Recoil Effect on the g Factor of Li-Like Ions

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(Received 21 September 2017; published 28 December 2017)

The nuclear recoil effect on the g factor of Li-like ions is evaluated. The one-electron recoil contribution is treated within the framework of the rigorous QED approach to the first order in the electron-to-nucleus mass ratio m/M and to all orders in the parameter αZ. These calculations are performed in a range $Z = 3$–92. The two-electron recoil term is calculated for low- and middle-Z ions within the Breit approximation using a four-component approach. The results for the two-electron recoil part obtained in the Letter strongly disagree with the previous calculations performed using an effective two-component Hamiltonian. The obtained value for the recoil effect is used to calculate the isotope shift of the g factor of Li-like $^{A}\mathrm{Ca}^{17+}$ with $A = 40$ and $A = 48$ which was recently measured. It is found that the new theoretical value for the isotope shift is closer to the experimental one than the previously obtained value.

DOI: 10.1103/PhysRevLett.119.263001

High-precision measurements of the g factor of highly charged ions [1–8] have triggered a great interest in the corresponding theoretical calculations [9–26]. To date, these experiments and theory have allowed the most stringent tests of bound-state quantum electrodynamics (QED) in the presence of a magnetic field and have provided the most precise determination of the electron mass [7,27]. In Ref. [8] the isotope shift of the g factor of Li-like $^{A}\mathrm{Ca}^{17+}$ with $A = 40$ and $A = 48$ has been measured.

The theoretical value of the g-factor isotope shift is generally given by a sum of the nuclear recoil (mass shift) and nuclear size (field shift) contributions. For low- and middle-Z ions it is mainly determined by the mass shift, which in the case of the s states is of pure relativistic origin. The fully relativistic theory of the nuclear recoil effect can be formulated only in the framework of QED. Moreover, the mass shift is the only effect which requires the employment of the bound-state QED theory beyond the external field approximation, providing a unique access to QED beyond the Furry picture at strong-coupling regime [8].

In Ref. [8] the theoretical value for the g-factor mass shift of Li-like calcium was obtained combining the calculations of the one-electron recoil contribution to all orders in αZ and the two-electron recoil contribution within the Breit approximation. While the one-electron contribution was directly evaluated using the QED theory [13,28], the two-electron part was obtained by extrapolating the lowest-order relativistic results from Refs. [29,30]. Combined with the nuclear size effect, the calculation of which causes no problem, the theoretical prediction for the isotope shift of the g factor of $^{A}\mathrm{Ca}^{17+}$ with $A = 40$ and $A = 48$ was found to be in agreement with the experimental one but at the edge of the experimental error bar.

In the present Letter we perform the most accurate to date evaluation of the nuclear recoil contribution to the g factor of highly charged Li-like ions. First, we improve the accuracy of the calculation of the one-electron QED recoil contribution for Li-like calcium [8] and extend it to a wide range of the nuclear charge number, $Z = 3$–92. Second, we calculate the two-electron recoil contribution to the g factor in a range $Z = 3$–20 within the Breit approximation using a four-component approach and investigate reasons for a strong disagreement between the obtained results and the previous calculations [29,30]. Finally, we present the theoretical prediction for the isotope shift of the g factor of Li-like $^{A}\mathrm{Ca}^{17+}$ with $A = 40$ and $A = 48$, which also includes the nuclear size effect, and compare it with experiment [8].

The QED theory for the nuclear recoil effect on the atomic g factor to first order in the electron-to-nucleus mass ratio m/M and to all orders in αZ was developed in Ref. [13]. This theory was employed to derive a complete αZ-dependent formula for the recoil effect on the g factor of a H-like ion. The obtained formula can be also applied to a many-electron ion (atom) with one electron over closed shells, provided the electron propagators are defined for the vacuum including the closed shells [28]. In this case, the formula also incorporates the two-electron nuclear recoil contributions to zeroth order in $1/Z$.

