Nuclear Shape Effect on the *g* Factor of Hydrogenlike Ions

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The nuclear shape correction to the *g* factor of a bound electron in the 1*S* state is calculated for a number of nuclei in the range of charge numbers from $Z = 6$ up to $Z = 92$. The leading relativistic deformation correction has been derived analytically, and also its influence on one-loop quantum electrodynamic terms has been evaluated. We show the leading corrections to become significant for mid-Z ions and for very heavy elements to even reach the 10^{-6} level.

The ever-increasing precision of measurements and theory of the *g* factor of a bound electron has recently delivered a new value for the electron mass [1,2] and keeps providing stringent tests for quantum electrodynamics (QED) in strong fields [1–3]. It also allows us to access electromagnetic properties of nuclei such as charge radii, as demonstrated in a very recent proof-of-principle study with a Si^{13+} ion [3], or, as suggested theoretically, magnetic moments [4]. Also, it is anticipated that *g* factor studies will yield a value for the fine-structure constant α that is more accurate than the presently established one when extending the experiments to elements with a high charge number Z [5].

In a few years, measurements with the heaviest elements will be possible [6]. As higher-order nuclear and QED contributions to the theoretical value of the *g* factor are strongly boosted with increasing Z, at the present 10^{-10} level of relative experimental accuracy [3,7] or even below, our present understanding of atomic structure will not be satisfactory. In such strong Coulomb fields, nuclear effects beyond a simple spherical model arise. Furthermore, QED and nuclear structural contributions are intertwined.

In this Letter, we consider the nuclear shape effect and find that, while it can be safely neglected in predictions for low-Z systems, it greatly influences the *g* factor value already for mid-Z elements. At high nuclear charges, its inclusion in the theoretical description is mandatory; for example, for U^{91+}, its relative contribution to the total *g* factor reaches the 10^{-6} level. We furthermore evaluate mixed nuclear-QED terms, i.e., the nuclear shape effect on the one-loop QED terms of self-energy (SE) and vacuum polarization (VP). Even these contributions will be highly relevant for the interpretation of experimental values to be obtained within a few years [6]. Furthermore, a comparison of theory and experiment may even yield more accurate values for nuclear shape parameters, relevant in explaining shape phase transitions in nuclear structure theory [8].

We account for the nuclear quadrupole and hexadecapole deformation and derive a formula describing the nuclear shape correction to the *g* factor of a bound electron in hydrogenlike ions in the 1*S* state. Then we focus on systems where the nucleus is spinless and in its ground state. Let us start with the definition of the electron *g* factor [we use units with $c = 1$, $\hbar = 1$, $\alpha = e^2/(4\pi)$, and $e = -|e|$ unless otherwise stated]

$$\delta E = -\frac{e}{m}\langle \vec{s}\,\vec{B}\rangle \frac{g}{2}, \qquad (1)$$

where δE stands for the energy correction due to the coupling of the electron spin operator $\vec{s}$ to the external magnetic field $\vec{B}$, m is the mass of the electron, and $\langle\ldots\rangle$ stands for the expectation value. The nuclear deformation (ND) correction to the *g* factor, which we present, is closely related to the finite-size (FS) effect, which is well known in the context of atomic levels. The correction emerges when one accounts for a deviation of a nucleus from the spherical shape.

Let us consider now a relativistic Hamiltonian of the bound system of an electron and a nucleus in the presence of an external, constant, and homogeneous magnetic field. The interaction of the nucleus with the external magnetic field is negligible, so that we can write

$$H = H_a + H_N + \delta V_C - e\vec{\alpha}\,\vec{A}, \qquad (2)$$

where $\vec{A} = \frac{1}{2}(\vec{B}\times\vec{r})$, H_a is the atomic Dirac-Coulomb Hamiltonian $H_a = \vec{\alpha}\,\vec{p} + \beta m - \frac{Z\alpha}{r}$, $\vec{r}$ is the vector describing the electron's position with respect to the mass center of the system, H_N is the (unknown) nuclear Hamiltonian, and δV_C is the deviation from the monopole term of the exact Coulomb potential of our system, i.e.,

