Improved access to the fine-structure constant with the simplest atomic systems

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discussed below, the weight is known analytically as $x = \frac{4}{3} (2 \sqrt{1 - (Z \Delta)^2} + 1)$, following from basic properties the Dirac equation [15].

Modern measurements of the $g$ factor of HCI have reached a relative accuracy of $3 \times 10^{-11}$ [10, 12, 16, 18]. It is important to note that $E = m_e - E_B$ is the total ground-state (1s) energy of the electron, i.e. the rest energy minus the binding energy $E_B$, thus $E$ is known to higher relative precision than $E_B$ alone. The ground-state binding energy can be determined e.g. with x-ray spectroscopy [19, 30], using the theoretical value of the excited-state energy. As an example, with an error bar of 14 meV for the Ly$_\alpha$ transition energy of Ar$^{17+}$ [25], $E$ can be extracted with a fractional uncertainty of $2.7 \times 10^{-8}$. Very recently, it was demonstrated that electronic binding energies of HCI can also be measured by mass spectrometry [31].

Accompanied by corresponding foreseeable improvements in the QED description of one-electron systems, such experiments would become sensitive to the uncertainty of the fine-structure constant $\alpha$. An important advantage of our scheme based on the reduced $g$ factor [1], compared to those relying on few-electron ions [7, 8], is that the theory of one-electron ions is more advanced than that of many-body systems. Further progress is anticipated to be achieved faster, rendering decreasing the uncertainty of $\alpha$ by orders of magnitude more likely. In what follows, we show how the individual nuclear structural terms, such as the leading and QED finite size effects, as well as the the nuclear polarization contribution, are suppressed in the difference $\tilde{g}$.

Leading finite nuclear size effect. — The leading Dirac contribution to the $g$ factor in the ground (1s) state H-like ions is [4]

$$g_{\text{ext}}^D = -\frac{8}{3} \int_0^\infty dr r G(r) F(r),$$

where $G$ and $F$ denote the upper and lower radial components of the bound wave function

$$\psi_{n\kappa m}(r) = \frac{1}{r} \left( \frac{G_{n\kappa m}(r) \Omega_{n\kappa m}(r/r)}{i F_{n\kappa m}(r) \Omega_{n\kappa m}(r/r)} \right),$$

with $\Omega_{n\kappa m}(r/r)$ denoting spherical spinors. $n$ and $\kappa$ are the principal and Dirac angular momentum quantum numbers, respectively, and $m$ is the magnetic quantum number. $\psi$ satisfies Dirac’s equation

$$(\alpha \cdot p + m_e \beta + V(r)) \psi = E \psi,$$
with the usual Dirac matrices $\alpha$ and $\beta$, the three-momentum operator $p$, and the radial nuclear potential $V(r)$. For a point-like nucleus with $V(r) = -Z\alpha/r$, the integral in Eq. (3) can be evaluated analytically, yielding the formula for $g_0$ given above.

For an extended nucleus, we calculate the integral in Eq. (3) numerically, solving the radial Dirac equation using the dual kinetic balance (DKB) approach [32] implemented in quadruple precision. The leading finite nuclear size (FNS) contribution to the $g$ factor is $g_D^{\text{fns}} = g_D^{\text{ext}} - g_0$. We use first the two-parameter Fermi function as the nuclear charge distribution and take root mean square (RMS) nuclear radii from Ref. [33]. There is an uncertainty $\delta_{\text{RMS}}g_D^{\text{fns}}$ resulting from the uncertainties of the RMS radii. Additionally, in order to estimate the dependence $\delta_{\text{model}}g_D^{\text{fns}}$ of the FNS effect on the nuclear model, we also calculate the radial distribution of protons performing Hartree-Fock-Skyrme nuclear structural calculations [34], and take the difference of the values obtained with the different distributions. In Ref. [35] it was observed that proton distributions resulting from Skyrme forces are in good agreement with distributions measured in electron scattering experiments. The total uncertainty of the FNS contribution is given as the quadratic sum of $\delta_{\text{RMS}}g_D^{\text{fns}}$ and $\delta_{\text{model}}g_D^{\text{fns}}$.

Fig. 1 compares the uncertainty of the $g$ factor — that of $g_0$ and the dominant radiative correction, the Schwinger term $\alpha/\pi$ — due to $\delta\alpha$, the absolute uncertainty of $\alpha$, and the uncertainty caused by the FNS effect. Already for low values of $Z$, the uncertainties due to FNS are approx. an order of magnitude larger than those due to $\delta\alpha$, and the discrepancy grows for heavier elements.