We consider an ion with one electron over closed shells which is put into the classical homogeneous magnetic field, $\mathbf{A}_{\mathrm{cl}}(\mathbf{r}) = [\boldsymbol{\mathcal{H}} \times \mathbf{r}]/2$. For simplicity, we assume that $\boldsymbol{\mathcal{H}}$ is directed along the z axis. According to Refs. [13,31], to zeroth order in $1/Z$, the m/M nuclear recoil contribution to the g factor for a state a is given by ($\hbar = c = 1$, $e < 0$)

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

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

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

is the transverse part of the photon propagator in the Coulomb gauge, $\boldsymbol{\alpha}$ is a vector incorporating the Dirac matrices, and the summation over the repeated indices is implicit. The tilde sign indicates that the corresponding quantity [the wave function, the energy, and the Coulomb Green's function $\tilde{G}(\omega)$] must be calculated in presence of the magnetic field. Since we consider an ion with one valence electron over the closed shells, the Coulomb Green's function is defined as $\tilde{G}(\omega) = \sum_{\tilde{n}} |\tilde{n}\rangle\langle\tilde{n}|[\omega - \tilde{\varepsilon}_n + i\eta(\tilde{\varepsilon}_n - \tilde{\varepsilon}_F)]^{-1}$, where $\tilde{\varepsilon}_F$ is the Fermi energy and $\eta \to 0$. Equation (1) includes both one- and two-electron nuclear recoil contributions to zeroth order in $1/Z$. For the $(1s)^2 2s$ state of a Li-like ion, the $(1/Z)^0$ two-electron contribution is equal to zero. However, this formula can be used to derive an effective two-electron recoil operator which describes the recoil effect on the g factor within the Breit approximation. The expression for this operator is given below.

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

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

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

Here $V(r) = -\alpha Z/r$ is the Coulomb potential of the nucleus, $\delta V(\mathbf{x}) = -e\boldsymbol{\alpha}\cdot\mathbf{A}_{\rm cl}(\mathbf{x})$, $G(\omega) = \sum_n |n\rangle\langle n|[\omega - \varepsilon_n(1-i0)]^{-1}$ is the Dirac-Coulomb Green's function, $\delta\varepsilon_a = \langle a|\delta V|a\rangle$, and $|\delta a\rangle = \sum_n^{\varepsilon_n\neq\varepsilon_a} |n\rangle\langle n|\delta V|a\rangle(\varepsilon_a - \varepsilon_n)^{-1}$. The low-order term can be derived from the relativistic Breit equation, while the derivation of the higher-order term requires the employment of QED beyond the Breit approximation. For this reason, we term them as non-QED and QED one-electron contributions, respectively.

To derive the effective two-electron recoil operator we need to consider in Eq. (1) the two-electron contributions which describe the interaction of the valence electron with the closed-shell electrons. It can easily be done according to the corresponding prescriptions in Refs. [28,32]. Within the Breit approximation, we obtain

$$\Delta g_{\rm int} = \Delta g_{\rm int}^{(1)} + \Delta g_{\rm int}^{(2)}, \tag{5}$$

where

$$\begin{aligned}\Delta g_{\rm int}^{(1)} = -\frac{2}{\mu_0\mathcal{H}m_a}\frac{1}{M}\sum_c(&\langle a|p^i|c\rangle\langle c|p^i|\delta a\rangle\\ &- \langle a|p^i|c\rangle\langle c|D^i|\delta a\rangle\\ &- \langle a|D^i|c\rangle\langle c|p^i|\delta a\rangle + \langle a|p^i|\delta c\rangle\langle c|p^i|a\rangle\\ &- \langle a|p^i|\delta c\rangle\langle c|D^i|a\rangle - \langle a|D^i|\delta c\rangle\langle c|p^i|a\rangle),\end{aligned} \tag{6}$$

$$\Delta g_{\rm int}^{(2)} = -\frac{1}{m_a}\frac{m}{M}\epsilon_{3kl}\sum_c(\langle a|x^l|c\rangle\langle c|(p^k - D^k)|a\rangle + \langle a|(p^k - D^k)|c\rangle\langle c|x^l|a\rangle). \tag{7}$$

Here

$$\mathbf{D} \equiv \mathbf{D}(0) = \frac{\alpha Z}{2r}\left(\boldsymbol{\alpha} + \frac{(\boldsymbol{\alpha}\cdot\mathbf{r})\mathbf{r}}{r^2}\right), \tag{8}$$

