Weighted difference of \(g\)-factors of light Li-like and H-like ions for an improved determination of the fine-structure constant

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A weighted difference of the \(g\)-factors of the Li- and H-like ion of the same element is studied and optimized in order to maximize the cancellation of nuclear effects. To this end, a detailed theoretical investigation is performed for the finite nuclear size correction to the one-electron \(g\)-factor, the one- and two-photon exchange effects, and the QED effects. The coefficients of the \(Z\alpha\) expansion of these corrections are determined, which allows us to set up the optimal definition of the weighted difference. It is demonstrated that, for moderately light elements, such weighted difference is nearly free from uncertainties associated with nuclear effects and can be utilized to extract the fine-structure constant from bound-electron \(g\)-factor experiments with an accuracy competitive with or better than its current literature value.

I. INTRODUCTION

Modern measurements of the bound-electron \(g\)-factor in H-like ions have reached the level of fractional accuracy of \(3 \times 10^{-11}\) [1]. Experiments have also been performed with Li-like ions [2]. In future it shall be possible to conduct similar experiments not only with a single ion in the trap, but also with several ions simultaneously. Such a setup would allow one to directly access differences of the \(g\)-factors of different ions, thus largely reducing systematic uncertainties and possibly gaining about two orders of magnitude in experimental accuracy [3]. So, experimental investigations of differences of the bound-electron \(g\)-factors on a sub-\(10^{-12}\) level look feasible in the future. Such measurements would become sensitive to the uncertainty of the fine-structure constant \(\alpha\), which is presently known up to the fractional accuracy of \(3 \times 10^{-10}\) [4]. It might be tempting to use such future experiments as a tool for an independent determination of \(\alpha\).

In order to accomplish a competitive determination of \(\alpha\) from the bound-electron \(g\)-factor experiments, one has to complete theoretical calculations to a matching accuracy, which is a challenging task. One of the important problems on the way is the uncertainty due to nuclear effects, which cannot be well understood at present. These uncertainties set a limitation on the ultimate accuracy of the theoretical description and, therefore, on the determination of \(\alpha\).

There is a way to reduce the nuclear effects and the associated uncertainties, by forming differences of different charge states of the same element. In Ref. [5], it was suggested to use a weighted difference of the \(g\)-factors of the H- and Li-like ions of the same element in order to suppress the nuclear size effects by about two orders of magnitude for high-\(Z\) ions. In Ref. [6], a weighted difference of the \(g\)-factors of B-like and H-like charge states of the same element was proposed. It was shown that the theoretical uncertainty of the nuclear size effect for ions around Pb can be reduced to \(4 \times 10^{-10}\), which was several times smaller than the uncertainty due to the fine-structure constant at the time of publication of Ref. [6]. Since then, however, the uncertainty of \(\alpha\) was decreased by an order of magnitude [7–9], thus making it more difficult to access it in the bound-electron \(g\)-factor experiments. In our recent Letter [10] we proposed a weighted difference of the \(g\)-factors of low-\(Z\) Li-like and H-like ions, for which a more significant cancellation of nuclear effects can be achieved. In the present paper we describe details of the underlying calculations and report extended numerical results for the finite nuclear size corrections.

In our approach, the weight \(\Xi\) of the specific difference of the \(g\)-factors is determined on the basis of studying the \(Z\alpha\) and \(1/Z\) expansions of various finite nuclear size (fns) corrections, in such a way that the cancellation of these undesirable contributions is maximized. We introduce the following weighted difference of the bound-electron \(g\)-factors of the Li-like and H-like charge states of the same element,

\[
\delta g = g(2s) - \Xi g(1s),
\]

where \(g(2s)\) is the \(g\)-factor of the Li-like ion, \(g(1s)\) is the \(g\)-factor of the H-like ion, and the parameter \(\Xi\) is defined as

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

with the notation \(\gamma = \sqrt{1 - (Z\alpha)^2}\). The justification of this choice of \(\Xi\) will be given later, after studying the contributions of individual physical terms to the fns effect.

This article is organized as follows. In Section II we describe our calculations of various fns contributions, namely, the leading one-electron fns effect, the fns correction from the one-electron QED effects, and the two- and three-electron fns corrections due to the exchange of one or more photons between the electrons. The resulting weighted difference of the \(g\)-factors and its utility in determining the fine-structure constant are discussed in Section III, which is followed by a short conclusion.
II. FINITE NUCLEAR SIZE CORRECTIONS

A. One-electron finite nuclear size

The leading one-electron fns correction to the bound-electron $g$-factor is defined as follows:

$$
\delta g_N^{(0)} = g_{\text{ext}}^{(0)} - g_{\text{pnt}}^{(0)},
$$

(3)

where $g_{\text{ext}}^{(0)}$ and $g_{\text{pnt}}^{(0)}$ are the leading-order bound-electron $g$-factor values calculated assuming the extended and the point-like nuclear models, respectively. The leading-order bound-electron $g$ factor is obtained for $n$s states as

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

(4)

where $g_s$ and $f_a$ are the upper and the lower radial components of the $n$s Dirac wave function, respectively [11].

The fns correction $\delta g_N^{(0)}$ has an approximate relation to the corresponding correction to the Dirac energy, which reads [12] for $n$s states as

$$
\delta g_N^{(0)} = \frac{4}{3} (2\gamma + 1) \frac{\delta E_N}{m},
$$

(5)

where $\delta E_N$ is the nuclear-size correction to the Dirac energy. Eq. (5) is exact in the nonrelativistic limit and also holds with a reasonable accuracy in the whole region of nuclear charge numbers $Z$. Using Eq. (5) and the result of Ref. [13] for $\delta E_N$, the leading one-electron fns effect for $n$s states can be parameterized as

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

(6)

where $R_{\text{sph}} = \sqrt{5/3} R$ is the radius of the nuclear sphere with the root-mean-square (rms) charge radius $R$ and $H_n^{(0,2+)}$ is the remainder due to relativistic effects. The superscript $(0,2+)$ indicates that its contribution is of zeroth order in $1/Z$ and of second and higher orders in $Z\alpha$. The nonrelativistic limit of Eq. (6) agrees with the well-known result of Refs. [14, 15].

