One-loop binding corrections to the electron *g* factor

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We calculate the one-loop electron self-energy correction of order $\alpha\,(Z\,\alpha)^5$ to the bound-electron g factor. Our result is in agreement with the extrapolated numerical value and paves the way for the calculation of the analogous, but as yet unknown, two-loop correction.

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I. INTRODUCTION

The g factor of a bound electron is the coupling constant of the spin to an external, homogeneous magnetic field. In natural units $\hbar = c = \varepsilon_0 = 1$, it is defined by the relation

$$\delta E = -\frac{e}{2\,m}\,\langle\vec\sigma\,\vec B\rangle\,\frac{g}{2}\,, \tag{1}$$

where δE is the energy shift of the electron due to the interaction with the magnetic field $\vec B$, m is the mass of the electron, and e is the electron charge ($e<0$). It was found long ago [1] that in a relativistic (Dirac) theory, the g factor of a bound electron differs from the value $g=2$ due to the so-called binding corrections. For an nS state, they are given by

$$g = \frac{2}{3}\left(1+2\,\frac{E}{m}\right) = 2-\frac{2}{3}\,\frac{(Z\,\alpha)^2}{n^2} + \left(\frac{1}{2\,n}-\frac{2}{3}\right)\frac{(Z\,\alpha)^4}{n^3}+\cdots\,, \tag{2}$$

where E is the Dirac energy. In addition, there are many QED corrections, and the dominant one comes from the so-called electron self-energy. When expanded in powers of $Z\,\alpha$ the one-loop electron self-energy correction reads (for the nS state)

$$g_{\rm SE} = \frac{\alpha}{\pi}\biggl[1+\frac{(Z\,\alpha)^2}{6\,n^2}+\frac{(Z\,\alpha)^4}{n^3}\left(\frac{32}{9}\,\ln[(Z\,\alpha)^{-2}]+b_{40}(n)\right) + \frac{(Z\,\alpha)^5}{n^3}\,b_{50}+\frac{(Z\,\alpha)^6}{n^3}(b_{62}\,\ln^2[(Z\,\alpha)^{-2}] + b_{61}(n)\,\ln[(Z\,\alpha)^{-2}]+b_{60}(n))+\cdots\biggr], \tag{3}$$

where $b_{40}(1S) = -10.236\,524\,32$ [2,3], $b_{50} = 23.6(5)$ [4], and higher-order coefficients remain unknown. What is approximately known, however, is the sum of b_{50} and higher-order terms for individual nuclear charges from all-order numerical calculations [4–7]. The subject of this work is the one-loop electron self-energy correction of the order of $\alpha\,(Z\,\alpha)^5$, namely, the coefficient b_{50}. Although it has been obtained by extrapolation of numerical results, we aim to calculate it directly, in order to find out the best approach for the analogous two-loop contribution, which currently is the main source of the uncertainty of theoretical predictions. Due to extremely accurate measurements in hydrogenlike carbon [8], the bound-electron g factor is presently used for the most accurate determination of the electron mass [9], and in the future it can be used for determination of the fine structure constant [10] and for precision tests of the standard model.

II. $\alpha\,(Z\,\alpha)^5$ CORRECTION TO THE LAMB SHIFT

Before turning to the g factor we present a simple derivation of the analogous correction to the Lamb shift as proof of concept because the computational approach for the g factor will be very similar. The one-loop electron self-energy contribution to the Lamb shift is

$$E_{\rm SE} = e^2\int\frac{d^4k}{(2\,\pi)^4\,i}\,\frac{1}{k^2}\,\langle\bar\psi|\gamma^\mu\,\frac{1}{\not p+\not k-\gamma^0\,V-m}\,\gamma_\mu|\psi\rangle, \tag{4}$$

where $V=-Z\,\alpha/r$. The $(Z\,\alpha)^5$ contribution is obtained from the hard two-Coulomb exchange