ϵ_{ikl} is the Levi-Civita symbol, $|\delta c\rangle = \sum_n^{\varepsilon_n\neq\varepsilon_c} |n\rangle\langle n|\delta V|c\rangle \times (\varepsilon_c - \varepsilon_n)^{-1}$, and the summation ($c$) runs over the closed shells. The $\Delta g_{\rm int}^{(1)}$ term corresponds to the combined interaction due to δV and the two-electron part of the effective recoil Hamiltonian (see Ref. [33] and references therein),

$$H_M = \frac{1}{2M}\sum_{i,k}\left[\mathbf{p}_i\cdot\mathbf{p}_k - \frac{\alpha Z}{r_i}\left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i\cdot\mathbf{r}_i)\mathbf{r}_i}{r_i^2}\right)\cdot\mathbf{p}_k\right]. \tag{9}$$

The one-electron part of this operator corresponds to the first term in Eq. (3). The $\Delta g_{\rm int}^{(2)}$ term leads to the following magnetic recoil operator:

$$H_M^{\rm magn} = -\mu_0\mathcal{H}\frac{m}{M}\sum_{i,k}\left\{[\mathbf{r}_i\times\mathbf{p}_k] - \frac{\alpha Z}{2r_k}\left[\mathbf{r}_i\times\left(\boldsymbol{\alpha}_k + \frac{(\boldsymbol{\alpha}_k\cdot\mathbf{r}_k)\mathbf{r}_k}{r_k^2}\right)\right]\right\}, \tag{10}$$

where we have added the corresponding one-electron part from Eq. (3). The first term in the right-hand side of Eq. (10) defines the nonrelativistic contribution derived previously by Phillips [34].

Thus, within the lowest-order relativistic (Breit) approximation, the recoil effect on the g factor to the first order in m/M can be evaluated by adding the operators (9) and (10) to the Dirac-Coulomb-Breit Hamiltonian, considered in the presence of the external magnetic field. As mentioned above, for the $(1s)^2 2s$ state of a Li-like ion the $(1/Z)^0$ two-electron recoil contribution equals zero. However, we can use the derived effective operators to evaluate the $1/Z$ and higher-order contributions to the recoil effect within the Breit approximation.

For a point-charge nucleus, the low-order one-electron term Δg_L can be evaluated analytically [13],

$$\Delta g_L = -\frac{m}{M}\frac{2\kappa^2\varepsilon^2 + \kappa m\varepsilon - m^2}{2m^2 j(j+1)}, \tag{11}$$

where ε is the Dirac energy and $\kappa = (-1)^{j+l+1/2}(j+1/2)$ is the angular momentum-parity quantum number. To leading order in αZ, we have

$$\Delta g_L = -\frac{m}{M}\frac{1}{j(j+1)}\left[\kappa^2 + \frac{\kappa}{2} - \frac{1}{2} - \left(\kappa^2 + \frac{\kappa}{4}\right)\frac{(\alpha Z)^2}{n^2} + \cdots\right]. \tag{12}$$

It can be seen that for an s state ($\kappa = -1$) the nonrelativistic contribution to Δg_L is equal to zero and, therefore, the low-order term is of pure relativistic [$\sim(\alpha Z)^2$] origin.

The numerical calculation of the higher-order one-electron contribution (4) was performed in the same way as in Refs. [14,35]. After the integration over angles, the summation over the intermediate electron states was carried out using the finite basis set method with the basis functions constructed from B splines [36]. The ω integration was performed analytically for the simplest "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) using the standard Wick's rotation. The higher-order (QED) contribution Δg_H for the $2s$ state is conveniently expressed in terms of the function $P^{(2s)}(\alpha Z)$,

$$\Delta g_H^{(2s)} = \frac{m}{M}\frac{(\alpha Z)^5}{8}P^{(2s)}(\alpha Z). \tag{13}$$

The corresponding numerical results are presented in Table I. The uncertainties have been obtained by studying the stability of the results with respect to a change of the basis set size. For $Z = 20$ the presented result agrees with that from Ref. [8] but is given to a higher accuracy.

To get the total one-electron recoil contribution, we should also account for the radiative ($\sim\alpha$) and second-order (in m/M) recoil corrections. To the lowest order in αZ these corrections were evaluated in Refs. [37–40].

TABLE I. The higher-order (QED) recoil contribution to the $2s$ g factor, expressed in terms of the function $P^{(2s)}(\alpha Z)$ defined by Eq. (13).

