Nuclear recoil effect on $g$ factor of heavy ions: prospects for tests of quantum electrodynamics in a new region

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Abstract

The nuclear recoil effect on the $g$ factor of H- and Li-like heavy ions is evaluated to all orders in $\alpha Z$. The calculations include an approximate treatment of the nuclear size and the electron-electron interaction corrections to the recoil effect. As the result, the second largest contribution to the theoretical uncertainty of the $g$-factor values of $^{208}\text{Pb}^{79+}$ and $^{238}\text{U}^{89+}$ is strongly reduced. Special attention is paid to tests of the QED recoil effect on the $g$ factor in experiments with heavy ions. It is found that, while the QED recoil effect on the $g$-factor value is masked by the uncertainties of the nuclear size and nuclear polarization contributions, it can be probed on a few-percent level in the specific difference of the $g$ factors of H- and Li-like heavy ions. This provides a unique opportunity to test QED in a new region — strong-coupling regime beyond the Furry picture.
I. INTRODUCTION

High-precision measurements of the Lamb shifts in highly charged heavy ions [1–5] have already provided tests of QED effects at strong Coulomb field on a few tenth percent level (see, e.g., Refs. [6, 7] and references therein). To date, there are also a number of high-precision measurements of the hyperfine splitting (HFS) in heavy H-like ions [8–13]. The main goal of these experiments was to test QED in a combination of the strongest electric and magnetic fields. However, due to a large uncertainty of the nuclear magnetization distribution correction (so-called Bohr-Weisskopf effect), direct tests of QED by comparison of theory and experiment on the HFS in H-like ions turned out to be impossible. The solution of the problem was found in Ref. [14], where it was proposed to study a specific difference of the HFS in H- and Li-like ions of the same heavy isotope. This difference can be calculated to a very high accuracy. It took about 15 years to reach the required level of accuracy for the HFS measurements in Li-like bismuth [15]. A large discrepancy between the obtained experimental result and the most elaborated theoretical prediction [16] for the specific difference has established the “hyperfine puzzle” [17], which is presently a subject of intensive investigations from both theoretical and experimental sides.

The current tests of bound-state QED by studying the Lamb shift and the HFS in heavy ions are limited to the region where the standard formalism of quantum electrodynamics in presence of external classical fields can be applied. This formalism is known as the Furry picture of QED. The nuclear recoil correction to the Lamb shift in heavy ions, whose evaluation requires QED beyond the Furry picture, is generally masked by the uncertainties of the nuclear size and polarization contributions. This fact and the limited experimental accuracy prevent presently any precise tests of the QED recoil effect on the Lamb shifts in heavy ions. Much higher accuracy is expected to be achieved in $g$-factor experiments with heavy ions which are anticipated in the nearest future at the HITRAP/FAIR facilities in Darmstadt and at the Max-Planck-Institut für Kernphysik (MPIK) in Heidelberg. To date, a number of high-precision measurements of the $g$ factor was performed for low- and middle-$Z$ highly charged ions ($Z$ is the nuclear charge number) [18–25]. The measurement of the isotope shift of the $g$ factor of Li-like $^{40}{\text{Ca}}^{17+}$ with $A = 40$ and $A = 48$ [25] has provided already the first test of the relativistic theory of the recoil effect in highly charged ions in the presence of magnetic field [26]. The precision of the experimental value is currently limited by the uncertainty of the $A = 48$ calcium atomic mass. Several worldwide initiatives are presently aiming to improve the atomic masses. The accuracy
improvement of the calcium masses will result in a direct test of the QED recoil effect in highly charged ions. Moreover, the $g$-factor experiments for heavy ions, which are anticipated in the nearest future, should provide a unique possibility to test the QED recoil effect in strongly nonperturbative in $\alpha Z$ regime, provided the total theoretical value is evaluated to the required accuracy. It is known \cite{27, 28}, however, that the uncertainty due to the nuclear size and polarization effects grows strongly with $Z$ and masks the recoil effect for heavy ions. In Refs. \cite{29–32}, it was shown that this uncertainty can be strongly reduced in specific differences of the $g$-factor values of H-, Li-, and B-like ions allowing for more precise tests of bound-state QED at strong fields. In the present paper we evaluate the nuclear recoil effect on the $g$ factor of H- and Li-like $^{208}$Pb and $^{238}$U ions and demonstrate that the QED recoil contribution to the specific difference in the case of Pb is two orders of magnitude bigger than the uncertainty to which the total theoretical value of the difference can be calculated. This will give a unique possibility to test QED at strong-coupling regime beyond the Furry picture.