$$E^{(5)}_{\rm SE} = e^2\,\phi^2(0)\,(Z\,\alpha)^2\int\frac{d^3q}{(2\,\pi)^3}\,\frac{f(\vec q^{\,2})}{\vec q^{\,4}}, \tag{5}$$

$$f(\vec q^{\,2}) = \int\frac{d^4k}{i\,\pi^2}\,\frac{1}{k^2}{\rm Tr}\biggl[(T_1+2\,T_2+T_3)\left(\frac{\gamma^0+I}{4}\right)\biggr], \tag{6}$$

where

$$T_1 = \gamma^\mu\,\frac{1}{\not t+\not k-m}\,\gamma^0\,\frac{1}{\not t+\not k+\not q-m}\,\gamma^0\,\frac{1}{\not t+\not k-m}\,\gamma_\mu,$$
$$T_2 = \gamma^0\,\frac{1}{\not t+\not q-m}\,\gamma^\mu\,\frac{1}{\not t+\not k+\not q-m}\,\gamma^0\,\frac{1}{\not t+\not k-m}\,\gamma_\mu,$$
$$T_3 = \gamma^0\,\frac{1}{\not t+\not q-m}\,\gamma^\mu\,\frac{1}{\not t+\not k+\not q-m}\,\gamma_\mu\,\frac{1}{\not t+\not q-m}\,\gamma^0, \tag{7}$$

and where $t=(m,0,0,0)$, $t\,q=0$, and $q^2=-\vec q^{\,2}$. Equation (5) as it stands is divergent at small $\vec q^{\,2}$. One subtracts leading terms in small $\vec q^{\,2}$, which correspond to lower-order contributions to the Lamb shift, so $f(\vec q^{\,2})\sim\vec q^{\,2}$, and

$$f(\vec q^{\,2}) = \vec q^{\,2}\int d(p^2)\,\frac{1}{p^2\,(\vec q^{\,2}+p^2)}\,f^A(p^2), \tag{8}$$

function f can be expressed in terms of its imaginary part f^A on a cut $\vec q^{\,2}<0$,

$$f^A(p^2) = \frac{f(-p^2+i\,\epsilon)-f(-p^2-i\,\epsilon)}{2\,\pi\,i}. \tag{9}$$

The correction to energy in terms of f^A becomes

$$E^{(5)}_{\rm SE} = e^2\,\phi^2(0)\,(Z\,\alpha)^2\int\frac{d\,p}{2\,\pi}\,\frac{f^A(p^2)}{p^2}. \tag{10}$$

The imaginary part f^A is much easier to evaluate because it does not involve any infrared or ultraviolet divergences in

k and has a much simpler analytic form than the f itself. The calculations go as follows. Traces are performed with FEYNCALC package [11]. The resulting expression is a linear combination of fractions with the numerator containing powers of k^2, q^2, $k\,t$, and $k\,q$, while $q\,t$ vanishes. Any k in the numerator can be reduced with the denominator with the help of

$$k\,q = \tfrac{1}{2}\,[(k+q+t)^2 - (k+t)^2 - q^2]\,, \quad k\,t = \tfrac{1}{2}\,[(k+t)^2 - k^2 - q^2]\,. \tag{11}$$

The resulting expression is a linear combination of

$$\frac{1}{i\,\pi^2}\int d^4k\,\frac{1}{[k^2]^n\,[(k+t)^2-1]^m\,[(k+t+q)^2-1]^l}, \tag{12}$$

with integers $n,m,l \geqslant 0$. Next, the powers n,m,l are reduced to 1 or 0 using integration by parts identities

$$\int d^4k\,\frac{\partial}{\partial k^\mu}\,\frac{p^\mu}{[k^2]^n\,[(k+t)^2-1]^m\,[(k+t+q)^2-1]^l} = 0, \tag{13}$$

with $p = k,q,t$. The resulting expression contains the integral

$$J = \frac{1}{i\,\pi^2}\int d^4k\,\frac{1}{k^2\,[(k+t)^2-1]\,[(k+t+q)^2-1]} \tag{14}$$

and simpler integrals without any of these denominators. Analytic expressions for all such integrals can be taken from [12], but it is much easier to calculate the imaginary part using Feynman parameters. For example, the imaginary part of the J integral is

$$J^A(p^2) = \frac{1}{p}\left[\arctan(p) - \Theta(p-2)\,\arccos\left(\frac{2}{p}\right)\right]. \tag{15}$$

