Magnetic moment of a bound electron

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Theoretical predictions underlying determinations of the fine structure constant \( \alpha \) and the electron-to-proton mass ratio \( m_e/m_p \) are reviewed, with the emphasis on the bound electron magnetic anomaly \( g - 2 \). The theory of the interaction of hydrogen-like ions with a magnetic field is discussed. The status of efforts aimed at the determination of \( O(\alpha(Z\alpha)^5) \) and \( O(\alpha^2(Z\alpha)^5) \) corrections to the \( g \) factor is presented. The reevaluation of analogous corrections to the Lamb shift and the hyperfine splitting is summarized.

1. Introduction

The world of our everyday experience is largely controlled by two dimensionless fundamental quantities: the fine structure constant \( \alpha \simeq 1/137 \) and the electron-to-proton mass ratio \( m_e/m_p \simeq 1/1836 \). The former describes the strength of the electromagnetic interaction. The two together relate the energy of atomic excitations to the bulk of the atomic mass.

Among the myriads of phenomena governed by these two constants, only a handful are suitable for their precise determination. Two characteristics are required: they have to be amenable to measurements and they must be theoretically very well understood. Most of such systems consist of only one, two, or three bodies.

In this talk we focus on the theoretical aspects of hydrogen-like ions. Measurements of their interaction with the magnetic field are a crucial ingredient in the best determination of \( m_e/m_p \), and indirectly help to determine \( \alpha \) with the second-best accuracy.

We first briefly review the present knowledge of both constants, to illustrate the level of accuracy already achieved. A system of ultimate simplicity is a single electron. It is studied with the Penning trap where it forms what is sometimes called a geonium atom \([1]\). The spectrum of lowest lying states is sensitive to the electron anomalous magnetic moment, \( g - 2 \), and thus to \( \alpha \) through the theoretical expression

\[
a = \frac{g - 2}{2} = 1 + \sum_{i=1}^{\infty} C_i \left( \frac{\alpha}{\pi} \right)^i + \Delta a,
\]

where \( C_i \) are the coefficients determined from an \( i \)-loop correction to the interaction of an electron with a weak homogeneous magnetic field, calculated in quantum electrodynamics (QED); and \( \Delta a \) are small corrections due to weak interactions and hadronic effects. The QED effects are now being studied at five-loops \([2,3]\). Indeed, the missing information about \( C_5 \) is the leading error in the present best value of \( \alpha \) \([4]\),

\[
\alpha^{-1}(g - 2) = 137.035999084(39)_{\text{th}}(33)_{\text{exp}}. \tag{2}
\]

The relative uncertainty of this evaluation is 0.37 part per billion (ppb).

The Penning trap can also be used to measure \( m_e/m_p \) by comparing the cyclotron frequency \( \omega_c = eB/m \) of an electron with that of a proton. The best value obtained in this way is accurate to 2.2 ppb \([5]\).

\[
\frac{m_p}{m_e}(\text{free } e^-) = 1836.1526665(40). \tag{3}
\]

The systematic limitation of this determination is the relativistic shift of the electron mass due to thermal excitations of the magnetron motion of the electron. For this reason, studies of electrons bound in a heavier ion, that will be discussed below, are superior: the thermal velocity of such a
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heavy system is eliminated as the source of relevant errors.

The second-best method for finding $\alpha$ is based on the excellent knowledge (to within 0.007 ppb) of the Rydberg constant [6],

$$R_\infty \equiv \frac{\alpha^2 m_e c}{2 \hbar} = 10973.731.568.527(73)/m,$$  (4)

where $\hbar$ denotes the Planck constant and $c$ the velocity of light. The latter being an exact number, $\alpha$ can be determined if the ratio of the electron mass to the Planck constant is measured. Such a direct measurement is difficult, but it is possible to measure the ratio of an atom mass $m_{\text{atom}}$ to $\hbar$ for atoms such as cesium and rubidium [7,8]. Then, if $m_e/m_p$ and $m_p/m_{\text{atom}}$ are known, one can determine $\alpha$. (This underscores again the importance of $m_e/m_p$.)

The best value obtained in this way, with rubidium atoms, is

$$\alpha^{-1}(\text{Rb}) = 137.035\,999\,450(620),$$  (5)

a 4.6 ppb determination. Efforts to reduce this error to about 1 ppb are being undertaken [9].