The leading relativistic correction $H_n^{(0,2)}$ has been given in a closed analytical form in Ref. [15]. We deduce from it that the difference of the relativistic corrections of relative order $(Z\alpha)^2$ for $2s$ and $1s$ states does not depend on the nuclear charge radius nor on the nuclear charge distribution model, and is just a constant:

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

(7)

In the present work we calculate the nuclear-size correction $\delta g_N^{(0)}$ numerically. For the extended nucleus, the radial Dirac equation is solved with the Dual Kinetic Balance (DKB) method [16], which allows us to determine $g_{\text{ext}}^{(0)}$ with a very high accuracy. The nuclear-size correction is obtained by subtracting the analytical point-nucleus result. In order to avoid loss of numerical accuracy in the low-$Z$ region, we used the DKB method implemented in the quadruple (about 32 digits) arithmetics.

In our calculations, we used three models of the nuclear charge distribution. The two-parameter Fermi model is given by

$$
\rho_{\text{Fer}}(r) = \frac{N}{1 + \exp[(r - r_0)/a]},
$$

(8)

where $r_0$ and $a$ are the parameters of the Fermi distribution, and $N$ is the normalization factor. The parameter $a$ was fixed by the standard choice of $a = 2.3/(4 \ln 3) \approx 0.52$ fm. The homogeneously charged sphere distribution of the nuclear charge is given by

$$
\rho_{\text{Sph}}(r) = \frac{3}{4\pi R_{\text{sph}}^3} \theta(R_{\text{sph}} - r),
$$

(9)

where $\theta$ is the Heaviside step function. The Gauss distribution of the nuclear charge reads

$$
\rho_{\text{Gauss}}(r) = \left( \frac{3}{2\pi R^2} \right)^{3/2} \exp \left( -\frac{3r^2}{2R^2} \right).
$$

(10)

The results of our calculations for the $2s$ and $1s$ states are presented in Table I, expressed in terms of the function $H_n^{(0,2+)}$. Experimental values of the rms nuclear charge radii $R$ are taken from Ref. [17]. For ions with $Z > 10$, we perform calculations with the Fermi and the homogeneously charged sphere models. The difference of the values obtained with these two models is taken as an estimation of the model dependence of the results. For ions with $Z < 10$, the Fermi model is no longer adequate and we use the Gauss model instead.

We observe that the model dependence of the relativistic fns correction $H_n^{(0,2+)}$ is generally not negligible; it varies from 1% in the medium-$Z$ region to 5% in the low-$Z$ region. However, the model dependence of the difference $H_2^{(0,2+)} - H_1^{(0,2+)}$ is tiny. According to Eq. (7), it is suppressed by a small factor of $(Z\alpha)^2$. Our calculations show that in addition it is suppressed by a small numerical coefficient.

We conclude that both the model dependence and the $R$ uncertainty of the one-electron fns correction can be cancelled up to a very high accuracy by forming a suitably chosen difference. The following weighted difference of the $2s$ and $1s$ one-electron $g$-factors cancels the one-electron fns contributions of relative orders $(Z\alpha)^0$ and $(Z\alpha)^2$,

$$
\delta g_{\Xi_0} = g^{(0)}(2s) - \Xi_0 \, g^{(0)}(1s),
$$

(11)

with the weight

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

(12)

The one-electron fns effects in the difference $\delta g_{\Xi_0}$ arise only in the relative order $(Z\alpha)^4$, with a numerically small coefficient.
TABLE I: The relativistic fns correction, in terms of function $H^{(0,2+)}_s$ defined by Eq. (6), for the $2s$ state ($n = 2$) and the $1s$ state ($n = 1$), for different models of the nuclear charge distribution. The rms charge radii $R$ and their errors are taken from the compilation of Ref. [17].

| $Z$ | $R$ [fm] | Model | $H^{(0,2+)}_s$ | $H^{(1,2+)}_s$ | $H^{(1,2+)}_s - H^{(0,2+)}_s - 3/16$ |
|-----|----------|-------|----------------|----------------|----------------------------------|
| 6   | 2.4702(22) | Gauss | 0.9296(3) | 0.7421(3) | 0.00003 |
| 6   | 2.4702(22) | Sphere | 0.9827(3) | 0.7951(3) | 0.00007 |
| 8   | 2.6991(52) | Gauss | 0.9912(6) | 0.8035(5) | 0.0001 |
| 10  | 3.0055(21) | Fermi | 1.0248 | 0.8370 | 0.0003 |
| 10  | 3.0055(21) | Sphere | 1.0700(2) | 0.8822(2) | 0.0003 |
| 12  | 3.0570(16) | Fermi | 1.0690 | 0.8810 | 0.0005 |
| 12  | 3.0570(16) | Sphere | 1.1067(1) | 0.9186(1) | 0.0006 |
| 14  | 3.1224(24) | Fermi | 1.1001(1) | 0.9118(1) | 0.0008 |
| 14  | 3.1224(24) | Sphere | 1.1327(1) | 0.9443(1) | 0.0009 |
| 20  | 3.4776(19) | Fermi | 1.1542(1) | 0.9647(1) | 0.0020 |
| 20  | 3.4776(19) | Sphere | 1.1764(1) | 0.9868(1) | 0.0021 |
| 25  | 3.7057(22) | Fermi | 1.1843 | 0.9934 | 0.0034 |
| 25  | 3.7057(22) | Sphere | 1.2030(1) | 1.0119(1) | 0.0035 |
| 30  | 3.9283(15) | Fermi | 1.2085 | 1.0159 | 0.0051 |
| 30  | 3.9283(15) | Sphere | 1.2246 | 1.0319(1) | 0.0053 |
| 35  | 4.1629(21) | Fermi | 1.2297(1) | 1.0350 | 0.0071 |
| 35  | 4.1629(21) | Sphere | 1.2438 | 1.0490(1) | 0.0073 |
| 40  | 4.2694(10) | Fermi | 1.2518 | 1.0548 | 0.0095 |
| 40  | 4.2694(10) | Sphere | 1.2652(1) | 1.0679 | 0.0098 |
| 45  | 4.4945(23) | Fermi | 1.2714(1) | 1.0718 | 0.0121 |
| 45  | 4.4945(23) | Sphere | 1.2834(1) | 1.0836(1) | 0.0123 |
| 50  | 4.6519(21) | Fermi | 1.2920 | 1.0897 | 0.0148 |
| 50  | 4.6519(21) | Sphere | 1.3033(1) | 1.1006 | 0.0151 |
| 55  | 4.8041(46) | Fermi | 1.3129(1) | 1.1077 | 0.0177 |
| 55  | 4.8041(46) | Sphere | 1.3235(1) | 1.1180(1) | 0.0180 |
| 60  | 4.9123(25) | Fermi | 1.3346(1) | 1.1265 | 0.0206 |
| 60  | 4.9123(25) | Sphere | 1.3447 | 1.1363(1) | 0.0209 |

