Finite-nuclear-size contribution to the g factor of a bound electron: Higher-order effects

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A precision comparison of theory and experiments on the g factor of an electron bound in a hydrogenlike ion with a spinless nucleus requires a detailed account of finite-nuclear-size contributions. While the relativistic corrections to the leading finite-size contribution are known, the higher-order effects need an additional consideration. Two results are presented in the paper. One is on the anomalous-magnetic-moment correction to the finite-size effects and the other is due to higher-order effects in $Z\alpha m R_N$. We also present here a method to relate the contributions to the g factor of a bound electron in a hydrogenlike atom to its energy within a nonrelativistic approach.

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I. INTRODUCTION

Recent experiments on the g factor of a bound electron in a hydrogenlike ion with a spinless nucleus have reached a really fantastic accuracy at the level of a few parts in 10^{11} [1]. The most suitable for the precision studies are the results at low and middle values of the nuclear charge Z, since in that range the theoretical uncertainty is competitive with the actual or potential experimental one. The theoretical uncertainty is due to higher-order effects of bound-state quantum electrodynamics (QED) (see, e.g., [2]) and due to the nuclear structure and, first of all, due to the distribution of the nuclear charge. Because of those nuclear effects, we do not expect to reach the accuracy at the level of a few parts in 10^{11} at high values of Z. (The situation with lithiumlike ions is in many respects similar, but it is beyond the scope of this paper.)

Meanwhile, it would be interesting to consider higher-order finite-nuclear-size (FNS) effects at low and middle Z in order to improve the accuracy and reliability of the calculations of the FNS effects. The finite-nuclear-size contribution is a small one. To reach the uncertainty of 10^{-11} for the bound electron g factor in a hydrogenlike carbon ion ($Z = 6$) we have to obtain the related finite-size contribution with the fractional uncertainty of 5%, while for a silicon ion ($Z = 14$) the required uncertainty is 0.1% (see, e.g., [3,4]).

The state of the art in calculation of the FNS effects is presented in Ref. [3]. The claimed theoretical accuracy of the considered there nuclear-size contributions is estimated as about 0.1%. As we show below the higher-order FNS effects, missed in Refs. [3,4], can deliver us the contributions comparable with the claimed uncertainty. The situation has to be clarified.

To find the FNS contribution to the bound electron g factor at the level better than one part per thousand one has to look for higher-order corrections. The FNS term for the g factor in the ground state of a hydrogenlike ion was found in Ref. [5] in the form of a relation between the contributions to the bound electron g factor and to the binding energy

$$\frac{\Delta g_{\rm fns}(1s)}{2} = \frac{2}{3}\frac{\partial E_{\rm fns}(1s)}{\partial m}, \tag{1}$$

where m is the electron mass and $E_{\rm fns}$ is the FNS contribution to the energy of the electronic state of interest. Here and throughout the paper the relativistic units, in which $\hbar = c = 1$, are applied.

The expression is valid within the external field approximation as far as the electron is a pointlike particle and therefore it satisfies a Dirac equation with no anomalous magnetic moment, while its interaction with the nucleus is described by a local electrostatic potential [5]. The relation between a contribution to the bound g factor and the related contribution to the binding energy is not restricted by the consideration of the FNS effects and it is actually applicable to the pure Coulomb potential as well. (Speaking, e.g., about the QED effects we recall that the electron self-energy cannot be described by such a local potential, while the vacuum polarization can.) The approximation allows us to account for the FNS effects, which are described by a certain effective potential. The expression is exact in $Z\alpha$. It delivers us the leading finite-nuclear-size contribution, all the relativistic corrections to it, and some other higher-order finite-size corrections.

This identity allows us to derive immediately the leading FNS term (cf. [6])

$$\frac{\Delta g_{\rm fns:lead}(1s)}{2} = \frac{4}{3}(Z\alpha)^4 m^2 R_N^2, \tag{2}$$

where R_N is the rms nuclear charge radius. To obtain (2) one has to utilize the expression for the leading term for the

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finite-size contribution to the energy

$$\Delta E_{\rm fns:lead}(1s) = \frac{2}{3}(Z\alpha)^4 m^3 R_N^2. \quad (3)$$

It also provides a possibility to find various corrections to (2), while applying a more advanced expression for $E_{\rm fns}$ than the leading term (3).

