the uncertainty is caused by the approximate treatment of the nuclear size correction to

TABLE III. The Breit, QED, and total recoil contributions to the g factor of the $(1s)^2 2s$ state of Li-like ions expressed in terms of the function $F(\alpha Z)$ defined by Eq. (15).

Z	F_{Breit}	F_{QED}	F_{total}
10	0.1962(1)	0.0003(1)	0.1965(1)
12	0.2056	0.0005(1)	0.2061(1)
14	0.2123	0.0008(1)	0.2131(1)
16	0.2173	0.0012(1)	0.2185(1)
18	0.2213	0.0016(2)	0.2229(2)
20	0.2245	0.0022(2)	0.2266(2)
24	0.2294	0.0035(3)	0.2330(3)
28	0.2332	0.0054(3)	0.2385(3)
30	0.2348	0.0065(4)	0.2412(4)
32	0.2362	0.0077(4)	0.2439(4)
40	0.2411	0.0142(6)	0.2553(6)
48	0.2452	0.0240(8)	0.2692(8)
50	0.2461	0.0271(9)	0.2732(9)
56	0.2487(1)	0.0383(11)	0.2871(11)
60	0.2503(1)	0.0478(13)	0.2982(13)
64	0.2517(2)	0.0593(15)	0.3110(16)
70	0.2533(3)	0.0814(20)	0.3347(20)
72	0.2536(4)	0.0904(22)	0.3440(22)
80	0.2533(10)	0.1372(30)	0.3904(32)
82	0.2525(12)	0.1523(33)	0.4048(36)
90	0.2446(28)	0.2331(54)	0.4777(61)
92	0.2410(35)	0.2597(65)	0.5007(73)

the recoil effect. It was estimated in the same way as for the Breit recoil contribution. As one can see from Table III, for very heavy ions the QED recoil effect becomes even bigger than the Breit recoil contribution.

The total recoil contribution to the g factor should also include small corrections of order $\alpha(\alpha Z)^2(m/M)$ and $(\alpha Z)^2(m/M)^2$ and the related corrections of higher order in αZ and in $1/Z$. To the lowest order in αZ the corresponding one-electron corrections were evaluated in Refs. [48–51].

IV. CONCLUSION

In this paper we have evaluated the nuclear recoil effect of first order in m/M on the ground-state g factor of highly charged Li-like ions. The Breit-approximation contributions have been calculated to all orders in $1/Z$ by employing recursive perturbation theory. The one-electron higher-order (QED) recoil contribution was evaluated to all orders in αZ with the wave functions which partly account for the electron-electron interaction effects. As the result, the most precise theoretical predictions for the recoil effect on the g factor of highly charged Li-like ions are presented.

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