B. One-electron QED fns correction

The one-electron QED fns correction $\delta g^{(0)}_{\text{QED}}$ to the bound-electron $g$ factor can be conveniently parameterized by means of the dimensionless function $G_{N\text{QED}}^{(0)}$ [18],

$$\delta g^{(0)}_{\text{QED}} = \delta g^{(0)}_N \frac{\alpha}{\pi} G_{N\text{QED}}^{(0)}(Z\alpha, R),$$

where $\delta g^{(0)}_N$ is the leading-order fns correction discussed in Sec. II A, and $G_{N\text{QED}}^{(0)}$ is a slowly varying function. The correction can be divided into four parts,

$$G_{N\text{QED}}^{(0)} = G_{\text{NSE}} + G_{\text{NUe,el}} + G_{\text{NWK,el}} + G_{\text{NVP,ml}},$$

where $G_{\text{NSE}}$ is the contribution of the electron self-energy, $G_{\text{NUe,el}}$ is induced by the insertion of the Uehling potential into the electron line, $G_{\text{NWK,el}}$ is the analogous correction by the Wichmann-Kroll potential, and $G_{\text{NVP,ml}}$ is the so-called magnetic-loop vacuum-polarization correction.

The QED fns correction was studied in detail in our previous investigation [18], where we reported numerical results for the $1s$ state of H-like ions. In the present work, we extend our calculations to the $2s$ state, which is required for describing the Li-like ions. The numerical results obtained for the $2s$ state are listed in Table II. The results for the $1s$ state are taken from Ref. [18]. We observe that the QED fns corrections for the $1s$ and $2s$ states, expressed in terms of the function $G_{N\text{QED}}^{(0)}$, are very close to each other. Therefore, they largely cancel in the weighted difference $\delta_{\Sigma g}$ introduced in Eq. (11).

C. One-photon exchange fns correction

The one-photon exchange fns correction is the dominant two-electron contribution to the total fns effect. It is suppressed by the factor of $1/Z$ with respect to the leading one-electron fns contribution $\delta g^{(0)}_N$. The one-photon exchange fns correction can be obtained as a difference of the one-photon exchange contributions to the $g$-factor evaluated with the extended nuclear charge distribution and with the point nucleus,

$$\delta g^{(1)}_N = \delta g^{(1)}_{\text{ext}} - \delta g^{(1)}_{\text{pnt}}.$$
TABLE II: One-electron QED fns corrections to the bound-electron \( g \) factor, expressed in terms of \( G_{\text{QED}}^{(0)} \) defined by Eq. (13). The abbreviations are as follows: “NSE” denotes the self-energy contribution, “NUe,el” denotes the Uehling electric-loop vacuum-polarization correction, “NWK,el” stands for the Wichmann-Kroll electric-loop vacuum-polarization correction, and “NVP,ml” denotes the magnetic-loop vacuum-polarization correction.

| Z | NSE   | NUe,el | NWK,el | NVP,ml | Total, 2s  | Total, 1s  |
|---|-------|--------|--------|--------|------------|------------|
| 6 | -0.54 (20) | 0.179  | -0.011 | -0.010 (1) | -0.38 (20) | -0.80 (1) |
| 8 | -0.77 (10)  | 0.256  | -0.019 | -0.010 (1) | -0.55 (10) | -0.70 (1) |
| 10| -0.94 (4)   | 0.337  | -0.028 | -0.013 (1) | -0.65 (4)  | -0.807 (9) |
| 12| -1.14 (4)   | 0.430  | -0.040 | -0.017 (2) | -0.77 (4)  | -0.905 (8) |
| 14| -1.32 (4)   | 0.530  | -0.053 | -0.018 (2) | -0.86 (4)  | -0.996 (5) |
| 20| -1.86 (4)   | 0.863  | -0.098 | -0.025 (4) | -1.12 (4)  | -1.237 (3) |
| 25| -2.36 (4)   | 1.185  | -0.143 | -0.030 (4) | -1.35 (4)  | -1.404 (2) |
| 30| -2.82 (4)   | 1.543  | -0.191 | -0.035 (6) | -1.50 (4)  | -1.542 (2) |
| 35| -3.27 (2)   | 1.933  | -0.240 | -0.039 (8) | -1.62 (4)  | -1.655 (1) |
| 40| -3.75 (2)   | 2.376  | -0.295 | -0.044 (8) | -1.71 (2)  | -1.733 (1) |
| 45| -4.21 (1)   | 2.837  | -0.345 | -0.047 (10)| -1.79 (2)  | -1.793 (1) |
| 50| -4.73 (1)   | 3.348  | -0.398 | -0.050 (12)| -1.83 (1)  | -1.821 (1) |
| 55| -5.25 (1)   | 3.902  | -0.450 | -0.053 (12)| -1.85 (1)  | -1.819 (1) |
| 60| -5.79 (2)   | 4.515  | -0.502 (1) | -0.055 (14) | -1.83 (2)  | -1.780 (1) |