Any correction described by the Dirac equation for a (pointlike) electron at the Coulomb field of a distributed charge can be incorporated through (1). In particular, it may be used to derive the relativistic corrections to the leading FNS term (see, e.g., the discussion in Ref. [5]). In this paper we consider a higher-order correction of order $(Z\alpha)^5(mR_N)^3m$ to the leading finite-size term (see Sec. II). That is a correction to (2), which is the leading one in $Z\alpha mR_N$.

Another type of higher-order effects is due to the anomalous magnetic moment, which induces an additional interaction between the electron and the electric field of the nucleus. The bound-state contribution due to the anomalous magnetic moment was also considered in Ref. [5]. The result [see (22) in Ref. [5]] is valid for any potential and may be used for the potential of the extended nucleus. However, the related expression, being a fully relativistic one (i.e., being exact in $Z\alpha$) is somewhat more complicated than the expression (1) above.

We note that the combined correction due to the anomalous magnetic moment and the finite-nuclear-size potential is small. It is of order $\alpha(Z\alpha)^4(mR_N)^2$ [being $\sim 10^{-3}$ of the leading finite-size term (2)]. The expression (22) in Ref. [5] allows us in principle to find the result exactly in $Z\alpha$, however, while the contribution of the electron's anomalous magnetic moment is unique in order $\alpha(Z\alpha)^4(mR_N)^2$, there are others in order $\alpha(Z\alpha)^5(mR_N)^2$. So, a nonrelativistic consideration of this contribution is sufficient since the uncertainty is anyway of order $\alpha(Z\alpha)^5(mR_N)^2$ unless we take into account all the radiative correction to the finite-size effects.

We perform such a nonrelativistic consideration below (see Sec. III). The result for the g factor of an electron bound at the ns state in a hydrogenlike ion is

$$\frac{\Delta g_{a:\rm fns}(ns)}{2} = -\frac{a_e}{3}\frac{\partial E_{\rm fns}(ns)}{\partial m}, \quad (4)$$

where $a_e \equiv (g-2)/2 = \alpha/2\pi + \cdots$ is the anomalous magnetic moment of the electron. Note that, for the finite-size energy $E_{\rm fns}$, it is sufficient to use the leading term (3).

II. NEXT-TO-LEADING FINITE-NUCLEAR-SIZE CORRECTION TO THE g FACTOR OF A BOUND ELECTRON (WITHOUT ANY ANOMALOUS MAGNETIC MOMENT)

In this section we consider the pointlike Dirac's electron with a zero value of the anomalous magnetic moment and explore opportunities given by the general expression for the bound contribution to the g factor induced by a central potential $V(r)$ [5] [which is reduced to Eq. (2) for the FNS correction to the $1s$ state]. The fully relativistic expression reads

$$g_V(nl_j) = -\frac{\kappa}{2j(j+1)}\left[1 - 2\kappa - 2\kappa\frac{\partial E}{\partial m}\right], \quad (5)$$

where $\kappa = \pm(j+1/2)$ (the plus sign is for $l > j$ and the minus one is for $l < j$; for the s states $\kappa = -1$). The expression includes also the free value of the electron g factor (which is equal to two for the ns states).

The binding energy E of the electron is its full energy above the rest energy mc^2; E includes the leading Coulomb term and various corrections to it. As we mentioned, Eq. (5) is valid for electric potential-type contributions within the external-field approximation for a pointlike electron. As far as we consider the nuclear-finite-size contributions in the nonrecoil limit, to find a higher-order contribution to the g factor is sufficient to find a related contribution to the energy and to differentiate it.

