Bound-Electron g Factor

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Contents

- Theory of hydrogen and deuterium spectra and the determination of fundamental constants
- Theory of the bound-electron $g$ factor and the determination of the electron mass, and of the fine-structure constant
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Theory of Bound Systems: Hydrogen

- **Schrödinger theory**: nonrelativistic quantum theory
- **Dirac theory**: relativistic quantum theory; includes zitterbewegung, spin, and spin-orbit coupling.
- **QED** includes the *self-interaction of the electron* and tiny corrections to the Coulomb force law.
Lamb-Shift Phenomenology

- Shifts $nS$-$n'S$ transition frequencies:

  \[ E(2S_{1/2}) \rightarrow 2S_{1/2} + 1045 \text{ Mhz} \]

  \[ E(1S_{1/2}) \rightarrow 1S_{1/2} + 8173 \text{ Mhz} \]
Self-Energy: Feynman Diagram

- Dominant contribution to the Lamb shift: self-energy

- Crude approximation: Lamb-shift "potential"

\[ \Delta V_{\text{Lamb}}(r) = \frac{4\alpha}{3} (Z\alpha) \ln[(Z\alpha)^{-2}] \frac{\delta^{(3)}(r)}{m^2} \]
Scaling of the One-Loop Correction for non-$S$ States

Energy displacement:

$$\Delta E_{\text{one-loop}} = \frac{\alpha}{\pi} \frac{(Z\alpha)^4 m_e c^2}{n^3} F(Z\alpha)$$

For $P$ states and states with higher orbital angular momenta:

$$F(Z\alpha) = A_{40} + (Z\alpha)^2 \left\{ A_{61} \ln \left[(Z\alpha)^{-2}\right] + A_{60} \right\}$$

Now: Illustration of the separation of energy scales in different regularizations
Higher-Order Self-Energy for an 8D State: Three Regularizations
Results in Photon Energy Regularization

A high-energy physicist would calculate (example of 8D):

\[ F_{H}(8D_{3/2}) = -\frac{1}{20} + (Z\alpha)^2 \left[ -\frac{20893}{2419200} - \frac{31}{2520\epsilon} - \frac{31}{2520} \ln(2\epsilon) \right] \]

An atomic physicist would calculate:

\[ F_{L}(8D_{3/2}, Z\alpha) = -\frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ 0.024886 + \frac{31}{2520\epsilon} + \frac{31}{2520} \ln \left( \frac{\epsilon}{(Z\alpha)^2} \right) \right] \]

The complete result is obtained upon combining the two approaches:

\[ F(8D_{3/2}) = F_{H}(8D_{3/2}, Z\alpha) + F_{L}(8D_{3/2}, Z\alpha) \]

\[ = -\frac{1}{20} - \frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ \frac{31}{2520} \ln \left( (Z\alpha)^{-2} \right) + 0.007723 \right] \]
Transition to Photon Mass Regularization

A high-energy physicist would calculate (example of 8D):

\[
F_H(8D_{3/2}) = -\frac{1}{20} + (Z\alpha)^2 \left[ -\frac{20687}{806400} - \frac{31\pi}{8960\mu} - \frac{31}{2520} \ln\left(\frac{1}{\mu}\right) \right]
\]

An atomic physicist would calculate:

\[
F_L(8D_{3/2}, Z\alpha) = -\frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ 0.033376 + \frac{31\pi}{8960\mu} + \frac{31}{2520} \ln\left(\frac{\mu}{(Z\alpha)^2}\right) \right]
\]

The complete result is obtained upon combining the two approaches:

\[
F(8D_{3/2}) = F_H(8D_{3/2}, Z\alpha) + F_L(8D_{3/2}, Z\alpha)
\]

\[
= -\frac{1}{20} - \frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ \frac{31}{2520} \ln\left(\frac{1}{(Z\alpha)^2}\right) + 0.007723 \right]
\]
Transition to Dimensional Regularization

A high-energy physicist would calculate (example of 8D):

\[ F_H(8D_{3/2}) = -\frac{1}{20} + (Z\alpha)^2 \left[ -\frac{15727}{806400} - \frac{31}{5040\ \varepsilon_D} \right] \]