The one-photon exchange correction to the \( g \)-factor of the ground and valence-excited states of Li-like ions is given by [5]

\[
\delta g^{(1)} = 2 \sum_{\mu c} \sum_P (-1)^P \left[ \langle Pv Pc|I(\Delta_{\mu c})|v c \rangle \delta^{(1)}_V \right] \\
+ \langle Pv Pc|I(\Delta_{\mu c})|v c \rangle \right] \\
- \sum_{\mu c} \left[ \langle v|V_g|v \rangle - \langle c|V_g|c \rangle \right] \langle cv|I'(\Delta_{\mu c})|vc \rangle , \tag{16}
\]

where \( v \) and \( c \) denote the valence and the core electron states, respectively, \( \mu c \) is the momentum projection of the core electron, \( P \) is the permutation operator, \( \langle Pv Pc| = (vc) \) or \( (cv) \), \( (-1)^P \) is the sign of the permutation, \( \Delta_{\mu c} = \varepsilon_c - \varepsilon_b \), \( I(\omega) \) is the relativistic operator of the electron-electron interaction defined below, and \( I'(\omega) = dI(\omega)/d\omega \) at \( \omega = \omega_r \). Further notations used in Eq. (16) are as follows: \( \delta^{(1)}_V \) stands for the first-order perturbation of the wave function \( \alpha \) by the potential \( V_g \),

\[
\delta^{(1)}_V \alpha = \sum_n \frac{\varepsilon_n - \varepsilon_\alpha}{\varepsilon_\alpha - \varepsilon_n} |n\rangle \langle n|V_g|\alpha \rangle , \tag{17}
\]

and \( V_g \) is the effective \( g \)-factor potential (see, e.g., Eq. (14) of Ref. [19]),

\[
V_g(r) = 2m |r \times \alpha| z , \tag{18}
\]

where \( \alpha \) is the vector of Dirac matrices in the standard representation. The above form of the potential \( V_g(r) \) assumes that the momentum projection of the valence state \( v \) in Eq. (16) is fixed as \( \mu_v = 1/2 \).

The relativistic electron-electron interaction operator \( I(\omega) \) in the Feynman gauge reads

\[
I(\omega, r_1, r_2) = \alpha (1 - \alpha_1 \cdot \alpha_2) \exp \left[ i|\omega| |r_{12}| \right] / r_{12} , \tag{19}
\]

where \( r_{12} = |r_1 - r_2| \) is the distance between the two electrons and \( \omega \) is the frequency of the photon exchanged between them.

The calculation of the one-photon exchange contribution with the extended and the point nuclear models was reported in Ref. [5]. In the present work, we redo these calculations with an enhanced precision, which is necessary for an accurate identification of the fns effect. The one-photon exchange fns correction \( \delta g_N^{(1)} \) can be parameterized as

\[
\delta g_N^{(1)} = \delta g_N^{(0)} \frac{1}{Z} H^{(1)}(Z, R) , \tag{20}
\]

where \( \delta g_N^{(0)} \) is the one-electron nuclear-size correction introduced earlier, and \( H^{(1)} \) is a slowly varying function. The \( Z, R \) expansion of \( H^{(1)} \) reads

\[
H^{(1)} = H^{(1,0)} + (Z, R)^2 H^{(1,2)} , \tag{21}
\]

where \( H^{(1,0)} \) is the leading nonrelativistic contribution and \( H^{(1,2)} \) is the higher-order remainder.

The nuclear-size correction is evaluated in this work as the difference of Eq. (16) calculated with the extended vs. point-like nuclear models. The numerical evaluation of Eq. (16) with the extended nucleus is performed by using the DKB method [16]. For the point nucleus, we use the analytical expressions for the reference-state wave functions and for the diagonal (in \( \kappa \) \( g \)-factor perturbed wave function [20], and the standard implementation of the B-splines method [21] for the non-diagonal in \( \kappa \) part of the perturbed wave function. In order to avoid loss of numerical accuracy in the low-\( Z \) region,
TABLE III: The one-photon exchange fns correction to the bound-electron $g$ factor of the ground state of Li-like ions, in terms of the function $H^{(1)}$ defined by Eq. (20). The column $(R, c)$ contains results obtained with the actual values of the nuclear charge radii $R$ and the speed of light $c$. The column $(4R, c)$ presents results obtained with the nuclear charge radii multiplied by a factor of 4. The column $(40R, 10c)$ contains results obtained with the nuclear charge radii multiplied by a factor of 40 and the speed of light multiplied by 10.

| $Z$ | $(R, c)$ | $(4R, c)$ | $(40R, 10c)$ |
|-----|----------|-----------|---------------|
| 6   | $-2.8529$ | $-2.8529$ | $-2.8527$     |
| 8   | $-2.8538$ | $-2.8539$ | $-2.8533$     |
| 10  | $-2.8550$ | $-2.8552$ | $-2.8539$     |
| 12  | $-2.8566$ | $-2.8568$ | $-2.8545$     |
| 14  | $-2.8584$ | $-2.8586$ | $-2.8550$     |
| 20  | $-2.8654$ | $-2.8658$ | $-2.8569$     |
| 25  | $-2.8731$ | $-2.8735$ | $-2.8585$     |
| 30  | $-2.8824$ | $-2.8828$ | $-2.8601$     |
| 35  | $-2.8933$ | $-2.8936$ | $-2.8616$     |
| 40  | $-2.9057$ | $-2.9057$ | $-2.8629$     |
| 45  | $-2.9194$ | $-2.9191$ | $-2.8642$     |
| 50  | $-2.9346$ | $-2.9336$ | $-2.8653$     |
| 55  | $-2.9510$ | $-2.9491$ | $-2.8663$     |
| 60  | $-2.9686$ | $-2.9655$ | $-2.8670$     |

we employ the DK8 and the $B$-splines methods implemented in the quadruple arithmetics.

The accuracy of the obtained numerical results is checked as follows. We observe that the leading term of the $Z\alpha$ expansion of Eq. (21), $H^{(1,0)}$, should not depend on the nuclear charge radius $R$. It also cannot depend on the speed of light $c$. All dependence of $H^{(1,0+)}$ on $R$ and $c$ comes only through the relativistic effects, which are small corrections in the low-$Z$ region. Therefore, numerical calculations of $H^{(1,0+)}$ performed with different choices of $R$ and $c$ should have the same low-$Z$ limit.