Z	$P^{(2s)}_{\text{Coul}}$	$P^{(2s)}_{\text{tr1}}$	$P^{(2s)}_{\text{tr2}}$	$P^{(2s)}(\alpha Z)$
3	−1.082	37.719	−22.644	13.993(1)
4	−1.067	29.519	−15.755	12.697(1)
6	−1.0403	21.1043	−9.1264	10.9376(2)
8	−1.0160	16.7563	−5.9884	9.7519(1)
10	−0.9943	14.0726	−4.2021	8.8762(1)
12	−0.9749	12.2396	−3.0704	8.1943(1)
14	−0.9575	10.9033	−2.3010	7.6447(1)
16	−0.9422	9.8841	−1.7509	7.1911(1)
18	−0.9287	9.0809	−1.3421	6.8101(1)
20	−0.9169	8.4322	−1.0292	6.4860(1)
30	−0.8818	6.4789	−0.1810	5.4160(1)
40	−0.8836	5.5765	0.1911	4.8840(1)
50	−0.9244	5.1802	0.4168	4.6727(1)
60	−1.0150	5.1326	0.6005	4.7182(1)
70	−1.181	5.426	0.795	5.040(1)
80	−1.482	6.186	1.050	5.753(3)
90	−2.07	7.82	1.45	7.20(1)
92	−2.26	8.33	1.57	7.64(2)

As noted above, for the $(1s)^2 2s$ state of a Li-like ion the two-electron recoil contribution to the g factor is equal to zero, if one neglects the interaction between the electrons. This approximation corresponds to zeroth order in $1/Z$. The recoil contributions of the first and higher orders in $1/Z$ have been evaluated within the Breit approximation using the operators (9), (10) and the standard expression for the Dirac-Coulomb-Breit Hamiltonian,

$$H^{\text{DCB}} = \Lambda^{(+)}\left(\sum_i h_i^{\text{D}} + \sum_{i<k} V_{ik}\right)\Lambda^{(+)}, \tag{14}$$

where the indices i and k enumerate the atomic electrons, $\Lambda^{(+)}$ is the product of the one-electron projectors on the positive-energy states (which correspond to the potential $V + \delta V$, where V is the Coulomb potential of the nucleus and δV describes the interaction with the external magnetic field), h_i^{D} is the one-electron Dirac Hamiltonian including δV, and

$$\begin{aligned} V_{ik} &= e^2 \alpha_i^\rho \alpha_k^\sigma D_{\rho\sigma}(0, \mathbf{r}_{ik}) = V_{ik}^{\text{C}} + V_{ik}^{\text{B}} \\ &= \frac{\alpha}{r_{ik}} - \alpha\left(\frac{\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_k}{r_{ik}} + \frac{1}{2}(\boldsymbol{\alpha}_i\cdot\boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_k\cdot\boldsymbol{\nabla}_k)r_{ik}\right) \end{aligned} \tag{15}$$

is the sum of the Coulomb and Breit electron-electron interaction operators.

Let us consider first the calculation of the $1/Z$ recoil contribution, which can be evaluated using perturbation theory. This contribution is conveniently represented by a sum of four terms,

$$\Delta g_{\text{int}}^{(1/Z)} = \Delta g_{\text{int}}^{(1)} + \Delta g_{\text{int}}^{(2)} + \Delta g_{\text{int}}^{(1\text{m})} + \Delta g_{\text{int}}^{(2\text{m})}, \tag{16}$$

where $\Delta g_{\rm int}^{(1)}$ combines the one-electron nonmagnetic recoil term from Eq. (9) with the electron-electron interaction (15) and with the magnetic interaction δV, $\Delta g_{\rm int}^{(2)}$ combines the two-electron nonmagnetic recoil term from Eq. (9) with the electron-electron interaction (15) and with the magnetic interaction δV, $\Delta g_{\rm int}^{(1{\rm m})}$ combines the one-electron magnetic recoil term from Eq. (10) with the electron-electron interaction (15), and $\Delta g_{\rm int}^{(2{\rm m})}$ combines the two-electron magnetic recoil term from Eq. (10) with the electron-electron interaction (15). The numerical evaluation of all these terms has been performed for extended nuclei in the range $Z = 3$–20 using the finite basis set method with the basis functions constructed from B splines. The results, which are expressed in terms of the function $B(\alpha Z)$ defined by