The relativistic units ($\hbar = c = 1$, $e < 0$) are used in the paper.

II. BASIC FORMULAS

The complete $\alpha Z$-dependent formula ($\alpha$ is the fine structure constant) for the nuclear recoil effect on the $g$ factor of a H-like ion to the first order in the electron-to-nucleus mass ratio $m/M$ was derived in Ref. \cite{33}. As was noted in that paper, the obtained formula can partially account for the nuclear size correction to the recoil effect if the pure Coulomb potential of the nucleus $V = -\alpha Z/r$ is replaced with the potential of the extended nucleus. The replacement of the potential with an effective local potential $V_{\text{eff}}(r)$, which is the sum of the nuclear and screening potentials, allows one to partially account for the corrections to the one-electron recoil contribution due to the screening of the valence 2s electron by the closed 1s$^2$ shell in a case of Li-like ion. The $m/M$ one-electron nuclear recoil contribution to the $g$ factor for the state $a$ can be represented by the sum of the low-order and higher-order in $\alpha Z$ terms, $\Delta g = \Delta g_L + \Delta g_H$, where

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

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

Here \( \mu_0 \) 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, \( V(r) \) is the nuclear or effective potential (see the discussion above), \( |a\rangle \) — the Dirac wave function for the potential \( V(r) \), \( \varepsilon_a \) — the corresponding Dirac energy, \( \delta V(r) = -e\alpha \cdot A_{cl}(r) \) describes the interaction of the electron with the classical homogeneous magnetic field \( A_{cl}(r) = [H \times r]/2, G(\omega) = \sum_n |n\rangle \langle n| \omega - \varepsilon_n (1 - i0)^{-1} \), \( \delta\varepsilon_a = \langle a | \delta V | a \rangle \), \( |\delta a\rangle = \sum_n^{\varepsilon_n \neq \varepsilon_a} |n\rangle \langle n| \delta V | a \rangle (\varepsilon_a - \varepsilon_n)^{-1} \), \( D^k(\omega) = -4\pi\alpha Z\alpha^l D^{lk}(\omega), \) 

\[ D^{lk}(\omega, r) = -\frac{1}{4\pi} \left\{ \frac{\exp (i|\omega| r)}{r} \delta_{lk} + \nabla^l \nabla^k \left( \frac{\exp (i|\omega| r) - 1}{\omega^2 r} \right) \right\} \] (3)

is the transverse part of the photon propagator in the Coulomb gauge, \( \alpha \) is a vector of the Dirac matrices, and the summation over the repeated indices is implied. The low-order contribution \( \Delta g_L \), which can be derived from the Breit equation, we will refer to as the one-electron non-QED contribution. The higher-order term \( \Delta g_H \) is determined by quantum electrodynamics beyond the Breit approximation and will be termed as the one-electron QED contribution.

In the case of a few-electron ion, one should also consider the two-electron recoil contributions. For ions with one electron over closed shells the two-electron contributions can be easily taken into account within the framework of the one-electron approach by redefining the electron propagator \([26, 29, 34, 35]\). For the ground state of a Li-like ion the two-electron recoil term vanishes in the zeroth order in \( 1/Z \). The corresponding first- and higher-order corrections in \( 1/Z \) to the \( g \) factor can be evaluated employing the effective recoil operators derived within the framework of the Breit approximation \([26]\).
III. RESULTS AND DISCUSSION

According to the aforesaid, the nuclear recoil correction to the $g$ factor is represented as a sum of the term corresponding to the Breit approximation and the QED term. For the pure Coulomb field $V(r) = -\alpha Z/r$, the low-order (non-QED) one-electron term can be calculated analytically [14]:

$$
\Delta g_{L}(\text{p.n.}) = -\frac{m \, 2\kappa \varepsilon_a^2 + \kappa m \varepsilon_a - m^2}{2m^2 j(j+1)},
$$

(4)

where $\varepsilon_a$ is the Dirac energy and $\kappa = (-1)^{j+l+1/2}(j + 1/2)$ is the relativistic angular quantum number. In the present work the low-order (non-QED) one-electron term is calculated for extended nuclei using Eq. (1). The sums over the intermediate electron states have been evaluated using the dual-kinetic-balance (DKB) finite basis set method [36] with the basis functions constructed from B splines [37]. The results of the calculations for $Z = 82, 92$ expressed in terms of the function $F(\alpha Z)$,

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

(5)

are presented in Tables I and II for H- and Li-like ions, respectively. For H-like ions the results are presented for both point and extended nuclei, while for Li-like ions only the case of extended nuclei is considered. The root-mean-square (rms) nuclear charge radii were taken from Ref. [38].

