

One-loop electron self-energy for the bound-electron g factor

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We report calculations of the one-loop self-energy correction to the bound-electron g factor of the $1s$ and $2s$ states of light hydrogenlike ions with a nuclear charge number $Z \leq 20$. The calculation is carried out to all orders in the binding nuclear strength. We find good agreement with previous calculations and improve their accuracy by about two orders of magnitude.

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The bound-electron g factor in light hydrogenlike and lithiumlike ions has been measured with a high accuracy, which reached 3×10^{-11} in the case of C^{5+} [1]. Such measurements have yielded one of the best tests of the bound-state QED theory [2] and significantly improved the precision of the electron mass [1,3]. Further advance of the experimental accuracy toward the 10^{-12} level is anticipated in the near future [4].

One of the dominant effects in the bound-electron g factor is the one-loop electron self-energy. Its contribution to the total g factor value is so large that the effect needs to be calculated to all orders in the nuclear binding strength parameter $Z\alpha$, even for ions as light as carbon (Z is the nuclear charge number, α is the fine-structure constant). The numerical error in the evaluation of the electron self-energy is currently the second-largest source of uncertainty for hydrogenlike ions (the largest error stemming from the two-loop electron self-energy [5,6]). The error needs to be decreased in order to match the anticipated experimental precision.

The numerical accuracy of one-loop self-energy is also relevant for the determination of the electron mass [1,3]. The self-energy values actually used in electron-mass determinations were obtained by an extrapolation of the high- and medium- Z numerical results down to $Z = 6$ (carbon) and 8 (oxygen). Clearly, this situation is not fully satisfactory and a direct numerical calculation would be preferable.

All-order (in $Z\alpha$) calculations of the electron self-energy to the bound-electron g factor have a long history. The first calculations of this correction were accomplished two decades ago [7–9]. The numerical accuracy of these evaluations was advanced in later works [10,11], which was crucial at the time as it brought an improvement of the electron mass determination. This correction was revisited again in Refs. [12,13]. In the present Rapid Communication, we aim to advance the numerical accuracy of the one-loop electron self-energy and bring it to the level required for future experiments.

We consider the one-loop self-energy correction to the g factor of an electron bound by the Coulomb field of a pointlike and spinless nucleus. This correction can be represented [10,11] as a sum of the irreducible (ir) and the vertex+reducible (vr) parts,

$$\Delta g_{SE} = \Delta g_{ir} + \Delta g_{vr}. \quad (1)$$

The irreducible part is

$$\Delta g_{ir} = 2 \langle \delta_g a | \gamma^0 \tilde{\Sigma}(\varepsilon_a) | a \rangle, \quad (2)$$

where $\tilde{\Sigma}(\varepsilon) = \Sigma(\varepsilon) - \delta m$ is the (renormalized) one-loop self-energy operator (see, e.g., Ref. [13]) and $|\delta_g a\rangle$ is the perturbed wave function

$$|\delta_g a\rangle = \sum_{n \neq a} \frac{|n\rangle \langle n | \delta V_g | a \rangle}{\varepsilon_a - \varepsilon_n}, \quad (3)$$

with $\delta V_g = 2m[\mathbf{r} \times \boldsymbol{\alpha}]_z$ being the effective g -factor operator [13] that assumes that the spin projection of the reference state is $m_a = \frac{1}{2}$. The vertex+reducible part is

$$\Delta g_{vr} = \frac{i}{2\pi} \int_C d\omega \sum_{n_1 n_2} \left[\frac{\langle n_1 | \delta V_g | n_2 \rangle \langle a n_2 | I(\omega) | n_1 a \rangle}{(\Delta_{a n_1} - \omega)(\Delta_{a n_2} - \omega)} - \delta_{n_1 n_2} \frac{\langle a | \delta V_g | a \rangle \langle a n_1 | I(\omega) | n_1 a \rangle}{(\Delta_{a n_1} - \omega)^2} \right], \quad (4)$$

where $I(\omega)$ is the operator of the electron-electron interaction (see, e.g., Ref. [11]), ω is the energy of the virtual photon, $\Delta_{ab} = \varepsilon_a - \varepsilon_b$, and a proper covariant identification and cancellation of ultraviolet and infrared divergences is assumed. The integration contour C in Eq. (4) is the standard Feynman integration contour; it will be deformed for a numerical evaluation as discussed below.