The leading nonrelativistic FNS contribution to the bound g factor [see (2)] is well known. The higher-order effects can be presented in the external-field approximation with a function of two parameters

$$\Delta g_{\rm fns:lead}\mathcal{F}(Z\alpha, Z\alpha mR_N). \quad (6)$$

Let's briefly discuss the current accuracy of the calculation of the FNS contribution in terms of two-parameter presentation (6). The state of the art for the FNS effects in theory of the g factor of a hydrogenlike ion with medium Z can be found in Ref. [3]. The consideration is based on the relation between FNS contributions to the g factor and those to the related binding energy as found in Ref. [5].

The expression for the energy originates from the results of [7]. There are a number of results there. First, they solve the Dirac equation with a nucleus, the charge of which is homogenously distributed within a sphere. The result for the homogenous sphere explicitly depends on two parameters [cf. (6)]. It is exact in $Z\alpha$, but not in $Z\alpha mR_N$. That is easy to verify by expanding in both parameters. There should be a term of order $(Z\alpha)^2m(Z\alpha mR_N)^2\ln(Z\alpha)$. This term is well established. It was found in Ref. [8] and rederived in, e.g., [9,10]. The term is absent in the results of [7] for the homogenous-sphere distribution. That means that the latter does not treat the contributions of the second order in the extended charge distribution properly and the result is not exact in $Z\alpha mR_N$.

Secondly, the result for the homogenous sphere, which depends on two small parameters [cf. (6)] is expanded in $Z\alpha mR_N$ [7] and such an expanded result of [7] is mostly used in literature and in particular it is applied in Refs. [3,4].

Besides, we have to mention that, after a certain solution with a homogenous sphere, one has to compare its result with the result for an arbitrary charge distribution in order to find an effective value of the sphere radius, for which the homogenous-sphere result is equal to a result for an arbitrary charge distribution $\rho_E(\mathbf{r})$. As it is well established in low-Z physics, the complete FNS result, expanded in $Z\alpha$ and $Z\alpha mR_N$, should include various bi-local convolutions, such as

$$\iint d^3r\, d^3r' |\mathbf{r}-\mathbf{r}'|^n \rho_E(\mathbf{r})\rho_E(\mathbf{r}'),$$

which is called the "nth Zemach moment." One of such convolutions (for $n = 3$) is the leading contribution for the second-order (in the FNS effects) correction (see below). In the case of an arbitrary charge distribution, the convolutions with odd values of n cannot be reduced to a sum of combinations such as

$$\int d^3r|\mathbf{r}|^a\rho_E(\mathbf{r})\int d^3r'|\mathbf{r}'|^{n-a}\rho_E(\mathbf{r}').$$

To the best of our knowledge, the numerous combinations of that type appeared in the effective radius approach, but no bilocal convolutions. That makes all known results for the binding energy with an arbitrary charge distribution, based on [7], incomplete in order $(Z\alpha)^2m(Z\alpha mR_N)^3$. Fortunately, the results in Refs. [3,4] are based on the results from [7], expanded in $Z\alpha mR_N$, and do not contain the results of order $(Z\alpha)^2m(Z\alpha mR_N)^3$ at all. Therefore, it is sufficient to add to the results of [3,4], which are exact in $Z\alpha$ and of the leading order in $(Z\alpha mR_N)$, a complete result of order $(Z\alpha)^2m(Z\alpha mR_N)^3$.

Concluding the brief discussion of the available results, the relativistic corrections (i.e., the result of expansion in $Z\alpha$ for the leading term in $Z\alpha mR_N$) to the energy can be completely taken into account by using (5) as suggested in Ref. [5]. Such relativistic corrections to the finite-size contribution to the energy are discussed in Ref. [8] (through $Z\alpha$ expansion) and in Ref. [7] (exactly in $Z\alpha$).

The issue on the relativistic corrections to the g factor has been already covered in Ref. [3] and in this section we focus on the expansion in $Z\alpha mR_N$. Since the value of this parameter is very small [$\ll(Z\alpha)^2$], it is sufficient to consider the contribution of the next-to-leading order in $Z\alpha mR_N$ in the leading order in $Z\alpha$.