The leading contribution to the $1s$ electron energy assuming a point-like nucleus is given by [30] $E_D = m_e \sqrt{1 - (Z\alpha)^2} = m_e (1 - \frac{1}{2} (Z\alpha)^2 + \ldots)$. For an extended nucleus, we obtain the ground-state energy $E_D^{\text{ext}}$ from the numerical solution of the radial Dirac equation. The calculation of $E_D^{\text{fns}} = E_D^{\text{ext}} - E_D$ and the determination of its uncertainty is performed similarly as above.

Using the Dirac equation (5) and its radial counterpart, Eq. (3) for the relativistic $g$ factor may be rewritten as [15]

$$g_D^{\text{ext}} = \frac{2}{3} \left(1 + 2\langle \beta \rangle\right) = \frac{2}{3} \left(1 + 2 \frac{\partial^{\text{ext}}}{\partial m_e}\right). \quad (6)$$

The FNS correction to the energy can be approximated on the one per thousand level as [37] $E_D^{\text{fns}} \approx m_e (2Zam_eR)^{3/2}$ with $\gamma = \sqrt{1 - (Z\alpha)^2}$ and an effective nuclear radius $R$, therefore, the FNS effects of the $g$ factor and the energy can be accurately related via the formula [19]

$$g_D^{\text{fns}} \approx \frac{4}{3} \left(2\sqrt{1 - (Z\alpha)^2} + 1\right) \frac{E_D^{\text{fns}}}{m_e}. \quad (7)$$

This motivates the choice of the weighted difference of the $g$ factor and the dimensionless energy in Eqs. (12): we expect the FNS effect in $\tilde{g}$ to cancel to a significant degree. As expected from Eq. (7), Fig. 1d shows that the FNS uncertainties are of comparable magnitude as the ones for the $g$ factor. Also, as in the case of the $g$ factor, the FNS effect causes larger errors than $\delta\alpha$ in the (weighted) energy.
can be performed in the framework of perturbation theory as a result of 2–3 digits cancellation of the NP correction in the QED-FNS uncertainty of the reduced uncertainty of the QED-FNS effect typically raises the uncertainty of the electronic energy level as well as the QED finite nuclear size effect. For the NP correction to the reduced factor to be that of an isolated, bare nucleus. In an atom, additional small effects arise from the mutual polarization of protons and electrons. A simple approximation of this factor by a factor \( Z^{\alpha} \) in Ref. [39] for the Lamb shift and \( \tilde{g} \) in Ref. [38] for the strong suppression of nuclear effects remains true even when considering higher-order nuclear contributions. In Ref. [42], the dip in the \( \tilde{g} \) factors \( \alpha \)-sensitivity around \( Z = 5 \) is removed (see Fig. [4]). This gives some advantage to the reduced factor scheme over those employing weighted differences of \( g \) factors in different charge states, since in those cases the sensitivity to \( \delta \alpha \) is slightly reduced in the difference [41]. In the following, we show that the strong suppression of nuclear effects remains true even when considering higher-order nuclear contributions.

**QED finite nuclear size effect.** — QED corrections to the electronic energy level as well as the \( g \) factor arise from one-loop self-energy (SE) and vacuum polarization (VP) diagrams. The FNS corrections to these terms have been evaluated e.g. in Ref. [38] for the Lamb shift and in Ref. [39] for the \( g \) factor. We use the results of these papers to determine the uncertainty of the QED-FNS effect of the reduced \( g \) factor \( \tilde{g} \) as a quadratic sum of the Lamb shift and the \( g \) factor uncertainties. We find that the uncertainty of the QED-FNS effect typically raises the FNS uncertainty of the reduced \( g \) factor by a factor of 3 or below. Also, QED FNS has a purely calculational uncertainty, which can be improved further, and thus the statements of the previous paragraph remain unchanged.

**Nuclear polarization correction.** — In the above calculations, the protonic charge distribution was assumed to be that of an isolated, bare nucleus. In an atom, additional small effects arise from the mutual polarization of protons and electrons. A simple approximation of this nuclear polarization (NP) correction to energy levels can be found in Ref. [40], which can be also extended to the \( g \) factor [41]. For the NP correction to the reduced \( g \) factor we obtain the simple analytical formula

\[
\tilde{g}^{\text{NP}} \approx \frac{32}{3} m_e^3 \alpha_d (Z \alpha)^2 \left( 1 - \frac{2Z \alpha R_{\text{sym}}}{2Z \alpha R_{\text{sym}}} \right),
\]

expressed in terms of the radius \( R \) of the homogeneously charged sphere model and the dipole nuclear polarizability \( \alpha_d \). The latter can be approximated in Migdal’s theory [42] as \( \alpha_d = \zeta(A) \alpha_0 \frac{R^2}{4 \alpha_{\text{sym}}} \), with \( \alpha_{\text{sym}} = 23 \text{ MeV} \) and \( \zeta(A) = 0.76 + 2.79/A^{1/3} \). While this simple model yields an order-of-magnitude estimate of the effect, it shows a 2-3 digits cancellation of the NP correction in \( \tilde{g} \).