The vertex+reducible contribution is further divided into three parts: the zero-potential, one-potential, and many-potential contributions,

$$\Delta g_{vr} = \Delta g_{vr}^{(0)} + \Delta g_{vr}^{(1)} + \Delta g_{vr}^{(2+)}. \quad (5)$$

This separation is induced by the following identity, which splits the integrand according to the number of interactions with the binding Coulomb field in the electron propagators,

$$\begin{aligned} G \delta V_g G &\equiv [G^{(0)} \delta V_g G^{(0)}] + [G^{(0)} \delta V_g G^{(1)} + G^{(1)} \delta V_g G^{(0)}] \\ &+ [G \delta V_g G - G^{(0)} \delta V_g G^{(0)}] \\ &- [G^{(0)} \delta V_g G^{(1)} - G^{(1)} \delta V_g G^{(0)}], \end{aligned} \quad (6)$$

where $G \equiv G(\varepsilon) \equiv \sum_n |n\rangle \langle n| / (\varepsilon - \varepsilon_n)$ is the bound-electron propagator, $G^{(0)} \equiv G|_{Z=0}$ is the free-electron propagator, and

$$G^{(1)}(\varepsilon) \equiv Z \left[\frac{d}{dZ} G(\varepsilon) \right]_{Z=0}$$

is the one-potential electron propagator.

In the present work, we will be concerned mainly with the numerical evaluation of $\Delta g_{vr}^{(2+)}$, since all other contributions were computed to the required accuracy in our previous investigations [11,13].

After performing integrations over the angular variables analytically as described in Ref. [11], we obtain the result that can be schematically represented as

$$\Delta g_{\text{vr}}^{(2+)} = \lim_{|\kappa_{\text{max}}| \rightarrow \infty} \int_C d\omega \int_0^\infty dx dy dz \sum_{|\kappa|=1}^{|\kappa_{\text{max}}|} f_{|\kappa|}(\omega, x, y, z), \quad (7)$$

where x , y , and z are the radial integration variables, $|\kappa|$ is the absolute value of the angular momentum-parity quantum number of one of the electron propagators, and $f_{|\kappa|}$ is the integrand. Summations over other angular quantum numbers are finite and absorbed into the definition of $f_{|\kappa|}$.

The approach of the present work is to split $\Delta g_{\text{vr}}^{(2+)}$ into two parts,

$$\begin{aligned} \Delta g_{\text{vr}}^{(2+)} &= \Delta g_{\text{vr,a}}^{(2+)} + \Delta g_{\text{vr,b}}^{(2+)} \\ &= \int_{C_{\text{LH,a}}} d\omega \int_0^\infty dx dy dz \sum_{|\kappa|=1}^{\kappa_a} f_{|\kappa|}(\omega, x, y, z) \\ &\quad + \lim_{\kappa_{\text{max}} \rightarrow \infty} \int_{C_{\text{LH,b}}} d\omega \int_0^\infty dx dy dz \\ &\quad \times \sum_{|\kappa|=\kappa_a+1}^{\kappa_{\text{max}}} f_{|\kappa|}(\omega, x, y, z), \end{aligned} \quad (8)$$

where κ_a is an auxiliary parameter and $C_{\text{LH,a}}$ and $C_{\text{LH,b}}$ are two integration contours used for the evaluation of the two parts of Eq. (8). In the present work we used $\kappa_a = 120$, which corresponds to the maximal value of $|\kappa|$ used in Ref. [13], and $C_{\text{LH,a}}$ being the same contour as used in that work. So, the numerical evaluation of $\Delta g_{\text{vr,a}}^{(2+)}$ was mostly analogous to the one reported in Ref. [13], but we had to improve the accuracy of numerical integrations by several orders of magnitude. In the updated numerical integrations, extended Gauss-log quadratures [14] were employed, alongside the standard Gauss-Legendre quadratures.