The related contribution to the energy [of the leading order in $(Z\alpha)$ and the next-to-leading order in $Z\alpha mR_N$] is well known and it is referred to as the Friar term [8,11],

$$\Delta E_{\rm fns:3}(1s) = -\frac{(Z\alpha)^5\,m^4}{3}\,\langle r^3\rangle_2, \tag{7}$$

where

$$\langle r^3\rangle_2 \equiv \int d^3r\,d^3r'\rho_E(\mathbf{r})\rho_E(\mathbf{r}')|\mathbf{r}-\mathbf{r}'|^3 \tag{8}$$

is the third Zemach momentum or the Friar momentum (of the nuclear charge distribution). It is a convolution with involving the density of the nuclear charge distribution $\rho_E(\mathbf{r})$. The corresponding contribution to the bound electron g factor is

$$\frac{\Delta g_{\rm fns:3}(1s)}{2} = -\frac{8}{9}(Z\alpha)^5\,m^3\,\langle r^3\rangle_2. \tag{9}$$

The contribution for the other states is

$$\Delta g_{\rm fns:3}(nl) = \Delta g_{\rm fns:3}(1s)\,\frac{\delta_{l0}}{n^3}.$$

The FNS correction of order $(Z\alpha)^5$ was studied previously in Ref. [12]. The results (in the momentum space) were obtained there taking into account recoil effects and they have rather a cumbersome form, which makes a direct comparison complicated. Those complicated expressions of [12] are not consistent with our result here. In the nonrecoil limit, which should dominate in the numerical values in Table 2 of [12], the correction to the g factor of a bound lepton should be proportional to its mass cubed [see (9)]. The results are given there for electronic and muonic atoms and the ratio of their values for medium Z, for which the recoil effects are negligible, is $\sim 2\times 10^6$, while $(m_\mu/m_e)^3 \simeq 8.9\times 10^6$, which means that the result in Ref. [12] has a different scaling from ours in Eq. (9). Besides, the sign of the correction for the g factor of a bound muon in a muonic hydrogenlike atom and of a bound electron in ordinary hydrogenlike atoms differs in Ref. [12]. In principle, the violation of the m^3 scaling and the change of the sign could be assigned to enhanced recoil contributions. However, that would change the sign of the muon's g factor and keep the sign of the electron's one. The electron's correction in Ref. [12] is positive, while our result in Eq. (9) has a negative value. We conclude that the calculations of the FNS correction of order $(Z\alpha)^5$ in Ref. [12] is incorrect.

III. CALCULATION OF THE ANOMALOUS-MAGNETIC-MOMENT CORRECTION IN THE FINITE-NUCLEAR-SIZE CONTRIBUTION

We have considered above an electron, neglecting its anomalous magnetic moment. On the contrary, in this section we consider the finite-size contribution due to the anomalous moment. We do that in the nonrelativistic approximation, i.e., in the leading order in $Z\alpha$. The anomalous-magnetic-moment contribution is the leading radiative correction to the finite-size term for the bound g factor. It has order $\alpha(Z\alpha)^4(mR_N)^2$ and is *not* related to the contribution to the energy of order $\alpha(Z\alpha)^4m(mR_N)^2$. The related contribution to the energy is of higher order [namely, of order $\alpha(Z\alpha)^5m(mR_N)^2$]. The mechanism to produce the contribution to the g factor is not related to the contribution to the energy directly. It is due to behavior of an electron with a nonzero anomalous magnetic moment at a electrostatic field modified by FNS effects and the related modification of its wave function.

The problem has been previously discussed in Ref. [5] with a fully relativistic consideration. Here, we consider the leading nonrelativistic approximation, which is sufficient for a number of applications and easier to use. We start with a relativistic expression obtained in Ref. [5] [see Eq. (22) there] and perform a nonrelativistic reduction of the wave function. That gives us the expression for the leading anomalous-magnetic-moment correction to the bound g factor for an arbitrary state nl_j,

$$\Delta g_a(nl_j) = \frac{a_e}{2j(j+1)}\bigg[1-2\kappa + \frac{\partial E}{\partial m} - \frac{\kappa}{m}\int d^3r\,\phi^*(\mathbf{r})\,r\,\frac{\partial V(r)}{\partial r}\phi(\mathbf{r})\bigg], \tag{10}$$

where $\phi(\mathbf{r})$ is the wave function and E is the energy of an electron of the Schrödinger equation with the central electrostatic potential $V(r)$, but without any anomalous magnetic moment.