A more sophisticated evaluation of the NP correction can be performed in the framework of perturbation theory following Refs. [43–46]. In this formalism, the electronic reference and intermediate states are treated relativistically, and nuclear transition data are taken from tabulations. The NP correction to the level energy reads:

\[
E^{\text{NP}} = -\alpha \sum_{LM} \sum_{j} B(EL) \times \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{2\omega_L}{\omega^2 - \omega_L^2 + i0} \frac{|\langle 1s | F_L Y_{LM} | j \rangle|^2}{\epsilon_{1s} - \omega - \epsilon_{j}(1 - i0)},
\]

where the summation extends over all nuclear excitation energies \( \omega_L \) with the reduced electric multipole transition strengths \( B(EL; L \to 0) \) (\( L \) is the multipolarity of a \( 2^L \)-pole transition). The label \( j \) denotes intermediate electronic states in the Dirac spectrum, the \( \epsilon_{1s} \) are their unperturbed eigenvalues, and the \( Y_{LM} \) denote spherical harmonics. The radial part is given in the sharp-surface approximation [47],

\[
F_L = \left\{ \begin{array}{ll} \frac{5\sqrt{\pi}}{2\pi^2} \left[ 1 - \left( \frac{\pi}{\sqrt{2L+1}} \right)^2 \right] \Theta(R - r), & L = 0, \\
\frac{1}{(2L+1)^{3/2}} \frac{(\max(r,R))^{L}}{(\min(r,R))^{L+2}}, & L \geq 1. \end{array} \right.
\]

For the NP correction to the \( g \) factor, one can write

\[
g^{\text{NP}} = -m_e \frac{\alpha}{m} \sum_{LM} \sum_{j,k} B(EL) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{2\omega_L}{\omega^2 - \omega_L^2 + i0} \times \left\{ \langle 1s | F_L Y_{LM}^* | j \rangle \langle j | F_L Y_{LM} | k \rangle \left[ \epsilon_{1s} - \omega - \epsilon_{j}(1 - i0) \right] \left( \epsilon_{1s} - \epsilon_{k}(1 - i0) \right) \right\}
\]

\[
+ \left\{ \langle 1s | F_L Y_{LM}^* | j \rangle \langle j | \alpha | k \rangle \langle k | F_L Y_{LM} | 1s \rangle \left[ \epsilon_{1s} - \omega - \epsilon_{j}(1 - i0) \right] \left( \epsilon_{1s} - \epsilon_{k}(1 - i0) \right) \right\}
\]

| Ion       | \( R \) (fm) | \( E_{NP} \) (meV) | \( g_{NP} \) | \( \tilde{g}_{NP} \) |
|-----------|-------------|----------------|-----------|-------------|
| \( ^{22}_{10} \)Ne | 2.9525 | -0.00024 | -2.10[-12] | -2.39[-13] |
| \( ^{28}_{14} \)Si | 3.1224 | -0.00105 | -9.07[-12] | -8.77[-13] |
| \( ^{40}_{20} \)Ca | 3.4776 | -0.00607 | -5.11[-11] | -3.95[-12] |
| \( ^{64}_{30} \)Zn | 3.9283 | -0.0545 | -4.45[-10] | -2.56[-11] |
| \( ^{84}_{36} \)Kr | 4.1884 | -0.144 | -1.15[-9] | -5.87[-11] |
| \( ^{102}_{44} \)Ru | 4.4809 | -0.541 | -4.25[-9] | -1.66[-10] |
| \( ^{112}_{48} \)Cd | 4.5944 | -0.857 | -6.66[-9] | -2.34[-10] |
| \( ^{124}_{42} \)Nd | 4.9123 | -2.96 | -2.22[-8] | -5.53[-10] |
| \( ^{144}_{66} \)Nd | 5.1569 | -10.4 | -7.69[-8] | -1.62[-9] |
| \( ^{154}_{58} \)Gd | 5.2074 | -12.9 | -9.47[-8] | -1.86[-9] |
| \( ^{166}_{64} \)Dy | 5.2074 | -12.9 | -9.47[-8] | -1.86[-9] |
| \( ^{174}_{70} \)Yb | 5.3108 | -18.9 | -1.37[-7] | -2.32[-9] |
| \( ^{196}_{78} \)Pt | 5.4307 | -22.6 | -1.57[-7] | -1.74[-9] |
| \( ^{208}_{82} \)Pt | 5.5012 | -28.9 | -1.98[-7] | -1.54[-9] |
| \( ^{238}_{92} \)U | 5.5817 | -196.5 | -1.27[-6] | -2.09[-9] |
with $[\ldots]_z$ denoting the $z$ component of a vector. Here, the first summand in the brackets corresponds to the reducible ($k = 1s$) and irreducible ($k \neq 1s$) contributions, and the second to the vertex contribution.