We found it impossible to extend the partial-wave expansion significantly beyond the limit of $\kappa_a = 120$ within the same numerical scheme as used in Ref. [13]. The reason is that the integration contour $C_{\text{LH,a}}$ used there, as well as in our previous works [10,11], involved computations of the Whittaker functions of the first kind $M_{\alpha,\beta}(z)$ and their derivatives for large complex values of the argument z . The algorithms we use [15] for computing $M_{\alpha,\beta}(z)$ become unstable for large α (needed for large κ 's) and large and complex z , even when using quadruple-precision arithmetics. For this reason, in order to compute $\Delta g_{\text{vr,b}}^{(2+)}$, we had to switch to the contour $C_{\text{LH,b}}$, which was originally introduced by Mohr in his calculations of the one-loop self-energy [16,17]. The crucial feature of this contour is that it involves the computation of the Whittaker functions $M_{\alpha,\beta}(z)$ and $W_{\alpha,\beta}(z)$ of the *real* arguments z only. For real arguments, the computational algorithms were shown [17] to be stable even for very large κ 's (and hence α 's).

Specifically, the contours $C_{\text{LH,a}}$ and $C_{\text{LH,b}}$ consist of two parts, the low-energy and the high-energy ones. The low-energy part extends along $(\Delta, 0)$ on the lower bank of the cut of the photon propagator of the complex ω plane and along $(0, \Delta)$ on the upper bank of the cut. The high-energy

part consists of the interval $(\Delta, \Delta + i\infty)$ in the upper half plane and the interval $(\Delta, \Delta - i\infty)$ in the lower half plane. The difference between $C_{\text{LH,a}}$ and $C_{\text{LH,b}}$ is only in the choice of the parameter Δ . For $C_{\text{LH,a}}$, we use $\Delta = Z\alpha\epsilon_a$ (the same choice as in our previous works [10,11,13]), whereas for $C_{\text{LH,b}}$, we use $\Delta = \epsilon_a$ (Mohr's choice). A detailed discussion of the integration contour and the analytical properties of the integrand can be found in the original work [16].

We found that the price to pay for using the contour $C_{\text{LH,b}}$ was the oscillatory behavior of the integrand as a function of the radial variables for $\omega \sim \epsilon_a$. Because of this, we had to employ very dense radial grids for numerical integrations, which made computations rather time consuming.

The largest error of the numerical evaluation of Eq. (8) comes from the termination of the infinite summation over $|\kappa|$ and the estimation of the tail of the expansion. In the present work, we performed the summation over $|\kappa|$ *before* all integrations and stored the complete sequence of partial sums, to be used for the extrapolation performed on the last step of the calculation. The convergence of the expansion was monitored; in the cases when the series converged to the prescribed accuracy [i.e., the relative contribution of several consecutive expansion terms was smaller than, typically, 10^{-11} for $\Delta g_{\text{vr,a}}^{(2+)}$ and 10^{-6} for $\Delta g_{\text{vr,b}}^{(2+)}$], the summation was terminated. This approach reduced the computation time considerably as compared to our previous scheme [11], where the summation over $|\kappa|$ was performed *after* all integrations. If the convergence of the partial-wave expansion had not been reached, the summation was extended up to the upper cutoff $\kappa_{\text{max}} = 450$.

The remaining tail of the series was estimated by analyzing the $|\kappa|$ dependence of the partial-wave expansion terms *after* all integrations. We fitted the last m expansion terms (typically, $m = 20$) to the polynomial in $1/|\kappa|$ with one to three fitting parameters,

$$\delta S_{|\kappa|} = c_0/|\kappa|^3 + c_1/|\kappa|^4 + \dots$$

The uncertainty of the extrapolation was estimated by varying the cutoff parameter κ_{max} by 20% and multiplying the resulting difference by a conservative factor of 1.5. This procedure usually led to the expansion tail estimated with an accuracy of about 10%.

We observed an interesting feature, namely, that the tail of the expansion, with a high accuracy, is the same for the $1s$ and for the $2s$ states. For example, for $Z = 4$, we find the expansion tail of $\delta g(1s) = -1.88(19) \times 10^{-12}$ and $\delta g(2s) = -1.88(19) \times 10^{-12}$; for $Z = 16$, we obtain $\delta g(1s) = -3.00(27) \times 10^{-11}$ and $\delta g(2s) = -3.01(27) \times 10^{-11}$. We do not know the reason for this, but such an agreement shows a high degree of consistency of our numerical calculations for the $1s$ and $2s$ states.