$$\delta V_C = \frac{Z\alpha}{r} - \sum_{i=1}^{Z}\frac{\alpha}{|\vec{r}-\vec{r}_i|}, \qquad (3)$$

where $\vec{r}_i$ are the proton position vectors. Now we formulate the framework for the perturbative calculation of the energy correction due to the presence of the magnetic field and the deviation from the Coulomb potential. We start with the equation

$$(H_a + H_N + \delta V_C - e\vec{\alpha}\vec{A})|\Psi\rangle = (E_a^{(0)} + E_N^{(0)} + \delta E)|\Psi\rangle, \quad (4)$$

where $|\Psi\rangle$ denotes the perturbed state of the system, $E_a^{(0)}$ the unperturbed ground-state energy of the atom, $E_N^{(0)}$ the unperturbed ground-state energy of the nucleus, and δE the energy correction arising due to δV_C and the interaction with the external magnetic field. Next, we perform the following approximation: We assume that the potential δV_C does not induce any nuclear transition, which means that we neglect the nuclear polarizability (NP) effects. However, the derivation of the NP correction as well as its numerical values for a number of elements can be found in Ref. [9]. In principle, there are also mixed terms containing both the NP and nuclear deformation effects, but, since these effects are both already small, we neglect the mixed terms. Then we can write $|\Psi\rangle = |\phi'\rangle \otimes |\psi\rangle$, where $|\psi\rangle$ stands for the ground state of the nucleus, $|\phi'\rangle$ denotes the perturbed atomic state $|\phi'\rangle = |\phi\rangle + |\delta\phi\rangle$, and $|\delta\phi\rangle$ stands for the correction to the unperturbed atomic state $|\phi\rangle$. We substitute the state $|\Psi\rangle$ into Eq. (4) and act on the resulting equation with $\langle\psi|$. Following an obvious reduction, we obtain

$$[H_a + \delta\hat{V}(\vec{r}) - e\vec{\alpha}\vec{A}]|\phi'\rangle = (E_a^{(0)} + \delta E)|\phi'\rangle, \quad (5)$$

where $\delta\hat{V}(\vec{r}) \equiv \langle\psi|\delta V_C|\psi\rangle$.

Now we will express $\delta\hat{V}(\vec{r})$ in terms of a nuclear charge distribution $\rho(\vec{r})$. We do not focus on details here since the detailed derivation of the formula (6) can be found in Ref. [10]. If the nucleus is in the state of vanishing angular momentum $I = 0$, then the potential $\delta\hat{V}(\vec{r})$ can be written in terms of the simple formula

$$\delta\hat{V}(r) = \frac{Z\alpha}{r} + \frac{e}{4\pi}\int dr'r'^2\frac{\rho(r')}{r_>}, \quad (6)$$

where $r_> = \max(r, r')$. In Eq. (6), we have introduced the radial charge density, i.e., $\rho(r) = \int d\vec{n}\rho(\vec{r})$. The terms on the right-hand side of Eq. (6) correspond to the respective terms on the right-hand side of Eq. (3). Let us note that the resulting potential $\delta\hat{V}(r)$ depends solely on the radial variable r.

In our calculation, we consider axially symmetric nuclei and employ the two-parameter Fermi charge distribution with quadrupole and hexadecapole deformation, i.e.,

$$\rho_\beta(\vec{r}) = \frac{N}{1 + \exp[(r - c_\beta)/a]}, \quad (7)$$

where N is a normalization constant and the half-density radius is given in terms of spherical harmonics as $c_\beta = c_0(1 + \beta_2 Y_{20} + \beta_4 Y_{40})$, with β_2 and β_4 being the quadrupole and hexadecapole deformation parameters, respectively. Our assumption of the absence of the octupole deformation for nuclei considered in this work is based on Ref. [11].