A macroscopic effect that competes with the atomic scale phenomena in the possible accuracy of determining $\alpha$ is the quantum Hall effect [10], giving the value

$$\alpha^{-1}(\text{QHE}) = 137.036\,003\,700(3300),$$  (6)

whose uncertainty is 23 ppb.

The last method for $\alpha$ that we want to mention here is based on the comparison of the measurement [11] of the fine structure of helium with QED predictions [12], having at present a 31 ppb uncertainty,

$$\alpha^{-1}(\text{He}) = 137.036\,001\,900(3900)_{\text{th}}(1600)_{\text{exp}}.$$  (7)

2. Bound electron $g$ factor

2.1. Binding effects in $g - 2$

We now focus on one system: an electron bound in a hydrogen-like ion. We discuss its theoretical description, explain how the ion is used to determine the electron-to-proton mass ratio, and discuss prospects for improvements of the theoretical predictions.

Consider an ion consisting of a nucleus with zero spin and a single electron. We will be interested here in the ground state of this ion. Since the nucleus has no magnetic moment, the magnetic interaction of this system is very similar to that of a free electron, modulo small binding effects. We define the bound-electron gyromagnetic ratio $g$ by the correction to the energy of the ion, linear in the magnetic field $B$. In the ground...
state, the whole magnetic moment \( \mathbf{\mu} \) of the ion is due to the electron’s spin \( s \), so the energy shift is

\[
\delta E = -\langle \mathbf{\mu} \cdot \mathbf{B} \rangle = g \frac{e}{2m_e} \sigma \cdot \mathbf{B},
\]

where \(-e\) is the electron’s charge. The expectation value is to be calculated with the wave function of the ion.

In the lowest order, neglecting all effects except the Coulomb field, \( g \) was calculated \[16\] already in 1928, in one of the first applications of the Dirac equation \[17\]. To illustrate the influence of binding effects, we reproduce here that result, treating the interaction with the external magnetic field as a perturbation. A uniform field is described by the vector potential \( \mathbf{A} = \frac{1}{2} \mathbf{B} \times \mathbf{r} \), and the correction to the energy is

\[
\delta E (\text{Coulomb}) = e \int d^3\mathbf{r} \psi \mathbf{A} \cdot \gamma \psi,
\]

where \( \psi \) is the solution of the Dirac equation with the Coulomb potential \( V(r) = -\frac{Z\alpha}{r} \). Here \( Z \) is the number of protons in the ion’s nucleus and \( \mathbf{r} \) describes the position of the electron relative to the nucleus (we assume the nucleus to be very heavy and motionless). The ground state wave function can be written in the form \[18\]

\[
\psi(r) = f(r) \left( 1 + i\gamma^5 \Sigma \cdot \dot{\mathbf{r}} \right) \psi,
\]

where \( f(r) = N r^{-2Z\alpha} \exp(-Zam_e r) \),

\[
\gamma = 1 - \sqrt{1 - (Z\alpha)^2} \approx \frac{Z\alpha}{2},
\]

where \( \psi \) is a spinor such that \( \psi^\dagger \psi = 1 \) and \( N \) is a normalization constant such that

\[
(1 + \gamma^2) \int d^3 r f^2 = 1.
\]

\( N \) approximately equals the value of the non-relativistic Coulomb wave function at the origin, \( N^2 \approx \left( \frac{Zam_e}{2} \right)^2 \). In the standard (Dirac) representation, \( \Sigma = \left( \begin{array}{cc} \sigma & 0 \\ 0 & \sigma \end{array} \right) \) and \( \gamma^5 = \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \).

With this wave function, we find

\[
\delta E = \frac{8\pi}{3} e\gamma (v^s \mathbf{B} \cdot \sigma v) \int_0^\infty dr r^3 f^2(r).
\]

Radial integrals of this type are

\[
\int_0^\infty dr r^n f^2(r) = (2Zam_e)^2 \frac{\Gamma(n + 1 - 2Z\alpha \gamma)}{4\pi (1 + \gamma^2) \Gamma(3 - 2Z\alpha \gamma)},
\]

leading to

\[
g (\text{Coulomb}) = \frac{2}{3} \left( 1 + 2 \sqrt{1 - (Z\alpha)^2} \right),
\]

the result first obtained by Breit \[16\].