Our numerical results for the self-energy correction to the bound-electron g factor of the $1s$ and $2s$ states of hydrogenlike ions are presented in Table I. The values for the irreducible part Δg_{ir} are taken from our previous investigations (from Ref. [13] for $Z \leq 12$ and from Ref. [11] otherwise). Using the results of Ref. [11], we introduced small corrections that accounted for a different value of the fine-structure constant used in that work. In Table I we also present values of the higher-order

TABLE I. One-loop self-energy correction to the bound-electron g factor for the $1s$ and $2s$ states of H-like ions, multiplied by 10^6 . The value of the fine-structure constant used in the calculation is $\alpha^{-1} = 137.036$.

Z	δg_{ir}	$\delta g_{\text{vr}}^{(0)}$	$\delta g_{\text{vr}}^{(1)}$	$\delta g_{\text{vr}}^{(2+)}$	Total	$H(Z\alpha)$
$1s$						
4	17.216 132 6	2 300.997 357 2	4.459 445 1	0.502 585 3 (2)	2 323.175 520 1 (2)	22.487 (4)
6	34.064 668 1	2 280.737 822 5	7.795 347 6	1.074 584 5 (4)	2 323.672 422 7 (4)	22.166 (1)
8	54.781 703 2	2 256.697 710 8	11.165 707 2	1.797 002 1 (7)	2 324.442 123 2 (7)	21.861 4 (5)
10	78.743 788 6	2 229.826 130 5	14.349 045 7	2.617 542 (1)	2 325.536 507 (1)	21.566 3 (2)
12	105.511 685 3	2 200.798 139 6	17.216 228 5	3.483 762 (2)	2 327.009 815 (2)	21.279 5 (1)
14	134.760 370 (3)	2 170.119 540 6	19.693 048 7	4.344 533 (2)	2 328.917 492 (4)	21.000 5 (1)
16	166.242 092 (3)	2 138.182 197 1	21.740 396 0	5.150 896 (3)	2 331.315 581 (4)	20.729 03 (8)
18	199.764 465 (3)	2 105.296 890 3	23.342 539 0	5.856 557 (3)	2 334.260 452 (5)	20.465 04 (5)
20	235.176 430 (4)	2 071.714 411 8	24.499 708 2	6.418 172 (4)	2 337.808 723 (6)	20.208 29 (4)
$2s$						
4	5.053 860 6	2 315.988 700 0	1.337 877 4	0.524 654 7 (3)	2 322.905 092 6 (3)	22.78 (4)
6	10.186 275 6	2 309.230 319 4	2.428 638 8	1.173 119 8 (4)	2 323.018 353 7 (4)	22.48 (1)
8	16.629 185 2	2 300.885 484 0	3.600 384 8	2.070 636 5 (7)	2 323.185 690 5 (7)	22.221 (4)
10	24.208 822 9	2 291.216 226 1	4.777 844 0	3.210 248 (1)	2 323.413 141 (1)	21.972 (2)
12	32.796 260 4	2 280.416 694 2	5.909 016 2	4.584 979 (2)	2 323.706 950 (2)	21.727 (1)
14	42.290 335 (2)	2 268.638 681 0	6.956 360 9	6.188 074 (2)	2 324.073 450 (3)	21.486 (1)
16	52.608 698 (2)	2 256.005 047 5	7.892 134 5	8.013 144 (3)	2 324.519 024 (4)	21.250 5 (6)
18	63.682 502 (3)	2 242.617 687 9	8.695 612 8	10.054 280 (4)	2 325.050 083 (5)	21.020 3 (4)
20	75.453 014 (4)	2 228.562 653 6	9.351 303 3	12.306 120 (5)	2 325.673 091 (6)	20.794 9 (3)

remainder function $H(Z\alpha)$, obtained after separating out all known terms of the $Z\alpha$ expansion [5,6] from our numerical results,

$$\Delta g_{\text{SE}} = \frac{\alpha}{\pi} \left[1 + \frac{(Z\alpha)^2}{6n^2} + \frac{(Z\alpha)^4}{n^3} \left\{ \frac{32}{9} \ln[(Z\alpha)^{-2}] + b_{40} \right\} + \frac{(Z\alpha)^5}{n^3} H(Z\alpha) \right], \quad (9)$$

where $b_{40}(1s) = -10.236\,524\,32$ and $b_{40}(2s) = -10.707\,715\,60$. The results for the higher-order remainder function are plotted in Fig. 1.