The nuclear parameters $\omega_L$ and $B(EL)$ for low-lying nuclear states are taken from Refs. [48–61]. The contributions of giant nuclear resonances are estimated by means of phenomenological energy-weighted sum rules [62]. Monopole, dipole, quadrupole and octupole ($L = 0–3$) low-lying transitions and giant resonances were taken into account. The spectral summation over the electronic states $j, k$ was performed using the DKB method. The values obtained for $E^{NP}$ and $g^{NP}$ are in a good agreement with literature values [44–46] for all available ions. In Table I a significant cancellation of the NP effect can be observed in the reduced $g$ factor. Additionally, by analyzing the individual contributions from each nuclear transition, we found that, for the reduced $g$ factor, a detailed knowledge of the nuclear level structures is not needed. It is sufficient to take into account only the few strongest transitions with the largest $B(EL)$ to provide reasonably accurate predictions. Whereas relative uncertainties of $E^{NP}$ and $g^{NP}$ individually reach up to 30-50% [43–45], due to effective cancellations between them, we observe that the fractional uncertainty in $\tilde{g}$ can be conservatively estimated to be on the few % level. Assuming a 5% theoretical uncertainty for $\tilde{g}^{NP}$, we find that it is of the same magnitude as the uncertainty of the FNS effect (see Fig. 2), allowing an improved extraction of $\alpha$.

Feasibility. — The current status of theory is summarized in Table I listing the various contributions to the reduced $g$ factor for $^{28}$Si$^{13+}$. This numerical example reiterates that nuclear effects do not hinder the extraction of $\alpha$. To this end, one-loop $g$ factor and three-loop Lamb shift terms, as well as recoil corrections need to be improved by a factor of 1.5–2 at least. As for two-loop diagrams, the ongoing nonperturbative evaluation [73, 80, 81] of all diagrams needs to be continued, and an evaluation of terms of order $(\alpha/\pi)(Z\alpha)^6$ in the framework of nonrelativistic QED [69, 72] is desirable. We note that less substantial theoretical improvements are needed for lighter elements, e.g. for $^{12}$C$^{5+}$. As for the experimental prospects: the $g$ factor of HCI can be nowadays measured with relative uncertainties on the level of $10^{-11}$, and further improvement is possible [82], allowing a broad range of ions (see Fig. 1) as candidates. Fig. 1 shows that the current $\sim 10^{-9}$ fractional uncertainty of the total ground-state energy [25] has to be decreased by 3-4 orders of magnitude in order to determine $\alpha$ with its present error bar. Recent developments in x-ray spectroscopy of HCI, i.e. the application of synchrotron and x-ray free electron laser sources [27, 29], the development of XUV and x-ray frequency combs [33] as well as advanced laser cooling schemes [34, 35] indicate that this goal can be reached and surpassed. Furthermore, the difference of reduced $g$ factors for two ions with different nuclear charges $Z_1$ and $Z_2$ may also be considered: differential measurements are typically more accurate than absolute ones, while the corresponding sensitivity to $\alpha$, namely, $\partial g(Z_1) / \partial \alpha - \partial g(Z_2) / \partial \alpha \approx (8/3)\alpha (Z_1^2 - Z_2^2)$ is comparable to that of a single-ion measurement.

In summary, the reduced $g$ factor of a simple one-electron ion, i.e. a combination of the bound-electron $g$ factor and the ground-state energy [given by Eqs. (12)],
is put forward as an efficient means for the determination of the fine-structure constant from experimental data on these atomic quantities. The reduced $g$ factor features a strongly suppressed sensitivity to nuclear effects, and an enhanced sensitivity to $\alpha$ as compared to the regular $g$ factor. By evaluating and analyzing the finite nuclear binding energy, and their radiative corrections, we show that existing and currently developed experimental technology, together with theoretical progress, will allow improving the uncertainty of $\alpha$ by orders of magnitude in the foreseeable future.

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