As mentioned above, for the ground state of a Li-like ion the two-electron recoil contribution to the $g$ factor is equal to zero, if one considers the independent electron approximation. This approximation corresponds to zeroth order in $1/Z$. In Table III we present the two-electron recoil correction, which was evaluated to all orders in $1/Z$ within the Breit approximation, as described in our recent work [26].

In the point-nucleus case, the numerical calculations of the higher-order (QED) one-electron contribution $\Delta g_{H}$ have been performed for the $1s$ and $2s$ states in Refs. [26, 27]. In the present paper we have calculated this contribution for the extended nucleus case. To partially account for the electron-electron interaction effect on the QED recoil contribution for Li-like ions, the core-Hartree (CH), Perdew-Zunger (PZ), and local Dirac-Fock (LDF) potentials have been also employed. The construction methods and application examples for these potentials can be found in Refs. [39–43]. The $\omega$ integration in Eq. (2) was performed analytically for the term which does not contain the $D^k(\omega)$ operator (“Coulomb” term) and numerically, after the standard Wick’s rotation, for the other (“one-transverse-photon” and “two-transverse-photon”) terms.
The summation over the intermediate electron states was carried out using the DKB finite basis set method. The results of the calculations for $Z = 82, 92$ expressed in terms of the function $F(\alpha Z)$, defined by Eq. (5), are given in Tables I and II for H- and Li-like ions, respectively. It should be noted that in case of uranium ions the QED term is even bigger than the non-QED contribution.

For H-like ions (Table I), the uncertainty is mainly due to the approximate treatment of the nuclear size contribution to the recoil effect on the $g$ factor. We assume that this uncertainty should be on the level of the related correction to the binding energy which was studied in the Breit approximation in Ref. [44]. According to Ref. [44], this correction changes the nuclear size contribution to the recoil effect by 16% and 21% for the $1s$ state of H-like lead and uranium ions, respectively.

For Li-like ions (Table II), as the final theoretical value of the QED recoil contribution, we have chosen the value obtained for the LDF potential. The uncertainty is estimated as a sum of two contributions. The first one is caused by the approximate treatment of the electron-electron interaction corrections to the QED recoil effect. To estimate this uncertainty, we have performed the calculations of the non-QED one-electron recoil contribution with the LDF potential and compared the obtained results with the total non-QED recoil values presented in Table II. The ratio of the difference obtained to the non-QED LDF result is chosen as a relative uncertainty of the corresponding correction to the QED recoil contribution. The second contribution to the uncertainty is due to the approximate treatment of the nuclear size contribution to the recoil effect. It is estimated in the same way as for H-like ions in Table I.

In Table III, we present the total theoretical values for the $g$ factor of Li-like lead and uranium ions. Except for the recoil corrections, all other contributions have been taken from the previous compilations [45–48]. Compared to Ref. [45], we have strongly reduced the second largest theoretical uncertainty, which was due to the nuclear recoil effect. As one can see from Table III, the QED recoil effect is masked by uncertainties caused by the nuclear size and polarization contributions. The uncertainty of the nuclear size contribution is estimated as a quadratic sum of the uncertainty which is due to the rms radius error bar [38] and the difference between the results obtained for the Fermi and sphere nuclear charge distribution models. This is a rather conservative estimate of the uncertainty. It can be substantially reduced, provided the nuclear charge distribution parameters are known to a good accuracy from experiments with the corresponding muonic atoms. The more fundamental accuracy limit is actually set by the
nuclear polarization uncertainty. To reduce the uncertainty due to the nuclear effects, in Ref. \[29\], it was proposed to study a specific difference between the $g$ factors of Li- and H-like ions,

$$g' = g_{(1s)^22s} - \xi g_{1s},$$

where the parameter $\xi$ must be chosen to cancel the nuclear size correction in this difference. It can be shown that both the parameter $\xi$ and this difference are very stable with respect to variations of the nuclear parameters and nuclear models \[29, 30\].