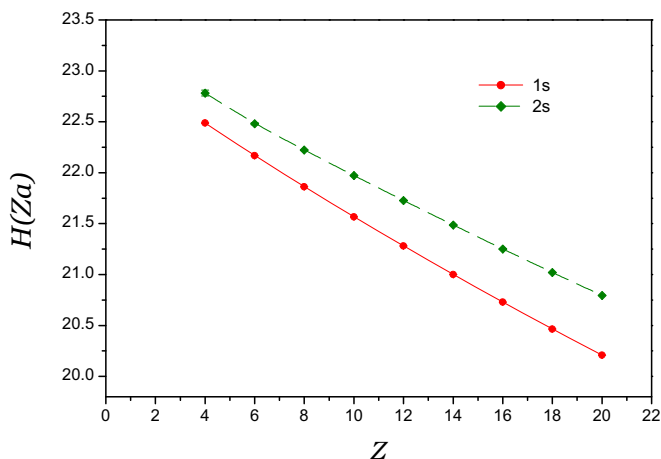


FIG. 1. The higher-order remainder function $H(Z\alpha)$, defined by Eq. (9), for the one-loop self-energy correction to the bound-electron g factor of the $1s$ and $2s$ states.

Our calculation represents an improvement in accuracy over previous works by about two orders of magnitude. Table II shows a comparison of various calculations for carbon. It is gratifying to find that all results are consistent with each other within the given error bars.

In the present work, we performed direct numerical calculations for ions with $Z \geq 4$. For smaller Z , numerical cancellations in determining the higher-order remainder become too large to make numerical calculations meaningful. Instead of direct calculations, we extrapolated the numerical values presented in Table I for $H(Z\alpha)$ down towards $Z \rightarrow 0$. Doing this, we assumed the following ansatz for $H(Z\alpha)$, which was inspired by the expansion of the one-loop self-energy for the Lamb shift,

$$H(Z\alpha) \approx c_{00} + (Z\alpha) \{ \ln^2[(Z\alpha)^{-2}] c_{12} + \ln[(Z\alpha)^{-2}] c_{11} + c_{10} \} + (Z\alpha)^2 c_{20}. \quad (10)$$

For the $2s - 1s$ difference, we use the form (10) with $c_{12} = 0$, assuming the leading logarithm to be state independent. The extrapolated results are presented in Table III. The uncertainties quoted for our fitting results are obtained under the

TABLE II. The higher-order remainder $H(Z\alpha)$ for the $1s$ and $2s$ states of H-like carbon ($Z = 6$), in different calculations.

$H_{1s}(6\alpha)$	$H_{2s}(6\alpha)$	Reference
22.166 (1)	22.48 (1)	This work
22.18 (9)	22.5 (1.3)	[13]
22.16 (1)		[5] ^a
22.2 (2)	18.(13.)	[10,11]
22. (2.)		[9]

^aExtrapolation of the numerical data from Ref. [10].

TABLE III. Extrapolated values of the higher-order remainder $H(Z\alpha)$ for small Z .

Z	H_{1s}	$H_{2s} - H_{1s}$
0	23.6 (5)	0.12 (5)
1	23.08 (9)	0.16 (3)
2	22.85 (3)	0.20 (2)

assumption that the logarithmic terms in the next-to-leading order of the $Z\alpha$ expansion of $H(Z\alpha)$ comply with Eq. (10). If we introduce, e.g., a cubed logarithmic term into Eq. (10), our estimates of uncertainties would increase by about a factor of 2.

In summary, we reported calculations of the one-loop self-energy correction to the bound-electron g factor of the $1s$ and $2s$ state of light hydrogenlike ions, performed to all orders in the binding nuclear strength parameter $Z\alpha$. The relative accuracy of the results obtained varies from 1×10^{-10} for $Z = 4$ to 3×10^{-9} for $Z = 20$. Our results agree well with previously published values, but their accuracy is by about two orders of magnitude higher.

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