### 2.2. Mixed binding-selfinteraction effects

In view of recent precise measurements with hydrogen-like ions, a variety of corrections have recently been studied, including electron selfinteraction loops \[19,20\], vacuum polarization \[21,22,23\], and recoil corrections \[24,25\]. Some effects have been determined to all orders in \( Z\alpha \) \[26,27,28,29\] while for others a few terms of the expansion around small \( Z\alpha \) have been calculated.

Here we take the nucleus to be infinitely heavy and neglect small hadronic and weak effects. The theoretical prediction for \( g \) in this limit can be organized as a double series expansion in \( \alpha/\pi \) (describing electron selfinteraction) and \( Z\alpha \), describing interactions between the electron and the nucleus, i.e., the binding effects.

If we neglect selfinteractions, \( g \) is given by Breit’s result \[14\]. On the other hand, if we neglect the binding, \( g \) is the same as for a free electron, \( g = 2 + 2a \), with the anomaly \( a \) described by eq. \[1\].

The interplay of the two types of effects occurs first at the order \( O \left( \frac{\alpha}{\pi} (Z\alpha)^2 \right) \). Interestingly, at this order in \( Z\alpha \), the correction is universal to all orders in \( \alpha \). It is found by considering the magnetic interaction of a bound particle, taking into account its anomalous magnetic moment. The result is \[30,31\]

\[
\delta g = 2a \left( 1 + \frac{(Z\alpha)^2}{8} \right),
\]

where \( a \) is given in \[1\].

There are no effects linear or cubic in \( Z\alpha \), but beginning with \( (Z\alpha)^4 \) all higher powers are present. In fact, in the approximation of a single-photon electron selfinteraction, it is possible to use the exact form of the electron propagator in the Coulomb field and numerically determine effects of \( O \left( \frac{\alpha}{\pi} (Z\alpha)^n \right) \) to all orders \( n \) \[26,27,28\].
It is still very interesting to compute analytically the coefficients of the $Z\alpha$ expansion to check the numerical evaluation. Such a calculation was performed for the terms $\frac{\alpha}{\pi}(Z\alpha)^4$ and $\frac{\alpha}{\pi}(Z\alpha)^4 \ln Z\alpha$ only in 2004 [19], which illustrates the difficulty of performing even one-loop calculations for bound particles.

The situation becomes even harder when two selfinteraction loops are included. In this case no numerical all-order study has been performed. The terms $(\frac{\alpha}{\pi})^2(Z\alpha)^4$ and $(\frac{\alpha}{\pi})^2(Z\alpha)^4 \ln Z\alpha$ are already known [20]. Together with measurements with carbon ions [32] the resulting theoretical prediction provides the best value of the electron-to-proton mass ratio,

$$\frac{m_p}{m_e} = 1836.152 672 9(10)$$

where we have used the CODATA recommended value of the proton mass in atomic units, $m_p = 1.00727646677(10)u$, which contributes an order of magnitude less to the uncertainty in (15) than the electron. We see that the error in (15) is four times smaller than in the determination using a free electron, eq. (3).

The uncertainty in (15) is dominated by the experiment; the theory is estimated to contribute only about three per cent of the total error. The reliability of the theoretical prediction is based on the numerical knowledge of higher-order binding effects in the one-loop selfinteraction.

It is thus very important to independently check the numerical studies by computing further terms in the $Z\alpha$ expansion. In particular, the coefficient of the contribution $\frac{\alpha}{\pi}(Z\alpha)^5$ to $g$ (for the principal quantum number $n = 1$, that is the ground state) is estimated to be $H_1(Z = 0) = 23.15(10)$ [23], in the notation of [26].

The two-loop effect $(\frac{\alpha}{\pi})^2(Z\alpha)^5$ is estimated to have the coefficient between $-118$ and $-75$ [23].

In order to verify these predictions, we have undertaken an explicit determination of the coefficients of $(Z\alpha)^5$ terms at one and two-loop selfinteraction level. In the next section we present some details of our method with examples of simpler observables, not involving an external magnetic field: the Lamb shift in hydrogen-like ions, and the hyperfine splitting (HFS) in muonium.