Using J^A and simpler formulas for other integrals, the result for f^A is

$$f^A(p^2) = \frac{7}{3} - \frac{16}{p^2} - \frac{1}{1+p^2} + \left(\frac{16}{p^3} + \frac{4}{p} - p\right)\arctan(p) + 4\left(1 + \frac{1}{p^2} - \frac{12}{p^4}\right)\frac{\Theta(p-2)}{\sqrt{1-4/p^2}} - \left(\frac{16}{p^3} + \frac{4}{p} - p\right)\Theta(p-2)\,\arccos\left(\frac{2}{p}\right). \tag{16}$$

The one-dimensional integration in Eq. (10) leads to

$$\int \frac{d\,p}{2\,\pi}\,\frac{f^A(p^2)}{p^2} = \frac{139}{128} - \frac{\ln 2}{2} \equiv C. \tag{17}$$

Finally, the result for the $\alpha\,(Z\,\alpha)^5$ electron self-energy contribution to the Lamb shift

$$E^{(5)}_{\rm SE} = m\,\frac{\alpha\,(Z\,\alpha)^5}{n^3}\,4\,C \tag{18}$$

is in agreement with the well-known value [9,13]. The same integration technique is used in the next section for the evaluation of the analogous correction to the g factor.

III. $\alpha\,(Z\,\alpha)^5$ CORRECTION TO THE g FACTOR

The one-loop correction to the g factor is similar to Eq. (4)

$$\delta E = e^2\int\frac{d^4k}{(2\,\pi)^4 i}\,\frac{1}{k^2} \times\langle\bar\psi|\gamma^\mu\,\frac{1}{\not p + \not k - e\,\not A - \gamma^0 V - m}\gamma_\mu|\psi\rangle, \tag{19}$$

where ψ is the electron wave function which includes perturbation due to external magnetic field A, and p^0 includes the corresponding energy shift

$$p_0 = E + \langle\bar\psi|e\,\not A|\psi\rangle. \tag{20}$$

The $(Z\,\alpha)^5$ contribution is given in analogy to the Lamb shift, by the hard two-Coulomb exchange

$$\begin{aligned}\delta E^{(5)} = e^2\int\frac{d^4k}{(2\,\pi)^4\,i}\,\frac{1}{k^2}\,\langle\bar\psi|\gamma^\mu\,&\frac{1}{\not p + \not k - e\,\not A - m}\,\gamma^0\,V\,\frac{1}{\not p + \not k - e\,\not A - m}\,\gamma^0\,V\,\frac{1}{\not p + \not k - e\,\not A - m}\,\gamma_\mu\\ &+ 2\,\gamma^0\,V\,\frac{1}{\not p - e\,\not A - m}\,\gamma^\mu\,\frac{1}{\not p + \not k - e\,\not A - m}\,\gamma^0\,V\,\frac{1}{\not p + \not k - e\,\not A - m}\,\gamma_\mu\\ &+ \gamma^0\,V\,\frac{1}{\not p - e\,\not A - m}\,\gamma^\mu\,\frac{1}{\not p + \not k - e\,\not A - m}\,\gamma_\mu\,\frac{1}{\not p + \not k - e\,\not A - m}\,\gamma^0\,V|\psi\rangle,\end{aligned} \tag{21}$$