The numerical results for the nuclear-size correction to the one-photon exchange are presented in Table III and shown graphically on Fig. 1. We observe that the results obtained with different values of $R$ and $c$ are in very good agreement for low $Z$. This agreement also indicates that the results for $H^{(1)}$ are practically independent of the nuclear model.

The results obtained with enlarged speed of light show very weak $Z$ dependence, which might have been anticipated since the $Z$ dependence of $H^{(1)}$ comes through the relativistic corrections only. These results can be easily extrapolated to $Z \to 0$, yielding

$$H^{(1,0)} = -2.8512 \, (10).$$

On the basis of this result, we conclude that the following weighted difference of the $2s$ and $1s$ $g$-factors cancels most of the fns contribution of order $1/Z$ for light ions,

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

D. Two and more photon exchange fns correction

The fns correction with two and more photon exchanges between the electrons is suppressed by the factor of $1/Z^2$ with respect to the leading fns contributions. A parametrization of this term can be given as

$$\delta g_N^{(2+)} = \delta g_N^{(0)} \frac{1}{Z^2} H^{(2+)}(Z\alpha, R),$$

where $\delta g_N^{(0)}$ is the one-electron nuclear-size correction defined in Eq. (3), and $H^{(2+)}$ is a slowly varying function of its arguments.

In order to compute the fns correction, we need to calculate the two and more photon exchange correction for the extended and the point nucleus and take the difference,

$$\delta g_N^{(2+)} = \delta g_{\text{ext}}^{(2+)} - \delta g_{\text{pnt}}^{(2+)}.$$

In this work, we calculate $\delta g_{\text{ext}}^{(2+)}$ and $\delta g_{\text{pnt}}^{(2+)}$ within the Breit approximation. The whole calculation is performed in three steps. In the first step, we solve the no-pair Dirac-Coulomb-Breit Hamiltonian by the Configuration-Interaction Dirac-Fock-Sturm (CI-DFS) method [22]. In the second step, we subtract the leading-order terms of orders $1/Z^0$ and $1/Z^1$, thus identifying the contribution of order $1/Z^2$ and higher. The subtraction terms of order $1/Z^0$ and $1/Z^1$ were calculated separately by perturbation theory. In the third step, we repeat the calculation for the extended and the point nuclear models and, by taking the difference, obtain the fns correction.

The fns effect is very small in the low-$Z$ region, which makes it very difficult to obtain reliable predictions for this
TABLE IV: The two and more photon exchange fns correction to the bound-electron $g$ factor of the ground state of Li-like ions, in terms of the function $H^{(2+)}$ defined by Eq. (24). Notations are the same as in Table III.

| $Z$ | $(R,c)$ | $(4R,c)$ | $(40R,10c)$ |
|-----|---------|----------|-------------|
| 10  | 1.059 (20) | 1.081 (20) |             |
| 14  | 1.073 (20) | 1.075 (20) |             |
| 20  | 1.102 (20) | 1.110 (20) | 1.075 (20)  |
| 25  | 1.157 (20) | 1.149 (20) | 1.074 (20)  |
| 30  | 1.198 (20) | 1.195 (20) | 1.074 (20)  |
| 35  | 1.255 (20) | 1.249 (20) | 1.073 (20)  |
| 40  | 1.321 (20) | 1.312 (20) | 1.072 (20)  |
| 50  | 1.481 (20) | 1.466 (20) | 1.068 (20)  |
| 55  | 1.579 (20) | 1.560 (20) | 1.067 (20)  |
| 60  | 1.690 (20) | 1.672 (20) | 1.064 (20)  |

Correlation. In order to be able to monitor the numerical accuracy, we performed three sets of calculations. The first set $(R,c)$ was obtained with the actual values of the nuclear charge radii $R$ and the speed of light $c$; the second set $(4R,c)$ was obtained with the nuclear charge radii multiplied by a factor of 4; the third set $(40R,10c)$ was obtained with the nuclear charge radii multiplied by a factor of 40 and the speed of light multiplied by 10. The obtained results are listed in Table IV and presented in Fig. 2.

Similarly to the one-photon exchange fns correction, we assume that the low-$Z$ limit of $H^{(2+)}$, denoted as $H^{(2,0)}$, does not depend either on $R$ or on $c$. By extrapolating our numerical results in Table IV to $Z \to 0$, we obtain the nonrelativistic value of the $1/Z^2$ correction as

$$H^{(2,0)} = 1.070 (25).$$

(26)

Based on this result, we conclude that for light ions, the following weighted difference of the $2s$ and $1s$ $g$-factors cancels most of the $1/Z^2$ fns contribution:

$$\delta g = \delta g^{(2+)}(2s) - \Xi_0 \left( \frac{107}{100} \frac{1}{Z^2} \right) g^{(0)}(1s).$$

(27)

III. THE WEIGHTED DIFFERENCE OF THE 2S AND 1S $g$ FACTORS

Combining the results obtained in the previous section, we introduce the total $\Xi$-weighted difference as follows

$$\delta \Xi g = g(2s) - \Xi g(1s),$$

(28)

where $g(2s)$ is the $g$ factor of the ground state of the Li-like ion, $g(1s)$ is the $g$ factor of the ground state of the H-like ion, and the weight parameter $\Xi$ is defined by Eq. (2). Basing on the analysis of the preceding Section, we claim that in the $\Xi$-weighted difference $\delta \Xi g$, the nonrelativistic fns corrections to order $1/Z^0$, $1/Z^1$, and $1/Z^2$ and, in addition, the relativistic contribution to order $(Z\alpha)^2/Z^0$ are cancelled. A small remaining fns correction to $\delta \Xi g$ is calculated numerically. The definition of $\delta \Xi g$ is based on the $Z\alpha$ expansion of the fns corrections. Because of this, it is applicable for low- and medium-$Z$ ions. For heavy systems, the $Z\alpha$ expansion is no longer useful. In this case, the cancellation of the fns effect in the weighted difference is still possible but should be achieved differently [5, 6].

