g Factor of Light Ions for an Improved Determination of the Fine-Structure Constant

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A weighted difference of the g factors of the H- and Li-like ions of the same element is theoretically studied and optimized in order to maximize the cancellation of nuclear effects between the two charge states. We show that this weighted difference and its combination for two different elements can be used to extract a value for the fine-structure constant from near-future bound-electron g factor experiments with an accuracy competitive with or better than the present literature value.

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Precision measurements of the free-electron g factor have enabled the determination of the fine-structure constant α to a high accuracy [1,2]. An independent value of α may be extracted from the measurement of the g factor of an electron bound in an H-like ion. This can be accomplished by identifying the leading relativistic (Dirac) contribution $g_D = \frac{2}{3}\left(1 + 2\sqrt{1-(Z\alpha)^2}\right)$ with Z being the nuclear charge number, after subtracting corrections induced by quantum electrodynamics (QED) and nuclear effects from the measured value. The sensitivity of g_D to α is largest for heavy ions. For these ions, however, nuclear effects (charge distributions, polarizabilities, etc.) are not well understood and set a limitation on the ultimate accuracy of such a determination.

In Ref. [3], it was suggested to use a weighted difference of the g factors of the H- and Li-like charge states of the same element in order to reduce the nuclear size effect by about 2 orders of magnitude for high-Z ions. In Ref. [4] (see also Ref. [5]), a specific weighted difference of the g factors of heavy H- and B-like ions with the same Z was put forward. It was demonstrated that the theoretical uncertainty of the nuclear size effect in this difference can be brought down to 4×10^{-10} for heavy ions around Pb, which was several times smaller than the uncertainty due to α at that time. Since then, however, the uncertainty of α was reduced by an order of magnitude [6–8], making it more difficult to access α in such experiments. In this Letter we propose a weighted difference of the g factors of low-Z ions, for which a much stronger cancellation of nuclear effects can be achieved. The low-Z region also seems favorable from the experimental point of view, since experiments so far concentrated in this regime [9–11].

Measurements of the g factor of H-like ions have reached the fractional level of accuracy of 3×10^{-11} [9]. Experiments have also been performed for Li-like ions [10]. In the future, it should be possible to perform experiments not only with a single ion in the trap, but also with several ions simultaneously. Such a setup will directly access differences of g factors of different ions, greatly reducing systematic uncertainties and possibly gaining 2 orders of magnitude in accuracy [12]. Such experiments, complemented by corresponding improvements in the theoretical description, would become sensitive to the uncertainty of α.

In the present Letter we put forward a method to extract α to higher accuracy by employing the weighted difference of the g factors of the H- and Li-like charge states of the same (light) element. The weight Ξ of this difference will be determined by studying the $Z\alpha$ and $1/Z$ expansions of the finite nuclear size (fns) effects, in such a way that the cancellation of unwanted contributions is maximized. Specifically, we introduce the following Ξ-weighted difference of the g factors of the Li- and H-like charge states of the same element

$$\delta_\Xi g = g(2s) - \Xi g(1s), \tag{1}$$

where $g(2s)$ is the ground-state g factor of the Li-like ion, $g(1s)$ is the ground-state g factor of the H-like ion, and the weight parameter Ξ is defined as

$$\Xi = 2^{-2\gamma-1}\left[1 + \frac{3}{16}(Z\alpha)^2\right]\left(1 - \frac{2851}{1000}\frac{1}{Z} + \frac{107}{100}\frac{1}{Z^2}\right), \tag{2}$$

where $\gamma = \sqrt{1-(Z\alpha)^2}$. The justification of such a choice of Ξ will be given below by studying the individual contributions to the fns effect.

One-electron finite nuclear size $\delta g_N^{(0)}$.—The leading one-electron fns correction is defined by the difference $\delta g_N^{(0)} = g_{\rm ext}^{(0)} - g_{\rm pnt}^{(0)}$, where $g_{\rm ext}^{(0)}$ and $g_{\rm pnt}^{(0)}$ are the relativistic one-electron g factors evaluated with the extended and the point nuclear models, respectively. For ns states, they are given by the radial integral

$$g^{(0)} = -\frac{8}{3}\int_0^\infty dr r^3 g_a(r) f_a(r), \tag{3}$$

where g_a and f_a are the upper and the lower radial components of the reference-state wave function, respectively.

