Two-Loop Binding Corrections to the Electron Gyromagnetic Factor

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We compute corrections to the gyromagnetic factor of an electron bound in a hydrogenlike ion at order $\alpha^2 (Z\alpha)^5$. This result removes a major uncertainty in predictions for silicon and carbon ions, used to determine the atomic mass of the electron.

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The Dirac equation predicts the gyromagnetic factor of a pointlike electron to be g = 2. However, even in vacuum, self-interaction of the electron modifies its g. The deviation from Dirac's prediction, a dimensionless number known as g - 2, can be computed in QED and expressed as a perturbation series in the fine-structure constant $\alpha = 1/137.035\,999\,139(31)$ [1]. This research program earned the 1965 Nobel Prize [2] and has led to the stunning five-loop prediction of order $(\alpha/\pi)^5$ [3]. In another heroic development, the four-loop term has been calculated with very high precision [4]. On the experimental side, precision is so high that the electron g - 2 is currently the best source of α [5].

When the electron is bound in an atom, the presence of the electrically charged nucleus also influences the *q* factor. This matters greatly for studies of trapped ions. The q factor has been precisely measured in a range of hydrogen-, lithium-, and boronlike ions [6-13]. This experimental enterprise holds great potential for the determination of fundamental constants and tests of the standard model because of the variety of systems that can be measured [14]. Access to nuclei with diverse values of the atomic number Z, and multiple electronic configurations for a given Z, helps eliminate uncertainties. Already now the hydrogenlike carbon (combined with silicon) provides the most precise value of the electron mass [15,16]. In the future, also the fine-structure constant might be determined independently from the theory and measurements of the freeelectron g - 2 [17–19].

The leading binding effect on g in a hydrogenlike ion, related to the electron's motion, is known to all orders in Coulomb interactions between the electron and the nucleus [20]; with $\alpha_Z = Z\alpha$,

$$g^{(0)} = 2 - \frac{4}{3} \left(1 - \sqrt{1 - \alpha_Z^2} \right). \tag{1}$$

In our notation $g^{(a,b)}$, *a* denotes the power of α/π and *b*, if present, the power of α_Z . Considered together, self-interaction

and binding effects are described by a double expansion in α/π and α_Z .

At one-loop level of self-interaction, g is known analytically including the very recently computed terms of order $(\alpha/\pi)\alpha_Z^5$ [21]. Higher order terms in α_Z have been computed numerically [22]. Numerical methods work especially well for highly charged ions but struggle for low values of Z. On the other hand, the perturbative series in α_Z behaves best at small Z. Thus analytical and numerical methods are complementary.

There is a slight tension between the two approaches. Corrections of $\mathcal{O}[(\alpha/\pi)\alpha_Z^5]$ arise from diagrams similar to Fig. 1(a), with a single self-energy (SE) loop. For an *nS* state (*n* is the principal quantum number) they are

$$g^{(1,5)} = \frac{\alpha \alpha_Z^5}{n^3} \left(\frac{89}{16} + \frac{8\ln 2}{3}\right) = 23.28 \frac{\alpha \alpha_Z^5}{\pi n^3}.$$
 (2)



FIG. 1. Examples of new contributions to the *g* factor at order $\alpha^2 \alpha_Z^5$. Coupling of the external magnetic field is denoted with a circled cross. (a) SE: one of about 100 two-loop self-energy diagrams; (b) LBL: light-by-light scattering; (c,d) MLPH, MLVP: corrections to the so-called magnetic loop with a virtual photon and a vacuum polarization.

This result, first obtained in Ref, [21], is hereby confirmed. It agrees with the coefficient 23.6(5) found numerically [22] for the ground state n = 1. However, Ref. [22] finds a slight deviation from the scaling $1/n^3$, contrary to Ref. [21] and us. This seems to indicate a poorer convergence of the numerical calculation than assessed in Ref. [22].

Two-loop self-interactions are significantly more challenging. Numerically, they are known for the Lamb shift [23,24], but for the *g* factor only some classes of diagrams have been evaluated [25]. Analytical results are known for the full set of two-loop terms up to $(\alpha/\pi)^2 \alpha_Z^4$ [26,27] and for some vacuum-polarization diagrams [28].