An atomic physicist would calculate:

\[ F_L(8D_{3/2}, Z\alpha) = -\frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ 0.027226 + \frac{31}{5040\ \varepsilon_D} + \frac{31}{2520} \ln [(Z\alpha)^{-2}] \right] \]

The complete result is obtained upon combining the two approaches:

\[ F(8D_{3/2}) = F_H(8D_{3/2}, Z\alpha) + F_L(8D_{3/2}, Z\alpha) \]

\[ = -\frac{1}{20} - \frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ \frac{31}{2520} \ln [(Z\alpha)^{-2}] + 0.007723 \right] \]
Recent Progress for Two-Loop Diagrams
Progress in Eighth-Order Two-Loop Corrections for Excited States: Completion of Hydrogen Theory in the Order $\alpha^8$, Unpublished for $P$ and $D$

\[
\begin{align*}
    b_L(1S) &= -81.4(3) \\
    b_L(2S) &= -66.6(3), \quad b_L(2P) = -2.2(3) \\
    b_L(3S) &= -63.5(6), \quad b_L(3P) = -2.5(3), \quad b_L(3D) = -0.006(2), \\
    b_L(4S) &= -61.8(8), \quad b_L(4P) = -2.8(3), \quad b_L(4D) = -0.004(2), \\
    b_L(5S) &= -60.6(8), \quad b_L(5P) = -2.8(3), \quad b_L(5D) = -0.005(3), \\
    b_L(6S) &= -59.8(8), \quad b_L(6P) = -2.9(3), \quad b_L(6D) = -0.006(4).
\end{align*}
\]

For the eighth-order weighted $nS-1S$ difference of the Lamb shift and general operators, see [U.D.J., A. Czarnecki and K. Pachucki, PRA, 2005].
Determination of the Rydberg Constant

General paradigm: We take (at least) two measurements [which we assume to be $1S-2S$ and $2S-8D$]:

$$f_{1S-2S} = R_\infty c \left\{ e_D(2S) - e_D(1S) \right\} + \mathcal{L}_{2S} - \mathcal{L}_{1S}$$

$$f_{2S-8D} = R_\infty c \left\{ e_D(8D) - e_D(2S) \right\} + \mathcal{L}_{8D} - \mathcal{L}_{2S}$$

One may eliminate the $2S$ Lamb shift via the combination

$$\mathcal{L}_{2S} = \frac{\mathcal{L}_{1S} + \mathcal{W}_{21}}{8}$$

$$\mathcal{W}_{21} = 2^3 \mathcal{L}_{2S} - \mathcal{L}_{1S}$$

which is independent of the proton radius. We need a good theoretical value for the $8D$ Lamb shift and for the normalized (weighted) $1S-2S$ difference, and we solve for the Rydberg constant and the proton radius (= ground-state Lamb shift). Same trick later for the electron mass and the fine-structure constant. Other issue: The Rydberg constant “contains QED.”
It can hardly be overemphasized that...

...the 2002 CODATA recommended value for the proton charge radius has been obtained by applying a least-squares adjustment to the 23 most accurately measured transitions in hydrogen and deuterium:

\[ R_p = 0.8750(68) \text{ fm} \]

The least-squares adjustment works by relating a set of fundamental constants, stored in a vector \( Z \), by a set of relations \( F \), to a set of observed transition frequencies \( Q \), by minimizing a functional

\[
(Q - F(Z)) \, V^{-1} \, (Q - F(Z))
\]

Where \( V \) is the matrix of covariances.
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How is the Bound-Electron g-Factor Defined?

Put the electron in a weak magnetic field.

Measure the energy difference (resonance energy) for a change in the angular momentum projection of the electron.

Then by definition

\[ E = g \mu_0 B \mu_a \]

This is enough from a theorist's perspective.