We parametrize the leading one-electron fns effect for ns states as

$$\delta g_N^{(0)}(ns) = \frac{2}{5}\left(\frac{2Z\alpha R_{\rm sph}}{n}\right)^{2\gamma}\frac{(Z\alpha)^2}{n}\left[1 + (Z\alpha)^2 H_n^{(0,2+)}\right], \tag{4}$$

where $R_{\rm sph} = \sqrt{5/3}R$ is the radius of the sphere with the root-mean-square (rms) radius R and $H_n^{(0,2+)}$ is the remainder induced by relativistic effects. The superscript $(0,2+)$ indicates the contribution of zeroth order in $1/Z$ and second and higher orders in $Z\alpha$. The nonrelativistic limit of Eq. (4) agrees with the known result [13]. The leading relativistic correction $H_n^{(0,2)}$ was derived analytically in Ref. [14]. From that work, we deduce that the difference of the leading relativistic corrections for the $2s$ and $1s$ states is just a constant

$$H_{21}^{(0,2)} \equiv H_2^{(0,2)} - H_1^{(0,2)} = \frac{3}{16}. \tag{5}$$

In the present work we calculated $\delta g_N^{(0)}$ numerically. The Dirac equation for the extended nucleus was solved with the dual kinetic balance method [15]. In order to compensate large numerical cancellations occurring in the low-Z region, we implemented the dual kinetic balance method in quadruple-precision (32-digit) arithmetics. After that, we were able to determine $\delta g_N^{(0)}$ and, therefore, $H_n^{(0,2+)}$ to a very high accuracy.

We found that the model dependence of the relativistic fns correction $H_n^{(0,2+)}$ is generally not small; it varies from 1% in the medium-Z region to 5% in the low-Z region. On the contrary, the model dependence of the difference $H_2^{(0,2+)} - H_1^{(0,2+)}$ is very weak. We thus obtain that both the model dependence and the R dependence of $\delta g_N^{(0)}(ns)$ can be cancelled up to a very high accuracy by forming a suitably chosen difference. Specifically, the following difference of the one-electron g factors cancels the one-electron fns contributions of relative orders $(Z\alpha)^0$ and $(Z\alpha)^2$:

$$\delta_{\Xi_0} g = g^{(0)}(2s) - \Xi_0 g^{(0)}(1s) \tag{6}$$

with

$$\Xi_0 = 2^{-2\gamma-1}\left[1 + \frac{3}{16}(Z\alpha)^2\right]. \tag{7}$$

One-electron QED fns correction $\delta g_{\rm NQED}^{(0)}$.—The one-electron QED fns correction, arising from the one-loop self-energy and vacuum polarization diagrams, can be conveniently parametrized in terms of the dimensionless function $G_{\rm NQED}^{(0)}$ [16]:

$$\delta g_{\rm NQED}^{(0)} = \delta g_N^{(0)}\frac{\alpha}{\pi}G_{\rm NQED}^{(0)}(Z\alpha, R), \tag{8}$$

where $\delta g_N^{(0)}$ is the leading-order fns correction. The QED fns correction was studied in detail in Ref. [16], where we reported results for the $1s$ state of H-like ions. In the present work, we extend those calculations to the $2s$ state. The numerical results obtained are listed in Table I. We observe that the QED fns corrections for the $1s$ and $2s$ states, expressed in terms of the function $G_{\rm NQED}^{(0)}$, are very close to each other. Therefore, they are significantly cancelled in the difference $\delta_{\Xi_0} g$ introduced by Eq. (6).

One-photon exchange fns correction $\delta g_N^{(1)}$.—The one-photon exchange fns correction is the leading two-electron contribution to the fns effect. It is suppressed by the factor of $1/Z$ with respect to the leading fns contribution $\delta g_N^{(0)}$. The first calculation of the one-photon exchange correction was demonstrated in Ref. [3]. Here, we redid these calculations with an enhancement of the numerical accuracy by several orders of magnitude, which was necessary for an accurate identification of the fns effect in the low-Z region.