In Table V we present the individual fns contributions to the $g$-factor of the ground state of Li-like ions $g(2s)$, H-like ions $g(1s)$ and for the weighted difference $\delta \Xi g$. We observe that the uncertainty of the fns corrections for $g(2s)$ and $g(1s)$ is dominated by the nuclear-model and nuclear-radii errors, which means they cannot be significantly improved. On the contrary, the fns effect for $\delta \Xi g$ is much smaller, and its uncertainty is mainly numerical, meaning that it can be improved further.

FIG. 2: (Color online) The two and more photon exchange fns correction to the bound-electron $g$ factor of the ground state of Li-like ions, in terms of the function $H^{(2+)}$ defined by Eq. (24). Notations are the same as in Fig. 1.

In Table V we present the individual fns contributions to the $g$-factor of the ground state of Li-like ions $g(2s)$, H-like ions $g(1s)$ and for the weighted difference $\delta \Xi g$. We observe that the uncertainty of the fns corrections for $g(2s)$ and $g(1s)$ is dominated by the nuclear-model and nuclear-radii errors, which means they cannot be significantly improved. On the contrary, the fns effect for $\delta \Xi g$ is much smaller, and its uncertainty is mainly numerical, meaning that it can be improved further.
FIG. 3: (Color online) Comparison of the error $\delta g = (\partial g / \partial \alpha) \delta \alpha$ 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 panel); for the weighted difference $\delta g(Z)$ (middle panel); and for the weighted difference $\delta \Omega g = \delta g(Z) - \delta g([Z/2])$ (right panel).

TABLE V: The fns corrections to the bound-electron $g$ factor of the ground state of Li-like and H-like ions and their weighted difference, multiplied by a factor of $10^6$. The numbers in the parentheses denote the uncertainty in the last figure. When three uncertainties are specified, the first one is the numerical error, the second one the model-dependence error, and the third one the uncertainty induced by the error of the nuclear charge radius. In the case only one uncertainty is specified, it is the numerical uncertainty (whereas the other errors are significantly smaller and are not indicated).

| $Z$ | Term | $\delta g_N(2s)$ | $\Xi_i / Z \delta g_N(1s)$ | $\delta g_N(2s) - \Xi_i / Z \delta g_N(1s)$ |
|-----|------|-----------------|-----------------|----------------------------------|
| 6   | $1/Z^0$ | 0.000 050 99 (0)(1)(9) | 0.000 050 99 (0)(1)(9) | 0. |
|     | $\alpha / Z^0$ | $-0.000 000 05 (2)$ | $-0.000 000 071 (2)$ | $0.000 000 03 (2)$ |
|     | $1/Z^1$ | $-0.000 024 24 (0)(0)(4)$ | $-0.000 024 23 (0)(0)(4)$ | $-0.000 000 016 (1)(0)(0)$ |
|     | $1/Z^{2+}$ | 0.000 001 52 (4) | 0.000 001 515 | 0.000 000 000 (4) |
|     | Total | 0.000 028 2 (0)(0)(0)(1) | 0.000 0282 (0)(0)(0)(1) | 0.000 000 01 (4)(0)(0) |
| 8   | $1/Z^0$ | 0.000 194 7 (0)(0)(7) | 0.000 194 7 (0)(0)(7) | 0. |
|     | $\alpha / Z^0$ | $-0.000 000 25 (3)$ | $-0.000 000 317 (5)$ | $0.000 000 07 (3)$ |
|     | $1/Z^1$ | $-0.000 069 5 (0)(0)(3)$ | $-0.000 069 4 (0)(0)(3)$ | $-0.000 000 068 (1)(0)(0)$ |
|     | $1/Z^{2+}$ | 0.000 003 26 (8) | 0.000 003 256 | 0.000 000 000 (8) |
|     | Total | 0.000 128 3 (1)(0)(0)(8) | 0.000 128 3 (0)(0)(0)(8) | 0.000 000 000 (8)(0)(0) |
| 10  | $1/Z^0$ | 0.000 598 3 (0)(1)(8) | 0.000 598 3 (0)(1)(8) | $-0.000 000 002$ |
|     | $\alpha / Z^0$ | $-0.000 000 90 (8)$ | $-0.000 001 12 (1)$ | $0.000 000 22 (8)$ |
|     | $1/Z^1$ | $-0.000 170 8 (0)(0)(2)$ | $-0.000 170 6 (0)(0)(2)$ | $-0.000 000 241 (1)(0)(0)$ |
|     | $1/Z^{2+}$ | 0.000 006 4 (1) | 0.000 006 40 | 0.000 000 000 (1) |
|     | Total | 0.000 433 0 (2)(1)(9) | 0.000 433 0 (0)(1)(9) | 0.000 000 000 (2)(0)(0) |
| 12  | $1/Z^0$ | 0.001 307 (0)(0)(1) | 0.001 307 (0)(0)(1) | $-0.000 000 007$ |
|     | $\alpha / Z^0$ | $-0.000 002 3 (2)$ | $-0.000 002 74 (2)$ | $0.000 000 4 (2)$ |
|     | $1/Z^1$ | $-0.000 311 1 (0)(1)(3)$ | $-0.000 310 5 (0)(1)(3)$ | $-0.000 000 604 (1)(0)(1)$ |
|     | $1/Z^{2+}$ | 0.000 009 7 (2) | 0.000 009 71 | 0.000 000 000 (2) |
|     | Total | 0.000 003 (0)(0)(0)(1) | 0.000 003 (0)(0)(0)(1) | $-0.000 000 2 (3)(0)(0)$ |
| 14  | $1/Z^0$ | 0.002 580 (0)(1)(4) | 0.002 580 (0)(1)(4) | $-0.000 000 026 (0)(1)(0)$ |
|     | $\alpha / Z^0$ | $-0.000 005 1 (3)$ | $-0.000 005 96 (3)$ | $0.000 000 8 (3)$ |
|     | $1/Z^1$ | $-0.000 5267 (0)(2)(8)$ | $-0.000 525 3 (0)(2)(8)$ | $-0.000 001 353 (1)(0)(2)$ |
|     | $1/Z^{2+}$ | 0.000 014 1 (3) | 0.000 014 1 | 0.000 000 000 (3) |
|     | Total | 0.002 062 (0)(1)(4) | 0.002 062 (0)(1)(4) | $-0.000 000 6 (4)(0)(0)$ |
We would like now to address the question whether the weighted difference $\delta g$ might be useful for the determination of the fine-structure constant $\alpha$. The leading dependence of $\delta g$ on $\alpha$ is given by the expansion

$$\delta g = 2(1 - \Xi) - \frac{2}{3}(Z\alpha)^2 \left( \frac{1}{4} - \Xi \right) + \frac{\alpha}{\pi}(1 - \Xi) + \ldots,$$