The g factor corrections of interest to us for the systems described by Eq. (5) might be calculated with the help of the results of Ref. [12]. We will use Eq. (27) of Ref. [12], which for a $1S$ state reads

$$\delta g_{FS} = \frac{4(2\gamma + 1)}{3}\frac{E_{FS}}{m}. \quad (8)$$

This formula describes a correction to the g factor due to the FS effect for arbitrary radial distributions of the nuclear charge. E_{FS} denotes the energy shift due to the FS effect described by the perturbing scalar potential, and $\gamma = \sqrt{1 - (Z\alpha)^2}$. Equation (8) takes into account the interaction with the external magnetic field in the first order of perturbation theory, whereas the interaction with $\delta\hat{V}(r)$ is treated to all orders. In practice, the accuracy of Eq. (8) is limited by the accuracy of E_{FS}. In order to obtain E_{FS}, we use Eq. (17) of Ref. [13]. Namely, for the $1S$ state

$$E_{FS} = \frac{(\alpha Z)^2}{10}[1 + (\alpha Z)^2 f(\alpha Z)](2\alpha ZRm)^{2\gamma}m, \quad (9)$$

where $f(\alpha Z) = 1.380 - 0.162(\alpha Z) + 1.162(\alpha Z)^2$ and R is the effective radius of the homogeneously charged sphere that gives the same energy correction as the original nuclear shape. For states with $j = 1/2$

$$R = \sqrt{\frac{5}{3}\langle r^2\rangle\left[1 - \frac{3}{4}(\alpha Z)^2\left(\frac{3}{25}\langle r^4\rangle/\langle r^2\rangle^2 - \frac{1}{7}\right)\right]}, \quad (10)$$

where $\langle r^n\rangle \equiv \int dr r^2 r^n \rho_\beta(r)/(Z|e|)$. In our calculation, $\langle r^4\rangle$ is computed by numerical integration, whereas $\langle r^2\rangle$ is found in the literature [14].

It might be instructive to obtain the approximate formula expressing R in terms of the nuclear parameters. For this purpose, we substitute relations (24)–(26) from Ref. [10] into Eq. (10) and expand the result. In this way, we obtain

$$R \simeq \langle r^2\rangle^{1/2}\left\{\sqrt{\frac{5}{3}} - \frac{(Z\alpha)^2}{14\pi}\left[\frac{\sqrt{15}}{4}\beta_2^2 + \frac{5\sqrt{3}}{7\pi^{1/2}}\beta_2^3\right.\right.$$
$$+ \frac{9\sqrt{15}}{7\pi^{1/2}}\beta_2^2\beta_4 + \left(\frac{a}{c_0}\right)^2\left(\sqrt{\frac{5}{3}}\pi^2 - \frac{147\sqrt{5}\pi^2}{28\sqrt{3}}\beta_2^2\right.$$
$$\left.\left.\left. - \frac{355\pi^{3/2}}{28\sqrt{3}}\beta_2^3 - \frac{639\sqrt{5}\pi^{3/2}}{28\sqrt{3}}\beta_2^2\beta_4\right)\right]\right\}. \quad (11)$$

The values of R obtained with the help of numerical integration are in good agreement with those obtained with formula (11). Finally, the nuclear deformation correction to the g factor is defined as

$$\delta g_{ND} \equiv \delta g_{FS}\left(Z, \sqrt{\langle r^2\rangle}, a, \beta_2, \beta_4\right)$$
$$- \delta g_{FS}\left(Z, \sqrt{\langle r^2\rangle}, a, 0, 0\right), \quad (12)$$

where δg_{FS} depends on the nuclear parameters via R.