The one-photon exchange fns correction $\delta g_N^{(1)}$ is conveniently parametrized as follows:

$$\delta g_N^{(1)} = \delta g_N^{(0)}\frac{1}{Z}\left[H^{(1,0)} + (Z\alpha)^2 H^{(1,2+)}\right], \tag{9}$$

TABLE I. One-electron QED fns corrections to the bound-electron g factor, expressed in terms of $G_{\rm NQED}^{(0)}$ defined by Eq. (8). Abbreviations are as follows: "NSE" denotes the self-energy fns contribution for the $2s$ state, "NVP" denotes the vacuum-polarization fns correction for the $2s$ state, "2s" is the total QED fns correction for the $2s$ state, and"1s" is the total QED fns correction for the $1s$ state.

Z	NSE	NVP	2s	1s
6	−0.54(20)	0.158 (1)	−0.38(20)	−0.60(1)
8	−0.77(10)	0.226 (1)	−0.55(10)	−0.70(1)
10	−0.94(4)	0.296 (1)	−0.65(4)	−0.807(9)
12	−1.14(4)	0.373 (2)	−0.77(4)	−0.905(8)
14	−1.32(4)	0.459 (2)	−0.86(4)	−0.996(5)
20	−1.86(4)	0.740 (4)	−1.12(4)	−1.237(3)
25	−2.36(4)	1.012 (4)	−1.35(4)	−1.404(2)
30	−2.82(4)	1.318 (6)	−1.50(4)	−1.542(2)
35	−3.27(2)	1.654 (8)	−1.62(4)	−1.655(1)
40	−3.75(2)	2.037 (8)	−1.71(2)	−1.733(1)
45	−4.23(1)	2.445 (5)	−1.79(2)	−1.793(1)
50	−4.73(1)	2.900 (7)	−1.83(1)	−1.821(1)
55	−5.25(1)	3.400 (8)	−1.85(1)	−1.819(1)
60	−5.79(2)	3.958 (9)	−1.83(2)	−1.780(1)

where $\delta g_N^{(0)}$ is the one-electron fns correction given by Eq. (4), $H^{(1,0)}$ is the leading nonrelativistic contribution, and $H^{(1,2+)}$ is the higher-order remainder.

Results of our numerical calculations of $\delta g_N^{(1)}$ for different Z values were extrapolated to $Z \to 0$, yielding an accurate value of the nonrelativistic contribution, $H^{(1,0)} = -2.8512(10)$. Our calculations confirm that $H^{(1,0)}$ depends neither on the nuclear model nor on the charge radius. Because of this, the nonrelativistic contribution can be exactly cancelled in the weighted difference. Specifically, we conclude that the following difference of the g factors cancels the dominant part of the $1/Z$ fns contribution for light ions:

$$\delta_{\Xi_1} g = g^{(1)}(2s) - \Xi_0 \left(-\frac{2851}{1000}\frac{1}{Z}\right) g^{(0)}(1s). \quad (10)$$

Two- and more photon exchange fns correction $\delta g_N^{(2+)}$.—The fns correction with two and more photon exchanges is suppressed by the factor of $1/Z^2$ as compared to the one-electron fns contribution. It can be parametrized analogously to Eq. (9):

$$\delta g_N^{(2+)} = \delta g_N^{(0)} \frac{1}{Z^2}\left[H^{(2+,0)} + (Z\alpha)^2 H^{(2+,2+)}\right]. \quad (11)$$

In order to access $\delta g_N^{(2+)}$ in a numerical calculation, one needs to calculate the two and more photon exchange correction for the extended and the point nuclear models and take the difference $\delta g_N^{(2+)} = \delta g_{\rm ext}^{(2+)} - \delta g_{\rm pnt}^{(2+)}$. Here, we performed these calculations within the Breit approximation, in three steps. First, we solved the no-pair Dirac-Coulomb-Breit Hamiltonian by the configuration-interaction Dirac-Fock-Sturm method [17]. Second, we subtracted the leading-order contributions of orders $1/Z^0$ and $1/Z^1$ (calculated separately by perturbation theory), thus identifying the contribution of order $1/Z^2$ and higher. Third, we repeated the calculation for the extended and the point nuclear models and, by taking the difference, obtained $\delta g_N^{(2+)}$.