The expression (10) can be transformed (see the Appendix) into

$$\Delta g_{a:V}(nl_j) = \frac{a_e}{2j(j+1)}[1+2\kappa]\frac{\partial E}{\partial m} \tag{11}$$

for any central potential $V(r)$. [We drop out the free contribution in (10), which for the ns states is $g_a^{(0)}(ns) = 2a_e$.]

To check this expression we can consider the pure Coulomb potential ($V = V_C$) and obtain the standard anomalous-magnetic-moment correction

$$\Delta g_{a:C}(nl_j) = -\frac{a_e}{4j(j+1)}[1+2\kappa]\frac{(Z\alpha)^2}{n^2}\,, \tag{12}$$

which for the s states is reduced to the well-known result [13]

$$\Delta g_{a:C}(ns) = a_e \frac{(Z\alpha)^2}{3n^2}. \quad (13)$$

In the case of the anomalous-magnetic-moment correction to the finite-size term we find

$$\Delta g_{a:\mathrm{fns}}(ns) = -\frac{4}{3}\, a_e\, (Z\alpha)^4 \frac{(mR_N)^2}{n^3}. \quad (14)$$

As we have already mentioned in the Introduction, the contribution in (14) is the leading radiative correction to FNS effects. The anomalous-magnetic-moment FNS contribution is a unique contribution to the bound g factor of order $\alpha(Z\alpha)^4 m(mR_N)^2$. The radiative FNS contributions to the energy levels are of order $\alpha(Z\alpha)^5 m(mR_N)^2$ (see, e.g. [14]) and they may lead only to FNS corrections of order $\alpha(Z\alpha)^5(mR_N)^2$ to the bound g factor. Since they involve the electron's self-energy they cannot be presented in the terms of a local potential and therefore cannot be derived by the method applied here.

IV. CONCLUSIONS

A hydrogenlike ion is a simple atomic system which allows us to build an accurate theory based on QED. In particular, such a theory can accurately predict a value of the g factor of a bound electron. A comparison of the theoretical predictions with experimental results enables accurate tests of the bound-state QED and a determination of the relative atomic weight of the electron (see, e.g., [15]). To facilitate this, we have to control the finite-nuclear-size effects with a high accuracy, which includes a consideration of higher-order FNS effects.

Concluding, we find two higher-order corrections to the leading finite-nuclear-size contribution to the g factor of bound electron in a hydrogenlike ion with a spinless nucleus. For the electron in the ground state the results are

$$\Delta g_{\mathrm{fns:3}}(1s) = -\frac{2}{3}(Z\alpha m R_N)\frac{\langle r^3\rangle_2}{R_N^3}\,\Delta g_{\mathrm{fns:lead}}(1s),$$
$$\Delta g_{a:\mathrm{fns}}(1s) = -\frac{\alpha}{4\pi}\,\Delta g_{\mathrm{fns:lead}}(1s), \quad (15)$$

where the leading finite-nuclear-size contribution $\Delta g_{\mathrm{fns:lead}}$ is given in Eq. (2).

The anomalous-magnetic-moment correction in Eq. (15) is comparable with the uncertainty of the relativistic calculation in the leading order in $Z\alpha m R_N$ for hydrogenlike carbon and silicon (see, e.g., [3])

$$\Delta g_{a:\mathrm{fns}}(1s) \simeq -5.8\times 10^{-4}\,\Delta g_{\mathrm{fns:lead}}(1s). \quad (16)$$

For a rough estimation of the importance of higher order in $Z\alpha m R_N$ correction in Eq. (15) one can set $\langle r^3\rangle_2 = 3.3\,R_N^3$ (as it takes place for the homogenous-sphere charge distribution). That leads to the results for carbon and silicon ions

$$\Delta g_{\mathrm{fns:3}}(1s,{}^{12}\mathrm{C}^{5+}) = -6.2\times 10^{-4}\,\Delta g_{\mathrm{fns:lead}}(1s),$$
$$\Delta g_{\mathrm{fns:3}}(1s,{}^{28}\mathrm{Si}^{13+}) = -1.8\times 10^{-3}\,\Delta g_{\mathrm{fns:lead}}(1s), \quad (17)$$

which are comparable with the uncertainty of the relativistic calculation of the leading finite-size term.