We also take into account nuclear deformation corrections to the QED corrections. The QED corrections to the g factor of first order in α consist of SE and VP corrections. We mostly use the calculation scheme as in Refs. [15,16]. The SE term represents the sum of irreducible, reducible, and vertex parts: $\delta g_{\text{SE}} = \delta g_{\text{irr}} + \delta g_{\text{red}} + \delta g_{\text{ver}}$. The irreducible part is given by [17]

$$\delta g_{\text{irr}} = \frac{1}{m_\phi} \sum_n^{E_n \neq E_\phi} \frac{\langle \phi | [\Sigma(E_\phi) - \gamma^0 \delta m] | n \rangle \langle n | [\vec{\alpha} \times \vec{r}]_z | \phi \rangle}{E_\phi - E_n}.$$

(13)

Here, m_ϕ is an angular momentum of the state $|\phi\rangle$ and E_n the energy of state $|n\rangle$, $[\vec{\alpha} \times \vec{r}]_z$ describes the interaction with the external magnetic field, and δm is a mass counterterm. $\Sigma(E)$ denotes the unrenormalized self-energy operator defined as

$$\langle a | \Sigma(E) | b \rangle = \frac{i}{2\pi} \int d\omega \sum_n \frac{\langle an | I(\omega) | nb \rangle}{E - \omega - E_n(1 - i0)}, \quad (14)$$

where $I(\omega, x_1, x_2) = e^2 \alpha^\mu \alpha^\nu D_{\mu\nu}(\omega, x_1, x_2)$ with the Dirac matrices $\alpha^\mu = (1, \vec{\alpha})$ and the photon propagator $D_{\mu\nu}(\omega, x_1, x_2)$. The expressions for the reducible and vertex parts read [17]

$$\delta g_{\text{red}} = \frac{1}{m_\phi} \langle \phi | [\vec{\alpha} \times \vec{r}]_z | \phi \rangle \langle \phi | \frac{d}{dE} \Sigma(E) |_{E=E_\phi} | \phi \rangle, \quad (15)$$

$$\delta g_{\text{ver}} = \frac{1}{m_\phi} \frac{i}{2\pi} \int d\omega \sum_{n_1, n_2}$$
$$\times \frac{\langle \phi n_2 | I(\omega) | n_1 \phi \rangle \langle n_1 | [\vec{\alpha} \times \vec{r}]_z | n_2 \rangle}{[E_\phi - \omega - E_{n_1}(1 - i0)][E_\phi - \omega - E_{n_2}(1 - i0)]}.$$

(16)

Both the reducible and vertex parts are ultraviolet-divergent, whereas the sum $\delta g_{\text{vr}} = \delta g_{\text{red}} + \delta g_{\text{ver}}$ is finite. To separate the ultraviolet divergencies, the expression (13) is decomposed into zero-, one-, and many-potential terms, and the expression (15) is decomposed into zero- and many-potential terms. All zero- and one-potential terms are evaluated in momentum space. The remaining many-potential parts $\delta g_{\text{irr}}^{(2+)}$ and $\delta g_{\text{vr}}^{(1+)}$ are calculated in coordinate space [18]. The angular integration and the summation over intermediate angular projections in the many-potential terms $\delta g_{\text{irr}}^{(2+)}$ and $\delta g_{\text{vr}}^{(1+)}$ are carried out in a standard algebraic manner. The many-potential terms involve infinite summation over the relativistic quantum number $\kappa = \pm(j + 1/2)$. This summation is terminated at a maximum value $|\kappa| = 15 - 20$, and the residual part of the sum is evaluated by a least-square inverse-polynomial fitting. The summation over the Dirac spectrum at fixed intermediate κ was carried out with the dual-kinetic-balance method [19].

The VP correction consists of two parts, originating from the vacuum-polarization diagram with the magnetic interaction inserted into the external electron line (the electric-loop contribution δg_{VP}^e) and into the vacuum-polarization loop (the magnetic-loop contribution δg_{VP}^m). We took into account only the leading term, since it guarantees the accuracy needed in the present work. The leading term originates from the electric loop and can be described by the Uehling potential. The VP correction is calculated by using the dual-kinetic-balance method as well.

To calculate the nuclear deformation correction to QED corrections (QED-ND), we employed an effective radius for the nucleus via Eq. (10). We employed the shell, homogeneously charged sphere and Fermi nuclear distributions. Although the QED-ND-calculation results are numerically stable and do not depend on the nuclear model, they should be considered as an estimate.