### 3. Lamb shift and hyperfine splitting

In this section we describe our calculations of the radiative-nonrecoil corrections to the Lamb shift [31] and the hyperfine splitting [35] of hydrogen-like atoms. In both cases the shift of the energy levels is given by a delta function potential, which affects only $S$ states,

$$\delta E = -M |\psi(0)|^2 = -M \frac{(Z\alpha\mu)^3}{\pi n^3}. \quad (16)$$

$\psi(0)$ is the wave function of a bound $S$ state with principal quantum number $n$ and reduced mass $\mu$ at the origin. The amplitude $M$ is determined from the corresponding Feynman diagrams. Sample diagrams are shown in Fig. 2.

![Figure 2](image)

**Figure 2.** Sample diagrams for the Lamb shift and hyperfine splitting at order $\alpha^2(Z\alpha)^5$. Solid and wavy lines denote electrons and photons. The dotted lines denote the interaction with the nucleus (cf. Fig 3).

The interaction of the electron with the nucleus is depicted in Fig. 3. In our calculation we construct an expansion in the ratio of electron and nucleus mass, using the method of expansion by regions [36]. We are only interested in the leading term, which is given by the region where all loop momenta are of the order of the electron mass. Expanding the nucleus propagators we find
that to leading order the only difference between the diagrams with direct and crossed photon exchange is an overall sign and the sign of the \(\epsilon\) prescription of the latter. We have

\[
\frac{1}{(q+k)^2 - M^2 + i\epsilon} + \frac{1}{(q-k)^2 - M^2 + i\epsilon} \\
\rightarrow \frac{1}{2q \cdot k + i\epsilon} - \frac{1}{2q \cdot k - i\epsilon} + \ldots \\
= -\frac{2\pi}{2} \delta(2q \cdot k) + \ldots,
\]

where the ellipses stand for higher order terms. \(q\) and \(M\) are the momentum and mass of the nucleus with \(q^2 = M^2\), and \(k\) is the loop momentum. In the rest frame of the nucleus, the factor \(\delta(2q \cdot k) = \delta(k_0)/2M\) ensures that the photons exchanged between the electron and the nucleus carry no energy. The integration over the loop denoted with the dotted line in the Feynman diagrams in the Figures is only over the spatial components \(\vec{k}\).

Our calculation is automated to a large extent. We use the program QGRAF [37] to generate all Feynman diagrams. These are turned into FORM-readable [38] expressions by Q2E and EXP [39,40]. The program MATAD3 [41] is used to perform the traces and express the amplitude \(\mathcal{M}\) in terms of scalar integrals, using custom made routines. Finally, we use integration-by-parts identities [42,43] to express all scalar integrals in terms of 32 so-called master integrals. This is achieved with the help of the program FIRE [44], which implements the so-called Laporta algorithm [45,46]. Results for all master integrals and details of their calculation are given in Ref. [34].

4. Conclusions

Our results for the Lamb shift and hyperfine splitting at order \(\alpha^2(Z\alpha)^5\) are

\[
\delta E_{\text{Lamb}} = -6.86100(4) \frac{\alpha^2(Z\alpha)^5}{\pi n^3} \left(\frac{\mu}{m_e}\right)^3 m_e, \\
\delta E_{\text{HFS}} = 0.77099(2) \frac{\alpha^2(Z\alpha)^5}{\pi n^3} E_F,
\]

respectively. \(E_F = (8\mu^3(Z\alpha)^4 g_N)/(6m_e M)\) is the Fermi energy. \(g_N\) is the gyromagnetic factor of the nucleus. Our results improve the precision of the previous results in [47] by more than an order of magnitude. Results for individual diagrams, including new analytical results, are given in Refs. [34,35].

Our new results agree very well with [47], which gives us confidence in the values of master integrals we have derived. The same set of 32 integrals is sufficient to compute the bound electron \(g\) factor to the desired accuracy, \((Z\alpha)^5\). The only remaining obstacles are the larger number of diagrams and the necessity of determining corrections to the wave function of the ion.

As the first step, we have found the gauge invariant set of one-loop (vertex) corrections to the electron interaction with the magnetic field, an ingredient of the coefficient of \((Z\alpha)^5\), providing approximately a quarter of the estimated value of 23.15(10) [33]. Work on the remaining one and two-loop diagrams is in progress.

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