By performing numerical calculations for a series of ions and fitting the numerical results, we obtained the nonrelativistic value of the $1/Z^2$ correction as $H^{(2,0)} = 1.070(25)$. We also found that $H^{(2,0)}$ does not depend on the nuclear radius and, therefore, can be cancelled in the difference. We conclude that the following difference cancels the dominant part of the $1/Z^2$ fns contribution for low-Z ions:

$$\delta_{\Xi_2} g = g^{(2)}(2s) - \Xi_0 \left(\frac{107}{100}\frac{1}{Z^2}\right) g^{(0)}(1s). \quad (12)$$

The weighted difference of the $2s$ *and* $1s$ g *factors.*—Combining the weighted differences for specific fns contributions from Eqs. (6), (10), and (12), we arrive at the total Ξ-weighted difference of the g factors of the Li- and H-like charge states in Eq. (1), with the weight parameter Ξ defined by Eq. (2). Based on the preceding analysis, we claim that the Ξ-weighted difference $\delta_\Xi g$ cancels the nonrelativistic fns corrections to order $1/Z^0$, $1/Z^1$, and $1/Z^2$ and, in addition, the nuclear model-dependent contribution to order $(Z\alpha)^2/Z^0$. A small remaining fns correction to $\delta_\Xi g$ is calculated numerically. The leading nuclear model dependence of this correction comes only in the relative order $(Z\alpha)^2/Z$, with a numerically small coefficient.

We now address the question whether the weighted difference $\delta_\Xi g$ in light ions might be useful for the determination of α. Expanding $\delta_\Xi g$ in α and keeping Ξ fixed, we have

$$\delta_\Xi g = 2(1-\Xi) - \frac{2}{3}(Z\alpha)^2\left(\frac{1}{4} - \Xi\right) + \frac{\alpha}{\pi}(1-\Xi) + \ldots. \quad (13)$$

The sensitivity of $\delta_\Xi g$ to α comes, first, from the binding effects (the second term in the right-hand side) and, second, from the free-electron QED effects (the third term). By varying α in Eq. (13) within its current error bars $\delta\alpha/\alpha = 3.2 \times 10^{-10}$ [2], we obtain the corresponding error of $\delta_\Xi g$.

In Fig. 1 we compare the uncertainty due to α to the nuclear-model and nuclear-radius error of the fns effect, keeping in mind that the latter sets the ultimate limit of the accuracy of theoretical calculations. The left panel of Fig. 1 represents this comparison for the g factor of Li-like ions $g(2s)$, whereas the middle panel gives the same comparison for the Ξ-weighted difference $\delta_\Xi g$. The dip of the α sensitivity around $Z = 16$ is due to the fact that the dependences of the binding and the free-QED effects on α in Eq. (13) have different signs and cancel each other.

From Fig. 1 we observe that the cancellation of the fns effects in the Ξ-weighted difference $\delta_\Xi g$ yields an improvement of the ultimate limit of the achievable accuracy by about 3 orders of magnitude as compared to the g factor $g(2s)$ of the Li-like ion. Up to $Z \approx 45$, the weighted difference $\delta_\Xi g$ yields possibilities for an improved determination of α.

The extraction of α from $\delta_\Xi g$ may be argued to have two disadvantages. The first is the unfortunate cancellation of the α dependence around $Z = 16$, which leads to a loss of sensitivity to α of up to an order of magnitude. The second is that the theory of $\delta_\Xi g$ contains the same free-QED part as the determination of α from the free-electron g factor, meaning that these two methods are not completely independent. Both disadvantages can be circumvented by forming another difference

$$\delta_\Omega g = \delta_\Xi g(Z) - \delta_\Xi g([Z/2]), \quad (14)$$

where $\delta_\Xi g(Z)$ is the Ξ-weighted difference (1) for the atomic number Z, and $\delta_\Xi g([Z/2])$ is the corresponding difference for the atomic number $[Z/2]$ ($[\cdots]$ means the upper or lower integer part). By forming the difference $\delta_\Omega g$, we cancel the free-QED contributions (which do not depend on Z), thus