$$\Delta g_{\rm int}^{(1/Z)} = \frac{m}{M}\frac{(\alpha Z)^2}{Z}B(\alpha Z), \tag{17}$$

are presented in Table II. All digits presented in the table should be correct. The extrapolation to the limit $\alpha Z \to 0$ leads to $B(0) = -0.5155(2)$. This value disagrees with the corresponding coefficient $B(0) = -0.8603(8)$ which can be derived (see Ref. [26]) by fitting the lowest-order relativistic results of the fully correlated calculations within the framework of a two-component approach performed by Yan [29,30]. To find out the reasons for this disagreement, we have also evaluated the $1/Z$ recoil corrections using the effective two-component Hamiltonian approach [29,39, 41–43]. The calculations have been performed by perturbation theory starting with the nonrelativistic independent-electron approximation. The summations over electron spectra have been carried out using the finite basis set method for the Schrödinger equation with the basis functions constructed from B splines [36]. With this approach, we obtain $B(0) = -0.8603$, provided we account for the same contributions as described in Refs. [29,30,42]. This corresponds to the evaluation of the spin-dependent terms in the magnetic-field-dependent part of the effective two-component Hamiltonian with the Schrödinger wave function. In the previous calculations [29,30,42] it was assumed that only these terms contribute for the s states. Our study showed, however, that this is not the case. We have found that there exist some additional contributions to the lowest relativistic order. To the first order in $1/Z$, these contributions originate from the spin-independent terms in the magnetic-field-dependent part of the effective Hamiltonian [the first term in Eq. (10)] if they are combined with the spin-orbit and spin-other-orbit coupling terms in the nonmagnetic part of the two-component Hamiltonian (the expressions for these couplings see, e.g., in Ref. [41]). The spin-orbit coupling leads to a nonzero result if it is combined with the Coulomb electron-electron interaction. The evaluation of these terms gives additionally 0.3447 to $B(0)$. This leads to the total result $B(0) = -0.5156$ which agrees with the value obtained in our four-component approach.

The evaluation of the second and higher orders in $1/Z$ contributions within the Breit approximation was also based on the operators (9), (10) and the standard expression for the Dirac-Coulomb-Breit Hamiltonian (14). This was done by the use of a recently developed recursive perturbative approach [44,45]. The results, which are expressed in terms of the function $C(\alpha Z)$ defined by

$$\Delta g_{\rm int}^{(1/Z^{2+})} = \frac{m}{M}\frac{(\alpha Z)^2}{Z^2}C(\alpha Z), \tag{18}$$

are presented in Table III. The $C^{(1+2)}(\alpha Z)$ and $C^{(1{\rm m}+2{\rm m})}(\alpha Z)$ parts, presented in the table, correspond to the nonmagnetic and magnetic recoil contributions defined by operators (9) and (10), respectively. The indicated error bars are due to the numerical uncertainties of the computation.

To derive the total value of the isotope shift, we need also to evaluate the nuclear size effect. In case of Ca isotopes, this contribution can be calculated in the one-electron

TABLE II. The $1/Z$ recoil contribution to the g factor of the $(1s)^2 2s$ state of Li-like ions, expressed in terms of the function $B(\alpha Z)$ defined by Eq. (17). The individual contributions correspond to the related terms in Eq. (16).

Z	$B^{(1)}(\alpha Z)$	$B^{(2)}(\alpha Z)$	$B^{(1{\rm m})}(\alpha Z)$	$B^{(2{\rm m})}(\alpha Z)$	$B(\alpha Z)$
3	−0.8835	0.0213	0.0000	0.3466	−0.5157
4	−0.8836	0.0213	0.0000	0.3465	−0.5158
6	−0.8839	0.0214	0.0000	0.3464	−0.5161
8	−0.8844	0.0216	0.0000	0.3462	−0.5166
10	−0.8849	0.0218	0.0000	0.3459	−0.5172
12	−0.8856	0.0220	0.0001	0.3456	−0.5179
14	−0.8864	0.0223	0.0001	0.3453	−0.5187
16	−0.8873	0.0227	0.0001	0.3449	−0.5197
18	−0.8883	0.0231	0.0001	0.3444	−0.5207
20	−0.8894	0.0235	0.0001	0.3439	−0.5219

TABLE III. The $1/Z^2$ and higher-order recoil contribution to the g factor of the $(1s)^2 2s$ state of Li-like ions, expressed in terms of the function $C(\alpha Z)$ defined by Eq. (18). The $C^{(1+2)}(\alpha Z)$ and $C^{(1{\rm m}+2{\rm m})}(\alpha Z)$ parts correspond to the nonmagnetic and magnetic recoil contributions defined by operators (9) and (10), respectively.