Effects of $\mathcal{O}[(\alpha/\pi)^2 \alpha_Z^5]$ are becoming important for the determination of m_e . Since g enters linearly in the master formula for m_e [15,16], the relative error in g enters directly into the uncertainty of m_e . Numerically, $(\alpha/\pi)^2 \alpha_Z^5/(g=2)$ is 4×10^{-13} for carbon and 3×10^{-11} for silicon. The current relative error in m_e is 3×10^{-11} . Further improvements of m_e hinge on the knowledge of the coefficient of $(\alpha/\pi)^2 \alpha_Z^5$.

In the latest determination of m_e [15,16], that coefficient and m_e were treated as two unknowns and were fitted to the two available results for g, in H-like carbon and silicon. (This illustrates opportunities offered by systems with various values of Z.) To this end, two-loop corrections were assumed to have the following expansion in α_Z :

$$g^{(2)} = \left(\frac{\alpha}{\pi}\right)^2 \left[b_{00} \left(1 + \frac{\alpha_Z^2}{6}\right) + \alpha_Z^4 (b_{40} + b_{41}L) + \alpha_Z^5 b_{50} + \alpha_Z^6 b_{63}L^3 + \cdots \right],$$
(3)

The fit performed in Refs. [15,16] resulted in b_{50} (fit) = -4.0(5.1). Here, we directly determine contributions to b_{50} beyond the already known vacuum-polarization effects b_{50}^{VP} [25,28]. We write $b_{50} = b_{50}^{VP} + \Delta b_{50}$ and set out to compute

$$\Delta b_{50} = b_{50}^{\rm SE} + b_{50}^{\rm LBL} + b_{50}^{\rm ML},\tag{4}$$

where the various terms originate with Feynman diagrams shown in Fig. 1.

Numerically, the largest contribution to b_{50} has been expected from b_{50}^{SE} , generated by two-loop self-energy diagrams $\Sigma^{(2)}$. They correspond to the 19 diagrams contributing to the Lamb shift at $\mathcal{O}(\alpha^2 \alpha_Z^5 m_e)$ [29–31] (see, for example, Fig. 2 in Ref. [31]). Each such diagram has five virtual electron propagators as well as external electron lines, all of which can interact with the magnetic field. Thus, we must compute more than 100 diagrams, one example of which is Fig. 1(a).

The α_Z^5 corrections require at least two photons to be exchanged between the electron and the nucleus. The leading contribution arises when the momentum flowing in all three loops is of the order of the electron mass [rather

than, for example, $\mathcal{O}(\alpha_Z m_e)$ or $\mathcal{O}(\alpha_Z^2 m_e)$, characteristic for so-called soft and ultrasoft effects]. In this so-called hard region, exchanges of additional Coulomb photons are suppressed by α_Z so there is no need to resum them. The contribution is local from the perspective of the longdistance atomic scale set by the Bohr radius $\sim (1/\alpha_Z m_e)$ and can be modeled by a Dirac delta potential. Corrections to this approximation are expected to be powers and logarithms of the ratio of the Compton wavelength of the electron and the Bohr radius, $\mathcal{O}(\alpha_Z)$.

The contribution of such a short-distance potential to the g factor equals $4/m_e$ times its expectation value (its contribution to the Lamb shift) [32]; the same result follows from virial relations [33]. Using the Lamb shift result [31], we find (for the ground state 1S, all our results can be generalized to nS states by dividing by n^3)

$$g^{\text{SE;Lamb}} = -9.83426(5)\alpha^2 \alpha_Z^5.$$
 (5)

The uncertainty in this result comes from numerical errors in the master integrals computed in Ref. [31]. They affect all quantities we compute below using these three-loop integrals.

Self-energy diagrams influence g also in two other ways. Their value depends on the energy of the electron, and that energy is shifted by the external magnetic field **B** by $\delta E = -g(q/2m_e)\langle s \rangle \cdot B$. The resulting correction to g is called g_3 in the notation of Ref. [21],

$$g_3 = g \frac{\partial \Sigma}{\partial E} \Big|_{E=m_e} = g_3^{(1)} + g_3^{(2)},$$
 (6)

where $g_3^{(1)}$ arises from the energy derivative of the one-loop self-energy multiplied by Schwinger's correction $\Delta g = (\alpha/\pi)$,

$$g_3^{(1)} = \left(4\ln 2 - \frac{659}{64}\right)\frac{\alpha^2}{\pi}\alpha_Z^5,\tag{7}$$

and $g_3^{(2)}$ arises from the two-loop self-energy times the lowest order $g \rightarrow 2$.