In case of lead one obtains $\xi = 0.1670264 \[29\]$. The replacement of the Fermi model of the nuclear charge distribution with the sphere model changes the specific difference $g'$ by about $1 \times 10^{-9}$. But, as is mentioned above, this is a very conservative estimate of the uncertainty. If, instead, we consider a variation of the root-mean-square charge radius of the nucleus within its double error bar, we get the change of $g'$ by about $0.1 \times 10^{-9}$ only. The nuclear polarization correction contributes $-0.13(6) \times 10^{-9}$ to this difference \[28, 31\]. At the same time, the QED recoil contribution to the specific difference amounts to $8.7 \times 10^{-9}$. This means that tests of the QED recoil effect on the $g$ factor of heavy ions are possible on a few-percent level, provided all QED and electron-electron interaction corrections are calculated to the required accuracy.

IV. CONCLUSION

In this paper we have evaluated the nuclear recoil effect on the $g$ factor of H- and Li-like lead and uranium ions for the finite-size-nucleus potential and for the effective potentials which partially account for the electron-electron interaction effects in Li-like ions. As the result, the second largest uncertainty in the theoretical values of the $g$ factor of $^{208}\text{Pb}^{79+}$ and $^{238}\text{U}^{89+}$ is strongly reduced. The contribution of the QED recoil effect to the specific difference of the $g$ factors of H- and Li-like ions is compared with the uncertainties due to the nuclear size and polarization effects. It is shown that the QED recoil effect on the $g$ factor can be probed in experiments with heavy ions. This provides a unique opportunity for tests of QED in a new region — strong-coupling regime beyond the Furry picture.

V. ACKNOWLEDGMENTS

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TABLE I. The nuclear recoil contribution to the 1s $g$ factor of H-like lead and uranium ions, expressed in terms of the function $F(\alpha Z)$ defined by Eq. (5). The uncertainties are mainly due to the approximate treatment of the nuclear size correction to the recoil effect (see the text).

| Contribution                        | $^{208}$Pb$^{81+}$ | $^{238}$U$^{91+}$ |
|-------------------------------------|---------------------|---------------------|
| Non-QED recoil, point nucleus       | 0.9632              | 0.9504              |
| Non-QED recoil, extended nucleus    | 0.8746              | 0.7583              |
| QED recoil, point nucleus           | 0.8619              | 1.4456              |
| QED recoil, extended nucleus        | 0.8564              | 1.3491              |
| Total recoil, point nucleus         | 1.8251              | 2.3961              |
| Total recoil, extended nucleus      | 1.731(15)           | 2.107(61)           |

TABLE II. The nuclear recoil contribution to the 2s $g$ factor of Li-like lead and uranium ions, expressed in terms of the function $F(\alpha Z)$ defined by Eq. (5). All values are calculated for the extended nucleus case. The total uncertainties account for the approximate treatment of the electron-electron interaction and the nuclear size effects (see the text).

| Contribution                        | $^{208}$Pb$^{79+}$ | $^{238}$U$^{89+}$ |
|-------------------------------------|---------------------|---------------------|
| Non-QED one-electron recoil         | 0.2597              | 0.2471              |
| Non-QED two-electron recoil         | -0.0072             | -0.0061             |
| Total non-QED recoil                | 0.2525              | 0.2410              |
| QED recoil, Coulomb potential       | 0.1585              | 0.2693              |
| QED recoil, CH potential            | 0.1525              | 0.2598              |
| QED recoil, LDF potential           | 0.1523              | 0.2597              |
| QED recoil, PZ potential            | 0.1539              | 0.2622              |
| Total recoil                        | 0.405(5)            | 0.501(17)           |

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

|                                | $^{208}$Pb$^{79+}$     | $^{238}$U$^{89+}$     |
|--------------------------------|------------------------|------------------------|
| Dirac value (point nucleus)    | 1.932002904            | 1.910722624            |
| Finite nuclear size            | 0.00007857(14)         | 0.00024162(36)         |
| One-electron QED               | 0.0024081(5)           | 0.0024427(8)           |
| Screened QED                   | $-0.00000191(4)$       | $-0.00000218(6)$       |
| Interelectronic interaction    | 0.00213934(4)          | 0.00250005(6)          |
| Non-QED recoil                 | 0.000000239(2)         | 0.000000250(8)         |
| QED recoil                     | 0.000000144(3)         | 0.000000270(10)        |
| Nuclear polarization           | $-0.00000004(2)$       | $-0.00000027(14)$      |
| Total theory                   | 1.9366273(5)           | 1.9159051(9)           |
| Total theory from Ref. [45]    | 1.9366272(6)           | 1.9159048(11)          |

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