Table I presents numerical values of δg_{ND} obtained with formula (12) for various hydrogenlike ions. Depending on the availability of experimental data, the quadrupole deformation parameter β_2 was either taken from the literature or estimated with the help of the formula [24]

$$\beta_2 = \frac{4\pi}{3Z|e|R_s^2} \left[\sum_i B(E2; 0^+ \to 2_i^+) \right]^{1/2}, \quad (17)$$

where $B(E2; 0^+ \to 2_i^+)$ stands for the reduced probability of the $E2$ transition from the ground state 0^+ to a state 2_i^+,

TABLE I. The nuclear deformation correction to the g factor (δg_{ND}). The values of $\langle r^2 \rangle^{1/2}$ and their uncertainties originate from Ref. [14]. Unless otherwise stated, the value of a was obtained by the equation $a = t/(4 \log 3)$ (Ref. [20]), where $t = 2.30$ fm and rather conservative error bars were assumed. The parameters β_2 were estimated with the help of formula (17) unless a reference is given. For ^{234}U and ^{238}U, we employed, in accordance with Ref. [21], $\beta_4 = 0.08(5)$ and $\beta_4 = 0.07(5)$, respectively; for ^{28}Si, in accordance with Ref. [22], $\beta_4 = 0.08(5)$, and the same value for ^{30}Si; for other elements, we assumed $\beta_4 = 0.0(1)$ in accordance with Ref. [11]. The values of c_0 are set by the requirement that the numerically computed $\langle r^2 \rangle^{1/2}$ should be equal to the established ones [14]. See also the comments in the text on the uncertainty of δg_{ND}.

Z	Isotope	a (fm)	β_2	δg_{ND}
6	^{12}C	0.523(40)	0.44(10)	$-7.9(5.3) \times 10^{-16}$
14	^{28}Si	0.523(20)	$-0.349(20)^c$	$-2.85(52) \times 10^{-13}$
	^{30}Si	0.523(20)	$-0.314(20)^c$	$-2.48(49) \times 10^{-13}$
38	^{86}Sr	0.523(20)	0.134(10)	$-9.0(3.1) \times 10^{-11}$
	^{100}Sr	0.523(20)	0.435(11)	$-1.08(28) \times 10^{-9}$
60	^{142}Nd	0.523(20)	0.100(20)	$-2.0(1.1) \times 10^{-9}$
	^{150}Nd	0.523(20)	$0.278(20)^a$	$-1.70(53) \times 10^{-8}$
62	^{144}Sm	0.523(20)	$0.090(20)^a$	$-2.1(1.2) \times 10^{-9}$
	^{154}Sm	$0.498(20)^a$	$0.328(20)^a$	$-3.24(98) \times 10^{-8}$
92	^{234}U	$0.509(20)^b$	0.256(10)	$-1.12(27) \times 10^{-6}$
	^{238}U	$0.505(20)^b$	0.280(10)	$-1.28(28) \times 10^{-6}$

[a]Ref. [23].
[b]Ref. [21].
[c]The sign originates from Ref. [22].

TABLE II.   The isotopic shifts of various corrections to the g factor. The following notation for
an isotopic shift has been introduced: $\Delta g_X \equiv \delta g_X(A_1) - \delta g_X(A_2)$, where A_1 and A_2 are the first
and second mass numbers, respectively, given in the second column, and $X \in \{ND, ND - QED\}$.

Z	Isotopes	Δg_{ND}	Δg_{ND-QED}	$\Delta g_{ND,Total}$
38	^{100,86}Sr	$-9.9(2.8) \times 10^{-10}$	$1.4(3) \times 10^{-11}$	$-9.8(2.8) \times 10^{-10}$
60	^{150,142}Nd	$-1.50(54) \times 10^{-8}$	$1.1(4) \times 10^{-10}$	$-1.49(54) \times 10^{-8}$
92	^{238,234}U	$-1.6(3.9) \times 10^{-7}$	$1(4) \times 10^{-9}$	$-1.6(3.9) \times 10^{-7}$

R_s is the effective radius evaluated with the help of the
simplified formula $R_s = \sqrt{(5/3)\langle r^2 \rangle}$, and the values of
$B(E2; 0^+ \rightarrow 2_i^+)$ were evaluated with the help of the data
from Ref. [25]. The uncertainty of δg_{ND} is estimated as the
quadratic sum of uncertainties related to the nuclear pa-
rameters. We assume rather conservative error bars for the
parameters a, β_2, and β_4 to account for an uncertainty
caused by the fact that for some nuclei the parameters were
compiled from various experimental results.