In practice, it is difficult to measure a magnetic field strength accurately, so one relies on measurements of the ratio of the Larmor precession to the cyclotron frequency.
For $S$ states, the bound-electron $g$-factor is related to the energy change that an electron experiences under a spin flip in a magnetic field:

\[ \hbar = c = \epsilon_0 = 1 \]

\[ E = g \mu_0 B \mu_a \]

\[ \mu_a = \pm \frac{1}{2} \]

\[ \mu_0 = -\frac{q}{2m} \]

\[ q = e = -|e| = \text{physical electron charge} \]
Let’s Evaluate the $g$-Factor (Bound Electron, S State, Dirac Theory)

Basic formulas:

\[
A \quad = \quad \frac{1}{2} \ (B \times r)
\]

\[
B \quad = \quad \nabla \times A
\]

\[
E(\mu_\alpha) \quad = \quad \langle nL_J \mid -\frac{q}{2} \alpha \cdot (B \times r) \mid nL_J \rangle
\]

\[
| nL_J \rangle \quad = \quad \text{fully relativistic Dirac wave function}
\]

Result of an expansion in the electron-nucleus coupling, which is effectively an expansion in the $v/c$, where $v$ is a typical velocity of the electron in a bound state (relativistic expansion):

\[
g(nS) = 2 - \frac{2 \ (Z\alpha)^2}{3 \ n^2} + \frac{(Z\alpha)^4}{n^3} \left( \frac{1}{2n} - \frac{2}{3} \right) + O(Z\alpha)^6
\]
Free-Electron g-Factor

*Loop expansion:*

\[
g_{\text{free}} = 2 + \frac{\alpha}{\pi} \delta g^{(2)} + \left(\frac{\alpha}{\pi}\right)^2 \delta g^{(4)} + \mathcal{O}(\alpha^3)
\]

\[
\delta g^{(2)} = 1
\]

\[
\delta g^{(4)} = -0.656958
\]

Question: Is this result recovered for *bound* electrons in the case of vanishing nuclear charge number \(Z=0\)?
Bound-Electron g-Factor (S states)

Combination of the relativistic expansion with the loop expansion:

\[
g(nS) = 2 - \frac{2(Z\alpha)^2}{3n^2} + \frac{(Z\alpha)^4}{n^3} \left( \frac{1}{2n} - \frac{2}{3} \right) + \mathcal{O}(Z\alpha)^6
\]

Breit (1928), purely based on Dirac theory

\[
+ \frac{\alpha}{\pi} \left\{ 2 \times \frac{1}{2} \left( 1 + \frac{(Z\alpha)^2}{6n^2} \right) + \frac{(Z\alpha)^4}{n^3} \left\{ a_{41} \ln[(Z\alpha)^{-2}] + a_{40} \right\} + \mathcal{O}(Z\alpha)^5 \right\}
\]

one-loop correction

\[
+ \left( \frac{\alpha}{\pi} \right)^2 \left\{ -0.656958 \left( 1 + \frac{(Z\alpha)^2}{6n^2} \right) + \frac{(Z\alpha)^4}{n^3} \left\{ b_{41} \ln[(Z\alpha)^{-2}] + b_{40} \right\} + \mathcal{O}(Z\alpha)^5 \right\} + \mathcal{O}(\alpha^3)
\]

two-loop correction

Terms marked in black correspond to the loop expansion of the free-electron g-factor.
Analytic Results for the One-Loop Correction

The one-loop coefficients read:

\[ a_{41}(nS) = \frac{32}{9} \]

\[ a_{40}(nS) = \frac{73}{54} - \frac{5}{24n} - \frac{8}{9} \ln k_0(nS) - \frac{8}{3} \ln k_3(nS) \]

\[ \ln k_0(1S) = 2.984128555 \]

\[ \ln k_0(2S) = 2.811769893 \]

\[ \ln k_3(1S) = 3.272806545 \]

\[ \ln k_3(2S) = 3.546018666 \]

Using these results, one can enhance the accuracy of the one-loop self-energy remainder contribution for low and intermediate nuclear charge numbers (such as \( Z=6 \) and \( Z=8 \)).
Two-Loop Corrections to the g Factor
The logarithmic coefficient $b_{41}$ is generated exclusively by the displayed set of diagrams. Its value is surprisingly large and equal to $3.1$. 
The two-loop coefficients read:

\[
\begin{align*}
    b_{41}(nS) & = \frac{28}{9} \\
    b_{40}(nS) & = \frac{258917}{19440} - \frac{4}{9} \ln k_0 - \frac{8}{3} \ln k_3 + \frac{113}{810} \pi^2 - \frac{379}{90} \pi^2 \ln 2 + \frac{379}{60} \zeta(3) \\
    & \quad + \frac{1}{n} \left[ -\frac{985}{1728} - \frac{5}{144} \pi^2 + \frac{5}{24} \pi^2 \ln 2 - \frac{5}{16} \zeta(3) \right] \\
    b_{40}(1S) & = -16.436842
\end{align*}
\]