Z	$C^{(1+2)}(\alpha Z)$	$C^{(1{\rm m}+2{\rm m})}(\alpha Z)$	$C(\alpha Z)$
3	0.61(5)	−0.75(5)	−0.14(7)
4	0.59(3)	−0.76(3)	−0.17(4)
6	0.566(10)	−0.775(10)	−0.209(14)
8	0.556(5)	−0.782(5)	−0.226(7)
10	0.550(3)	−0.786(3)	−0.236(4)
12	0.546(2)	−0.789(2)	−0.243(3)
14	0.545(2)	−0.790(2)	−0.245(3)
16	0.543(2)	−0.791(2)	−0.248(3)
18	0.542(1)	−0.792(1)	−0.250(2)
20	0.542(1)	−0.792(1)	−0.250(2)

TABLE IV. Isotope shift of the g factor: ${}^{40}\mathrm{Ca}^{17+} - {}^{48}\mathrm{Ca}^{17+}$, in units of 10^{-9}.

One-electron non-QED nuclear recoil	12.240
Two-electron non-QED nuclear recoil	−1.302
QED nuclear recoil: $\sim m/M$	0.123(12)
QED nuclear recoil: $\sim\alpha(m/M)$	−0.009(1)
Finite nuclear size	0.004(11)
Total theory	11.056(16)
Experiment [8]	11.70(1.39)

approximation using the analytical formula from Ref. [17]. The root-mean-square nuclear charge radii and the related uncertainties were taken from Ref. [46].

The individual contributions to the isotope shift of the g factor for ${}^{40}\mathrm{Ca}^{19+} - {}^{48}\mathrm{Ca}^{19+}$ are presented in Table IV. The uncertainty of the finite nuclear size contribution includes both the nuclear radius and shape variation effects. The shape variation uncertainty was estimated as a difference between the calculations performed for the Fermi and sphere nuclear models. The total theoretical value of the isotope shift amounts to $\Delta g_{\mathrm{IS}}^{(\mathrm{theor})} = 11.056(16) \times 10^{-9}$. This value differs from its previous evaluation, $\Delta g_{\mathrm{IS}}^{(\mathrm{theor})} = 10.305(27) \times 10^{-9}$ [8], which included the two-electron recoil contribution obtained by extrapolating the corresponding results from Refs. [29,30], and is significantly closer to the experimental value, $\Delta g_{\mathrm{IS}}^{(\mathrm{exp})} = 11.70(1.39) \times 10^{-9}$ [8].

Concluding, in this Letter we have evaluated the nuclear recoil effect on the g factor of Li-like ions. The calculations included the m/M one-electron recoil correction in the framework of the fully relativistic formalism and the two-electron recoil contribution within the Breit approximation. A large discrepancy was found between the present result for the two-electron recoil contribution obtained using the four-component approach within the Breit approximation and its previous calculation performed using the effective two-component Hamiltonian. An analysis of the discrepancy showed that some important contributions were omitted in the previous works. As the result, we have obtained the most precise to date theoretical values for the recoil effect on the g factor of Li-like ions. Combining the nuclear recoil and size effects, the isotope shift of the g factor of Li-like ${}^{A}\mathrm{Ca}^{17+}$ with $A = 40$ and $A = 48$ has been evaluated providing better agreement between theory and experiment. We hope that the obtained results will also pave the way for QED tests beyond the Furry picture in experiments with highly charged ions which are planned at the Max-Planck-Institut für Kernphysik in Heidelberg and at the HITRAP/FAIR facilities in Darmstadt.

We thank Krzysztof Pachucki and Vladimir Yerokhin for valuable discussions. This work was supported by the Russian Science Foundation (Grant No. 17-12-01097).

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