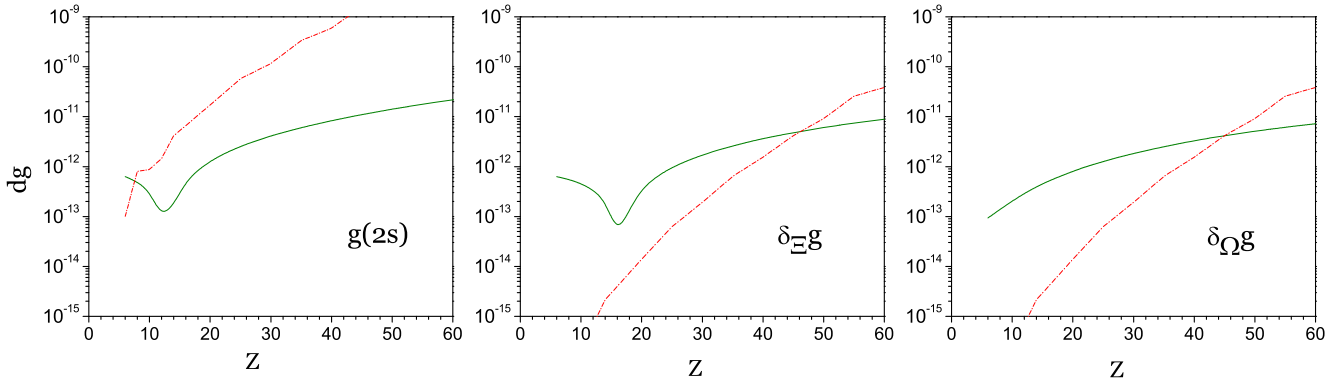

FIG. 1. Comparison of the error $dg = (\partial g/\partial\alpha)\delta\alpha$ due to the uncertainty of the fine-structure constant $\delta\alpha/\alpha = 3.2 \times 10^{-10}$ (solid line, green) and the error due to the finite nuclear size effect (dashed-dot line, red) for the g factor of the ground state of Li-like ions $g(2s)$ (left graph), for the weighted difference $\delta_\Xi g(Z)$ (middle graph), and for the weighted difference $\delta_\Omega g = \delta_\Xi g(Z) - \delta_\Xi g([Z/2])$ (right graph).

leaving the leading dependence on α through the binding effects only and rendering the determination of α independent of that employing the free-electron g factor.

The comparison of the uncertainty due to α and the error of the fns effect for the weighted difference $\delta_\Omega g$ is presented in the right panel of Fig 1. As expected, we find a smooth dependence of the sensitivity to α on Z, without any structure around $Z = 16$. We observe that in the region of nuclear charges $Z = 10$–20, the weighted difference $\delta_\Omega g$ offers better possibilities for determining α than $\delta_\Xi g$. $\delta_\Omega g$ can be effectively determined in an experiment by measuring two differences $g(1s, Z) - g(1s, [Z/2])$ and $g(2s, Z) - g(2s, [Z/2])$, and $g(1s, [Z/2])$, where the latter is suppressed in the weighted difference by a factor of $\Xi(Z) - \Xi([Z/2]) \approx 0.02$–$0.04$ in the region of interest. Thus, the experimental error of $\delta_\Omega g$ can be improved by more than an order of magnitude as compared to absolute g factors.

We now turn to the experimental consequences of our calculations. The only element for which the weighted difference $\delta_\Xi g$ has been measured is Si ($Z = 14$). In Table II we collect all available theoretical contributions to $\delta_\Xi g(^{28}\mathrm{Si})$, including our present results for the fns effect. Corrections due to the one- and two-electron QED effects were taken from Refs. [8,18–24]. Theoretical results are compared with the experimental value [10,11,25]. The error of the Dirac value and the free-QED correction is due to the uncertainty of the current value of $\alpha^{-1} = 137.035\,999\,074\,(44)$ [2]. The indicated uncertainty of the fns effect of 4×10^{-13} is already smaller than the uncertainty of the Dirac value due to α; it is of purely numerical origin and thus can be improved further in future calculations.

Table II shows that the present experimental and theoretical precision of $\delta_\Xi g(\mathrm{Si})$ is on the level of few parts in 10^{-9}, which is much lower than the precision achieved for other systems (in particular, in H-like C the present experimental and theoretical uncertainties are, correspondingly, 6×10^{-11} and 6×10^{-12} [9]). Such underperformance, however, was more due to a lack of motivation than due to principal obstacles. On the experimental side, the same precision as for H-like C can be obtained for Li-like C [and, therefore, $\delta_\Xi g(\mathrm{C})$], with the existing apparatus [12]. Moreover, a further experimental advance is anticipated that could bring 1 or 2 orders of magnitude of improvement [12]. On the theoretical side, the modern nonrelativistic quantum electrodynamics (NRQED) approach (see, e.g., Ref. [26]) can provide a theoretical prediction for Li-like C

TABLE II. Individual contributions to the weighted difference $\delta_\Xi g$ for ^{28}Si. $M/m = 50984.8327(3)$. $\Xi = 0.101136233077060$.