Because of the uncertainty in the calculation of the leading finite-size term at the level of a part in thousand, it is sufficient to find the (small) correction, discussed here, with a 10% accuracy. That completely justifies the use of the homogenous-sphere distribution for this correction. The values of the nuclear charge radii are taken from [16].

The combined higher-order contribution to the bound electron g factor is -4.8×10^{-13} for the carbon-12 ion and -4.6×10^{-11} for the silicon-28 one. A similar calculation for the hydrogenlike oxygen-16 gives -2.2×10^{-12}. These three ions are of the highest experimental interest [1,17,18].

Our results have been obtained by using relations between the contributions to the energy of a bound state and its electron's g factor. Those relations are derived here by using a nonrelativistic relativistic approach. We expect the same method can be applied for other nonrelativistic contributions.

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APPENDIX: NONRELATIVISTIC DERIVATION OF (11)

Here we do a "nonrelativistic" consideration of the bound electron g factor. That assumes that we consider an electron, described by the Dirac equation, but with use of a nonrelativistic expansion. To derive (11) or (5) within a nonrelativistic technique, we first note that usually the related contributions to the g factor for the nl_j state are expressed in terms of a linear combination of $\langle \mathbf{p}^2\rangle$, $\langle V(r)\rangle$, and $\langle r(\partial V(r)/\partial r)\rangle$, where $\langle\cdots\rangle$ stands for the diagonal matrix element over the state of interest. For example, the result for the anomalous-magnetic-moment contribution in Sec. III *is* expressed in Eq. (10) in terms of $\langle r(\partial V(r)/\partial r)\rangle$.

Once we have the initial expression with one or a few of the mentioned structures, we have to link all three matrix elements to the energy. One relation between them is obvious:

$$\left\langle \frac{\mathbf{p}^2}{2m}\right\rangle + \langle V(r)\rangle = E_{nlj}. \quad (A1)$$

Another relation is found by a transformation similar to a proof of a quantum virial theorem, by exploring

$$\langle [H, \mathbf{r}\cdot\mathbf{p}]\rangle = 0. \quad (A2)$$

The relation of interest is

$$\left\langle r\,\frac{\partial V(r)}{\partial r}\right\rangle = 2\left\langle\frac{\mathbf{p}^2}{2m}\right\rangle, \quad (A3)$$

which for $V(r)\propto r^k$ delivers us the quantum extension of the virial theorem.

Therefore, any linear combination of $\langle\mathbf{p}^2\rangle$, $\langle V(r)\rangle$, and $\langle r(\partial V(r)/\partial r)\rangle$ may be presented in the terms of $\langle\mathbf{p}^2\rangle$ and E_{nlj}.

To find $\langle\mathbf{p}^2\rangle$ we note that the potential $V(r)$ does not depend explicitly on the electron mass m. Therefore, we obtain

$$\left\langle\frac{\mathbf{p}^2}{2m}\right\rangle = -m\left\langle\frac{\partial}{\partial m}H\right\rangle = -m\,\frac{\partial E}{\partial m}. \quad (A4)$$

Combining this identity with the previous one we arrive at

$$\left\langle r\,\frac{\partial V(r)}{\partial r}\right\rangle = -2m\,\frac{\partial E}{\partial m}. \tag{A5}$$

To calculate the Coulomb contribution (with or without the anomalous magnetic moment) we have to set $V(r) = V_C(r)$, $E = E_C$, etc. To deduce the finite-nuclear-size correction we have to start with $V = V_C + V_{\rm fns}$, $E = E_C + E_{\rm fns}$, etc. and subtract the Coulomb term appropriately. The obtained nonrelativistic expressions for (5) and (11) are not exact in $Z\alpha$, but they are exact in the perturbation $V_{\rm fns}$.

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