and by the expansion in A and in the momentum carried by A. The expansion of ψ in A is not very trivial. Since only the low momenta of the wave function ψ contribute to $(Z\,\alpha)^5$ we apply the Foldy-Wouthuysen transformation in the presence of the magnetic field

$$S = -\frac{i}{2\,m}\,\vec\gamma\cdot\vec\pi, \tag{22}$$

and the wave function can be represented as

$$|\psi\rangle = e^{-{\rm i}\,S}\left|\begin{matrix}\phi\\0\end{matrix}\right\rangle = \left(I - \frac{1}{2\,m}\,\vec\gamma\,\vec\pi + \frac{e}{8\,m^2}\,\vec\sigma\,\vec B\right)\left|\begin{matrix}\phi\\0\end{matrix}\right\rangle, \tag{23}$$

where ϕ is the spinor wave function which corresponds to the transformed Hamiltonian

$$H' = e^{{\rm i}\,S}\,(H - i\,\partial_t)\,e^{-{\rm i}\,S} = \frac{p^2}{2\,m} - \frac{Z\,\alpha}{r} - \frac{e}{2\,m}\,\vec\sigma\,\vec B\left(1 - \frac{p^2}{2\,m^2} + \frac{Z\alpha}{6\,m\,r}\right). \tag{24}$$

We are now ready to perform an expansion in $\not A$ of Eq. (21), and split $\delta E^{(5)}$ in four parts

$$\delta E^{(5)} = E_1 + E_2 + E_3 + E_4\,. \tag{25}$$

E_1 comes from the last term in Eq. (23)

$$E_1 = \frac{e}{4\,m^2}\,\langle\vec{\sigma}\cdot\vec{B}\rangle\,E^{(5)} = -\frac{e}{2\,m}\,\langle\vec{\sigma}\cdot\vec{B}\rangle\,\frac{g_1}{2}, \tag{26}$$

where

$$g_1 = -\frac{E^{(5)}}{m} = -\frac{\alpha\,(Z\,\alpha)^5}{n^3}\,4\,C\,. \tag{27}$$

E_2 comes from perturbation of ϕ due to the last term in the transformed Hamiltonian (24)

$$E_2 = \frac{e}{m}\,\langle\vec{\sigma}\cdot\vec{B}\rangle\,C\,\alpha\,(Z\,\alpha)^5\left\langle\frac{5}{6\,r}\,\frac{1}{(E-H)'}\,4\,\pi\,\delta^{(3)}(r)\right\rangle, \tag{28}$$

where $p^2/2$ is replaced by $1/r$. Since

$$\frac{1}{(E-H)'}\,\frac{1}{r}\,\phi = -\frac{\partial}{\partial\alpha}\,\phi, \tag{29}$$

the above matrix element is

$$\left\langle\frac{1}{r}\,\frac{1}{(E-H)'}\,4\,\pi\,\delta^{(3)}(r)\right\rangle = -\frac{6}{n^3}\,, \tag{30}$$

and g_2 becomes

$$g_2 = \frac{\alpha\,(Z\,\alpha)^5}{n^3}\,20\,C\,. \tag{31}$$

E_3 comes from expansion of Eq. (21) in $p_0 - m = -e\,\langle\vec{\sigma}\,\vec{B}\rangle/(2\,m)$,

$$E_3 = -\frac{e}{2\,m}\,\langle\vec{\sigma}\cdot\vec{B}\rangle\,e^2\,\phi^2(0)\,(Z\,\alpha)^2\,C'\,, \tag{32}$$

where

$$\begin{aligned} C' &= \frac{\partial}{\partial E}\bigg|_{E=1}\int\frac{d^3q}{(2\,\pi)^3}\,\frac{1}{\vec{q}^{\,4}}\int\frac{d^4k}{i\,\pi^2}\,\frac{1}{k^2} \\ &\quad\times\mathrm{Tr}\left[(T_1+2\,T_2+T_3)\left(\frac{\gamma^0+I}{4}\right)\right] \\ &= -\frac{659}{256}+\ln(2)\,, \end{aligned} \tag{33}$$