Contribution	Order	Value
Dirac		1.796 687 854 216 5 (7)
One-loop QED	$\alpha(Z\alpha)^0$	0.002 087 898 255 0 (7)
	$\alpha(Z\alpha)^2$	0.000 000 601 506 0
	$\alpha(Z\alpha)^4$	0.000 000 014 797 0
	$\alpha(Z\alpha)^{5+}$	0.000 000 015 48 (52)
Two-loop QED	$\alpha^2(Z\alpha)^0$	−0.000 003 186 116 6
	$\alpha^2(Z\alpha)^2$	−0.000 000 000 917 9
	$\alpha^2(Z\alpha)^4$	−0.000 000 000 084 4
	$\alpha^2(Z\alpha)^{5+}$	0.000 000 000 00 (13)
≥ Three-loop QED	$\alpha^3(Z\alpha)^0$	0.000 000 026 517 7 (1)
	$\alpha^3(Z\alpha)^2$	0.000 000 000 007 6
	$\alpha^3(Z\alpha)^{4+}$	0.000 000 000 000 0 (11)
Recoil:		0.000 000 030 5 (10)
One-photon exchange		0.000 321 590 803 3
Two-photon exchange		−0.000 006 876 0 (5)
≥ Three-photon exchange		0.000 000 093 0 (60)
Two-electron QED		−0.000 000 236 0 (50)
Two-electron recoil		−0.000 000 012 1 (7)
Finite nuclear size		−0.000 000 000 000 6 (4)
Total theory		1.799 087 813 9 (79)
Experiment [10,11,25]		1.799 087 812 5 (21)

with the same accuracy as obtained for H-like C [27]. Moreover, a further theoretical advance is possible; namely, the two-loop QED correction of order $\alpha^2(Z\alpha)^5$ and the three-loop QED correction of order $\alpha^3(Z\alpha)^4$ can be calculated, both for H-like and Li-like ions [27].

Since we are presently interested in light ions, the best way for the theoretical advance is a combination of two complementary methods. The first one is the NRQED approach (used, e.g., in Ref. [28]), which accounts for the nonrelativistic electron-electron interactions to all orders but expands the QED and relativistic effects in α and $Z\alpha$. The second method (used, e.g., in Refs. [19,21–23]) accounts for the relativistic effects to all orders in $Z\alpha$ but uses perturbation expansions for QED effects (in α) and for the electron-electron interaction (in $1/Z$). Matching the coefficients of $Z\alpha$ and $1/Z$ expansions of these two methods allows one to merge them together, as was done for the energy levels in Ref. [29]. As a result, only higher-order corrections in $Z\alpha$ will be expanded in $1/Z$ and higher-order corrections in $1/Z$ will be expanded in $Z\alpha$, whereas the lower-order terms will be obtained complete both in $Z\alpha$ and in $1/Z$. Such an approach should allow one to advance the theory to the level required for the improved determination of α.

It is important that the theoretical progress in calculations of $\delta_\Xi g$ is not hampered by the nuclear size, and in fact by any other nuclear effects. Recent investigations of the nuclear deformation and polarization effects [23,30] demonstrated that these effects are of the same short-range nature as the nuclear size effects and that they are cancelled in the same weighted difference. In particular, we estimate the magnitude of the nuclear polarization contribution to $\delta_\Xi g(\mathrm{C})$ to be $\sim 5 \times 10^{-16}$, which is completely negligible at the level of interest.

In summary, specific weighted differences of the g factors of H- and Li-like ions were investigated. The weight parameter Ξ was determined by the condition of cancellation of the nonrelativistic finite nuclear size corrections to order $1/Z^0$, $1/Z^1$, and $1/Z^2$ and, in addition, the relativistic nuclear model-dependent contribution to order $(Z\alpha)^2/Z^0$. We demonstrated that the Ξ- and Ω-weighted differences (1) and (14) can be used for an effective cancellation of nuclear structural effects. This independent scheme may be used to extract the fine-structure constant from a comparison of experimental and theoretical bound-electron g factors with an accuracy competitive with or better than the current value.

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