(29)

where the second term in the right-hand-side stems from the
binding corrections, whereas the third term is due to the one-loop free-electron QED effect. In the above equation, we keep $\Xi$ fixed, ignoring its dependence on $\alpha$, since it does not contribute to the sensitivity of $\delta_{\Xi g}$ on $\alpha$ (the same value of $\Xi$ should be used when comparing the experimental and theoretical values of $\delta_{\Xi g}$). By varying $\alpha$ in Eq. (29) within its current error bars of $\delta\alpha/\alpha = 3.2 \times 10^{-10}$ [4], the corresponding error of $\delta_{\Xi g}$ can be obtained.

In Fig. 3 we compare the uncertainty due to $\alpha$ and the uncertainty due to the nuclear model and radius, keeping in mind that the latter defines the ultimate limit of the accuracy of theoretical calculations. The left panel of Fig. 3 shows this comparison for the $g$-factor of the ground state of Li-like ions $g(2s)$, whereas the middle panel gives the same comparison for the $\Xi$-weighted difference $\delta_{\Xi g}$. The dip of the $\alpha$-sensitivity curve around $Z = 16$ is caused by the fact that the dependence of the binding and the free-QED effects on $\alpha$ in Eq. (29) (second and third terms) have different signs, and thus cancel each other in this $Z$ region. From Fig. 3 we can conclude that up to $Z \approx 45$, the weighted difference $\delta_{\Xi g}$ yields possibilities for an improved determination of $\alpha$.

The determination of $\alpha$ from $\delta_{\Xi g}$ has two drawbacks. The first one is the cancellation of a $\alpha$ dependence of $\delta_{\Xi g}$ around $Z = 16$, leading to a loss of sensitivity to $\alpha$ in this $Z$ region. The second one is that $\delta_{\Xi g}$ contains the same free-QED part which is used for the determination of $\alpha$ from the free-electron $g$ factor, which means that these two determinations cannot be regarded as fully independent. Both drawbacks can be avoided by introducing another difference,

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

with $\delta_{\Xi g}(Z)$ being the weighted difference (28) for the nuclear charge $Z$, and $\delta_{\Xi g}([Z/2])$ is the corresponding difference for the nuclear charge $[Z/2]$, where $[\ldots]$ stands for the upper or the lower integer part. In the difference $\delta_{\Omega g}$, most free-QED contributions vanish. So, by a small sacrifice of the sensitivity of the binding effects to $\alpha$, we removed the dip around $Z = 16$ and made the theory of the weighted difference (almost) independent on the theory of the free-electron $g$-factor.

The right panel of Fig 3 presents the comparison of the uncertainty due to $\alpha$ with the error of the fns effect for the weighted difference $\delta_{\Omega g}$. One finds a smooth dependence of the sensitivity to $\alpha$ on $Z$, without any dip in the region around $Z = 16$. We observe that in the region $Z = 10 - 20$, the weighted difference $\delta_{\Omega g}$ offers better possibilities for determining $\alpha$ than $\delta_{\Xi g}$.

Employing the difference $\delta_{\Omega g}$ can be also advantageous from the experimental point of view. It can be rewritten as

$$\delta_{\Omega g} = g(2s, Z) - g(2s, Z_2)$$

$$- \Xi(Z)[g(1s, Z) - g(1s, Z_2)]$$

$$- g(1s, Z_2)[\Xi(Z) - \Xi(Z_2)],$$

with $Z_2 = [Z/2]$. We thus observe that $\delta_{\Omega g}$ can be effectively determined in an experiment by measuring two equal-weight $g$-factor differences (namely, the ones in the first and second rows of the above equation) and $g(1s, Z_2)$. The equal-weight differences may be measured with largely suppressed systematic errors and thus can be determined in near-future experiments much more accurately than the $g$-factors of individual ions. The last term in Eq. (31) is suppressed by a small factor of $\Xi(Z) - \Xi(Z_2) \approx 0.02 - 0.04$ in the region of interest. Therefore, the experimental error of $\delta_{\Omega g}$ can be significantly improved as compared to that of the absolute $g$-factors.

Let us now turn to the experimental consequences of the present calculations. So far, the only element for which the weighted difference $\delta_{\Xi g}$ has been measured is silicon. In Table VI we collect the individual theoretical contributions to $\delta_{\Xi g}(^{29}\text{Si})$. Theoretical results for various effects were taken from the literature, Refs. [9, 23–28]. The total theoretical value is compared to the experimental result [2, 29, 30]. The errors of the Dirac value and of the one-loop free QED ($\sim \alpha(Z\alpha)^6$) result specified in the table are due to the uncertainty of the current value of $\alpha^{-1} = 137.035\ 999\ 074\ (44)$ [4]. The uncertainty of the fns effect specified in the table is $6 \times 10^{-13}$, which is already smaller than the uncertainty of the Dirac value due to $\alpha$. The fns uncertainty is of purely numerical origin, i.e., it does not influence by the errors due to the rms charge radius and the nuclear charge distribution, and thus it can be further improved in future calculations.

Table VI illustrates another advantage of the $\Xi$-weighted difference: the contributions of one-electron binding QED effects to $\delta_{\Xi g}$ are much smaller than those to $g(2s)$. This is explained by the fact that these effects largely originate from short distances, similarly to the fns effect, and thus are significantly canceled in the difference. In particular, the uncertainty of $\delta_{\Xi g}(\text{Si})$ due to three-loop binding QED effects is on the $10^{-12}$ level, implying that these effects do not need to be known to a high degree of accuracy for the determination of $\alpha$.