and where T_i are defined in Eq. (7) with $t=(E,0,0,0)$. The corresponding correction to the g factor is

$$g_3 = \frac{\alpha\,(Z\,\alpha)^5}{n^3}\,8\,C'\,. \tag{34}$$

The last term E_4 comes from the expansion of $\delta E^{(5)}$ in $\vec{\gamma}\cdot\vec{A}$. A typical contribution is of the form

$$\begin{aligned} E_4 &= e^2\int\frac{d^4k}{i\,\pi^2}\,\frac{1}{k^2}\int\frac{d^3p}{(2\,\pi)^3}\,\frac{Z\,\alpha}{(-\vec{p}-\vec{q}/2)^2}\,\frac{Z\,\alpha}{(\vec{p}-\vec{q}/2)^2}\,\phi^2(0)\,e\,i\,\epsilon^{ijk}\,\sigma^k \\ &\quad\times\mathrm{Tr}\left[\gamma^\mu\,\frac{1}{\not t+\not k-m}\,\gamma^0\,\frac{1}{\not t+\not p+\not q/2+\not k-m}\,\not A(q)\,\frac{1}{\not t+\not p-\not q/2+\not k-m}\,\gamma^0\,\frac{1}{\not t+\not k-m}\,\gamma_\mu\,\frac{(\gamma^0+I)}{16}\,[\gamma^i\,,\gamma^j]\right]+\cdots, \end{aligned} \tag{35}$$

where by dots we denote all other diagrams. In addition, we perform an expansion in the momentum $\vec{q}$ transferred by A and obtain

$$\begin{aligned} E_4 &= e^2\,(Z\,\alpha)^2\,\phi^2(0)\,C''\,(A^i\,q^j - A^j\,q^i)\,e\,i\,\epsilon^{ijk}\,\sigma^k \\ &= -2\,e^2\,(Z\,\alpha)^2\,\phi^2(0)\,C''\,e\,\vec{\sigma}\,\vec{B}, \end{aligned} \tag{36}$$

where

$$C'' = \frac{281}{1024}+\frac{\ln(2)}{12}\,. \tag{37}$$

The corresponding correction to the g factor is

$$g_4 = \frac{\alpha\,(Z\,\alpha)^5}{n^3}\,32\,C''\,. \tag{38}$$

The total $\alpha\,(Z\,\alpha)^5$ contribution to the bound-electron g factor is the sum of individual corrections, namely,

$$\begin{aligned} g^{(5)} &= g_1+g_2+g_3+g_4 \\ &= \frac{\alpha\,(Z\,\alpha)^5}{n^3}\,(16\,C+8\,C'+32\,C'') \\ &= \frac{\alpha\,(Z\,\alpha)^5}{n^3}\left(\frac{89}{16}+\frac{8\,\ln(2)}{3}\right). \end{aligned} \tag{39}$$

The numerical value for the coefficient multiplied by π is $b_{50} = 23.282\,005$, in agreement with Yerokhin's very recent result of 23.6(5) [4]. However, what is not in agreement is the difference for $b_{50}(2S) - b_{50}(1S)$, which according to our calculations vanishes, but Yerokhin *et al.* [4] give 0.12(5). All the assumptions in performing the fit in Ref. [4] were correct, so this small discrepancy needs further investigation.

IV. SUMMARY

We have calculated the one-loop electron self-energy contribution of order $\alpha\,(Z\,\alpha)^5$ to the bound-electron g factor, and found that it is state independent. The principal result, however, is a presentation of the computational approach, which can be extended to the yet unknown two-loop correction. This correction is presently the main source of theoretical uncertainty. The extension of the direct one-loop numerical calculation to the two-loop case is presently out of reach. In contrast, the analytic approach with an expansion in $Z\,\alpha$ is technically as difficult as the two-loop self-energy correction to the Lamb shift, which has been known for some time [13].

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