Also the wave function of the electron is modified by the magnetic field. This effect, together with the coupling of **B** inside self-energy diagrams like in Fig. 1(a) provides the last SE correction g_4 .

To evaluate the three-loop diagrams required for $g_3^{(2)}$ and g_4 , we use the approach developed for the Lamb shift [31]. All three-loop diagrams are expressed in terms of 32 master integrals with the so-called Laporta algorithm [34,35] implemented in the program FIRE [36]. Results for the master integrals and details of their computation can be found in Ref. [31]. Separately gauge-dependent, $g_3^{(2)}$ and g_4 add up to give a gauge-invariant result,

$$g_3^{(2)} + g_4 = 12.816667(72)\alpha^2 \alpha_Z^5.$$
(8)

The total SE correction is the sum of Eqs. (5), (7), and (8),

$$g^{\rm SE} = 0.58735(9)\alpha^2 \alpha_Z^5. \tag{9}$$

We note the remarkable cancellation of sizable partial contributions to g^{SE} in this sum.

The next correction comes from light-by-light scattering diagrams, one example of which is Fig. 1(b). They can be viewed as a term in the external-field expansion of self-energy diagrams with a vacuum-polarization insertion. In principle, they can be calculated numerically along the lines of Ref. [25]. However, the numerical treatment of virtual (unbound) electrons is challenging. Thus, we include them here in the same manner as the SE corrections, again considering their Lamb-shift contribution and its energy dependence. Together with the direct magnetic field coupling effect, we find

$$g^{\text{LBL}} = -0.1724526(1)\alpha^2 \alpha_Z^5. \tag{10}$$

Diagrams with the external magnetic field coupling to the virtual electron loop are expected to be small [25]. In this class, we consider only the so-called magnetic loop contributions [37], examples of which are shown in Figs. 1(c) and 1(d). Their origin and evaluation differs from the diagrams we have discussed so far. Rather than modifying the response of the electron to a given external magnetic field, they represent the modification of the strength of the magnetic field caused by the electrostatic field of the nucleus.

There are three types of corrections to the leading-order magnetic loop result $\Delta g^{\text{ML}} = \frac{7}{216} \alpha \alpha_Z^5$ found in Ref. [37]. Like in Eq. (7), there is a one-loop SE correction on the main electron line that provides

$$g^{\text{MLSE}} = \frac{7}{432} \frac{\alpha^2}{\pi} \alpha_Z^5. \tag{11}$$

Diagrams with a virtual photon inside the electron loop, see, for example, Fig. 1(c), give

$$g^{\text{MLPH}} = \left(-\frac{7543}{16200} - \frac{303587}{10125\pi} + \frac{92368}{2025\pi}\ln 2\right)\alpha^2\alpha_Z^5.$$
(12)

The third magnetic-loop contribution comes from inserting a second electron loop in one of the Coulomb-photon propagators, as in Fig. 1(d),

$$g^{\rm MLVP} = \left(\frac{628}{8505\pi} - \frac{1}{54}\right) \alpha^2 \alpha_Z^5.$$
 (13)

The total magnetic-loop correction is the sum of Eqs. (11), (12), and (13),

$$g^{\rm ML} = 0.064387 \cdots \alpha^2 \alpha_Z^5,$$
 (14)

a small effect, as expected [25]. Finally, we sum Eqs. (9), (10), and (14) and get the total new correction

$$\Delta g^{(2,5)} = 0.479287(90)\alpha^2 \alpha_Z^5,\tag{15}$$

or, equivalently, a new contribution to b_{50} , defined in Eq. (4),

$$\Delta b_{50} = 4.7304(9). \tag{16}$$

The error estimate in this coefficient refers to the numerical uncertainty in the three-loop master integrals. We estimate the additional error due to the yet uncalculated vacuum-polarization (VP) diagrams at about 13% of the value in Eq. (16), on the basis of the part we did evaluate, Eq. (14). This error is presently negligible in comparison with unknown higher-order effects and we neglect it in the numerical analysis.

We note that the magnitude of the numerical coefficient in Eq. (15) is much smaller than in the previous order, see Eq. (2). This smallness may have complicated the experimental fit [15,16]. Our final result (16) has opposite sign but similar magnitude to the fitted result [15,16] b_{50} (fit) = -4.0(5.1). The difference between central values is 1.7 times the error assigned to the fit. Of course, the fit includes VP effects that we have not considered, but the known VP contributions are predominantly positive [25] and increase our discrepancy with the fit. On the other hand, the fit was done before the $O(\alpha_Z^2)$ light-by-light scattering effect was computed [27]; including it may improve the agreement [38].