Table VI shows that the present experimental and theoretical precision of $\delta_{\Xi g}(\text{Si})$ is on the level of few parts in $10^{-9}$, which is significantly worse than the precision achieved for other systems (in particular, H-like carbon, where the present experimental and theoretical uncertainties are, correspondingly, $6 \times 10^{-11}$ and $6 \times 10^{-12}$ [1]). This underperformance is, however, more due to a lack of motivation than due to principal obstacles.

On the experimental side, the same precision as for H-like carbon can be also obtained for $\delta_{\Xi g}(C)$, with an existing ion trap [3]. Further experimental advance is anticipated that could bring one or two orders of magnitude of improvement [3]. On the theoretical side, the modern nonrelativistic quantum electrodynamics (NRQED) approach (see, e.g., [31]) can apparently provide a theoretical result for Li-like carbon with the same accuracy as obtained for its H-like counterpart [32]. Moreover, further theoretical advance is possible: the two-loop QED corrections of order $\alpha^2(Z\alpha)^3$ and the three-loop QED corrections of order $\alpha^3(Z\alpha)^4$ can be calculated, both for H-like and Li-like ions [32].

As we are presently interested in light ions, the best way for the advancement of theory would be a combination of two complementary methods. The first one is the NRQED method (used, e.g., in [33]) that accounts for the nonrelativistic electron-electron interactions to all orders in $1/Z$, but ex-
pands the QED and relativistic effects in powers of $\alpha$ and $Z\alpha$. The second approach (used, e.g., in [24, 26–28]) accounts for the relativistic effects to all orders in $Z\alpha$ but employs perturbation expansions in $\alpha$ (QED effects) and in $1/Z$ (electron-electron interaction). Matching the coefficients of the $Z\alpha$ and $1/Z$ expansions from the two methods allows one to combine them together, as it was done for energy levels in Ref. [34]. As a result of this procedure, only higher-order corrections in $Z\alpha$ will be expanded in $1/Z$ and only higher-order corrections in $1/Z$ will be expanded in $Z\alpha$. This approach should allow one to advance theory to the level required for a determination of $\alpha$.

The principal limitation for the theory is set by the non-trivial nuclear structural effects, such as the nuclear deformation, nuclear polarization, etc. For light ions, the leading nuclear effects are described by effective operators proportional to the Dirac delta function $\delta(r)$. Such effects are canceled in the weighted difference $\delta g$. We estimate that the uncertainty due to the remaining nuclear effects in $\delta g$ should be of the same order as the nuclear-model dependence error of the $\alpha$ effect. From the breakdown in Table V we deduce that for silicon, this error is by about two orders of magnitude smaller than the uncertainty due to $\alpha$. We thus conclude that the nuclear effects do not represent any obstacles for the determination of $\alpha$ from $\delta g$ and $\delta \alpha g$.

IV. CONCLUSION

In this work we investigated specific weighted differences of the $g$-factors of H- and Li-like ions of the same element. An accurate formula was obtained for the weight parameter $\Xi$, determined by requiring cancellation of the nonrelativistic finite nuclear size corrections to orders $1/Z^0$, $1/Z^1$, and $1/Z^2$ and, in addition, the relativistic contribution to order $(Z\alpha)^2/Z^0$. The coefficients of the $Z\alpha$ expansion of the finite nuclear size corrections were obtained by performing accurate numerical calculations and fitting the results to the known expansion form. It was demonstrated that the $\Xi$- and $\Omega$-weighted differences, as given by Eqs. (28) and (30), can be used for an efficient suppression of nuclear effects. The residual uncertainty due to nuclear effects is smaller than the uncertainty due to the currently accepted value of the fine-structure constant $\alpha$. The $\Xi$- and $\Omega$-weighted differences may be used in future to determine $\alpha$ from a comparison of theoretical and experimental bound-electron $g$-factors with an accuracy competitive with or better than the present literature value.

Acknowledgments

V.A.Y. and Z.H. acknowledge helpful conversations with Sven Sturm. V.A.Y. acknowledges support by the Ministry of Education and Science of the Russian Federation (program for organizing and carrying out scientific investigations) and by RFBR (grant No. 16-02-00538). E.B. acknowledges support from G-RISC, project No. P-2014a-9.

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TABLE VI: Individual contributions to the weighted difference $\delta \Xi$ for $^{29}$Si, $M/m = 52806.93396$, $\Xi = 0.101136233077060$.  

| Contribution Order | Value               |
|--------------------|---------------------|
| Dirac              | 1.796 687 854 216 5 (7) |
| 1-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) |
| 2-loop QED $\alpha^2(Z\alpha)^{0}$ | −0.000 003 186 116 6 |
| $\alpha^2(Z\alpha)^{2}$ | −0.000 000 009 179 0 |
| $\alpha^2(Z\alpha)^{4}$ | −0.000 000 000 844 4 |
| $\alpha^2(Z\alpha)^{5+}$ | 0.000 000 000 000 0 (13) |
| $\geq$ 3-loop QED $\alpha^3+(Z\alpha)^{0}$ | 0.000 000 026 514 9 (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 $m/M(Z\alpha)^{2+}$ | 0.000 000 029 4 (10) |
| 1-photon exchange $(1/Z)(Z\alpha)^{2+}$ | 0.000 321 590 803 3 |
| 2-photon exchange $(1/Z^2)(Z\alpha)^{2+}$ | −0.000 006 876 0 (5) |
| $\geq$ 3-photon exchange $(1/Z^3)(Z\alpha)^{2+}$ | 0.000 000 093 0 (60) |
| 2-electron QED $(\alpha/Z)(Z\alpha)^{2+}$ | −0.000 000 023 6 (50) |
| 2-electron Recoil $(m/M)(1/Z)(Z\alpha)^{2+}$ | −0.000 000 011 6 (7) |
| Finite nuclear size | −0.000 000 000 000 0 (14) |
| Total theory | 1.799 087 813 2 (79) |
| Experiment [2, 29] | 1.799 087 812 5 (21) |

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