As for the QED-ND effect, it is significantly smaller
than the leading ND correction. For example, we obtained
the following values: $5(3) \times 10^{-9}$, $4(2) \times 10^{-9}$, $1.2(4) \times 10^{-10}$, $1.3(1.1) \times 10^{-11}$, $1.5(3) \times 10^{-11}$, and $1.6(6) \times 10^{-12}$ for ^{238}U, ^{234}U, ^{150}Nd, ^{142}Nd, ^{100}Sr, and ^{86}Sr, respec-
tively. The accuracy of the results for the ND and QED-ND
corrections is such that the comparison with the experi-
mental values of the g factor could serve as a method for
the determination of β_2 and β_4 for heavy nuclei, provided
that all other relevant corrections, i.e., the currently un-
known higher-order QED corrections, the FS and mixed
FS-QED effects, and the NP effect, as well as remaining
nuclear parameters are known with sufficient accuracy.

Table II contains the values of the isotopic shift of δg_{ND}
for various chosen isotopes. For a comparison with
experimental results, values of other isotope-dependent

effects are required. The leading FS effect as well as the
mixed FS-VP effect can be found in Ref. [20], the mixed
FS-SE correction in Ref. [26], the recoil effects in
Refs. [27–29], and the NP effect in Ref. [9].

For comparison, Fig. 1 presents a plot of δg_{ND} and some
other contributions to the g factor. It is apparent that δg_{ND}
grows quickly with Z and that it becomes prominent for
heavy ions.

In summary, we have developed the theory of the nu-
clear deformation correction to the bound electron g factor
and calculated this term for a wide range of elements. It
turns out that already for ^{100}Sr^{37+}, the relative nuclear
shape contribution exceeds 10^{-10}, which is the level that
has just been reached in experiment [3]. For high-Z ele-
ments, the correction becomes large, e.g., on the level of
10^{-6} for ^{238}U^{91+}, and definitely will be important for the
comparison between theory and experiment for high-Z
elements, which are expected within a few years [6].
These results are likely to allow in future for the extraction
of nuclear deformation parameters from experimental val-
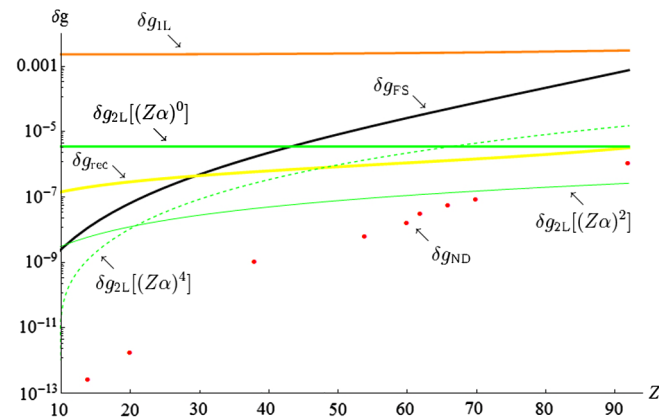ues of the g factor.

FIG. 1 (color online).   Various contributions to the g factor:
δg_{1L} stands for one-loop all-order QED corrections, δg_{FS} for the
finite-size effect, δg_{rec} for the recoil correction, and δg_{ND} for the
nuclear deformation correction, and $\delta g_{2L}[(Z\alpha)^n]$ represents two-
loop QED corrections at order $(Z\alpha)^n$ (see [30]).

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