How does the new correction in Eq. (15) influence the determination of the electron mass? In the case of the carbon ion, the relative size of the change in g is 2×10^{-12} . The atomic electron mass is directly proportional to g so this change increases m_e by the same relative amount, well below the current error of 3×10^{-11} [15,16], in absolute terms, by about 10^{-15} atomic mass units.

This stability of the electron mass should not be taken for granted. Partial results such as Eq. (8) correspond to relative shifts as large as 5×10^{-11} , larger than the current uncertainty in m_e . They have, however, been canceled by other effects such as $g^{\text{SE;Lamb}}$ in Eq. (5).

In Table I we summarize results for hydrogenlike helium, carbon, and silicon ions. The first line corresponds to Breit's formula (1). The second line includes additionally all known corrections preceding this work, as given in Ref. [16]: finite nuclear size [39], one-loop QED corrections obtained by combining numerical and analytical computations [22,26,37,40–48], two-loop QED corrections evaluated up to order α_Z^4 [27,46,47], higher order terms for diagrams with vacuum polarization insertions [25], three and more QED loops up to order α_Z^2 [3], recoil and radiative recoil [49–51] (see also Ref. [52]), nuclear polarizability [53] and susceptibility [54], as well as leading weak [55] and hadronic effects [56,57].

Contribution	⁴ He ⁺	$^{12}C^{5+}$	²⁸ Si ¹³⁺	Source
Dirac/Breit value + other known corrections g ^{SE} g ^{LBL} M	1.999 857 988 825 37(6) 2.002 177 406 711 41(55) 0.000 000 000 000 002 -0.000 000 000 000 01	1.998 721 354 392 1(6) 2.001 041 590 168 6(12) 0.000 000 000 005 0 -0.000 000 000 001 5	1.993 023 571 557(3) 1.995 348 957 825(39) 0.000 000 000 348 -0.000 000 000 102	Ref. [20] Refs. [16,22] ⁴ This work This work
$\frac{g^{\text{WL}}}{(\alpha/\pi)^2 \alpha_Z^6 \ln^3 \alpha_Z^{-2}}$ Total	0.000 000 000 000 000 00 0.000 000 000 0	0.000 000 000 000 6 0.000 000 000 000 0(93) 2.001 041 590 172 7(94)	0.000 000 000 038 0.000 000 000 000(583) 1.995 348 958 109(584)	This work

TABLE I. Bound electron g factor for helium, carbon, and silicon ions. The error related to missing higher order contributions is estimated by $(\alpha/\pi)^2 \alpha_5^2 \ln^3 \alpha_7^{-2}$.

^aThe only change with respect to Ref. [16] is that we used the new evaluation of Ref. [22] for the one-loop corrections.

For carbon and silicon the theoretical error in the second row of Table I is dominated by the finite nuclear size effects, whose error is respectively $\delta g = 7 \times 10^{-13}$ and $\delta g = 31 \times 10^{-12}$. For helium, the main uncertainty comes from the poorly known one-loop corrections extrapolated from numerical computation.

We estimate the remaining error due to still missing higher order terms by the leading logarithm $(\alpha/\pi)^2 \alpha_Z^6 \ln^3 \alpha_Z^{-2}$. In carbon and silicon, this logarithmic term exceeds other uncertainties as well as our correction. It also exceeds the uncertainty estimated in Ref. [16], where for Si ion the error was 139×10^{-12} .

It may seem ironic that after all the effort of computing Δb_{50} our predictions for *g* have larger uncertainties than before our work. We believe however that this conservative treatment of unknown higher orders is necessary.

In Ref. [15], b_{50} was fitted and the higher-order terms were neglected. This procedure raises some concerns since the next term b_{63} is logarithmically enhanced. For small Z, that enhancement may overshadow the b_{50} term. Yet, with experimental results available only for carbon and silicon it was impossible to constrain that higher-order term. Now that the b_{50} term is at hand, one can fit the logarithmically enhanced term b_{63} while neglecting parametrically suppressed terms starting from b_{62} .

In this way, our result will help derive full benefit from future measurements of g factors, an effort we admire and encourage.

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