The coefficient \( b_{50} \) might also be within the reach of current analytic methods.
# Current Theoretical Predictions for the g-Factor

A careful analysis of all contributing physical effects leads to the following table:

<table>
<thead>
<tr>
<th></th>
<th>( ^{12}C^{5+} )</th>
<th>( ^{16}O^{7+} )</th>
<th>( ^{40}Ca^{19+} )</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \langle r^2 \rangle^{1/2} \text{[fm]} )</td>
<td>2.4703 (22)</td>
<td>2.7013 (55)</td>
<td>3.4764 (10)</td>
<td></td>
</tr>
<tr>
<td>Dirac value (point nucleus)</td>
<td>1.998 721 354 39 (1)</td>
<td>1.997 726 003 06 (2)</td>
<td>1.985 723 203 7 (1)</td>
<td></td>
</tr>
<tr>
<td>Finite nuclear size</td>
<td>0.000 000 000 41</td>
<td>0.000 000 001 55 (1)</td>
<td>0.000 000 113 0 (1)</td>
<td></td>
</tr>
<tr>
<td>1-loop QED ( (Z \alpha)^0 )</td>
<td>0.002 322 819 47 (1)</td>
<td>0.002 322 819 47 (1)</td>
<td>0.002 322 819 5</td>
<td></td>
</tr>
<tr>
<td>( (Z \alpha)^2 )</td>
<td>0.000 000 742 16</td>
<td>0.000 001 319 40</td>
<td>0.000 008 246 2</td>
<td></td>
</tr>
<tr>
<td>( (Z \alpha)^4 )</td>
<td>0.000 000 093 42</td>
<td>0.000 000 240 07</td>
<td>0.000 002 510 6</td>
<td></td>
</tr>
<tr>
<td>h.o., SE</td>
<td>0.000 000 008 28</td>
<td>0.000 000 343 43 (1)</td>
<td>0.000 003 107 7 (2)</td>
<td></td>
</tr>
<tr>
<td>h.o., VP-EL</td>
<td>0.000 000 006 56</td>
<td>0.000 000 002 24</td>
<td>0.000 000 172 7</td>
<td></td>
</tr>
<tr>
<td>h.o., VP-ML</td>
<td>0.000 000 004 04</td>
<td>0.000 000 000 16</td>
<td>0.000 000 014 6</td>
<td></td>
</tr>
<tr>
<td>( \geq 2 )-loop QED ( (Z \alpha)^0 )</td>
<td>-0.000 003 515 10</td>
<td>-0.000 003 515 10</td>
<td>-0.000 003 515 1</td>
<td></td>
</tr>
<tr>
<td>( (Z \alpha)^2 )</td>
<td>-0.000 000 001 12</td>
<td>-0.000 000 002 00</td>
<td>-0.000 000 012 5</td>
<td></td>
</tr>
<tr>
<td>( (Z \alpha)^4 )</td>
<td>0.000 000 000 06</td>
<td>0.000 000 000 08</td>
<td>-0.000 000 010 9</td>
<td>TW</td>
</tr>
<tr>
<td>h.o.</td>
<td>0.000 000 000 00 (3)</td>
<td>0.000 000 000 00 (11)</td>
<td>0.000 000 000 00 (100)</td>
<td></td>
</tr>
<tr>
<td>Recoil ( m/M )</td>
<td>0.000 000 087 70</td>
<td>0.000 000 117 07</td>
<td>0.000 000 297 3</td>
<td></td>
</tr>
<tr>
<td>h.o.</td>
<td>-0.000 000 000 08</td>
<td>-0.000 000 000 10</td>
<td>-0.000 000 000 3</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>2.001 041 590 18 (3)</td>
<td>2.000 047 020 32 (11)</td>
<td>1.988 056 946 6 (100)</td>
<td></td>
</tr>
</tbody>
</table>
What can we do with the bound-electron g factor?

Answer: Determine the electron mass, but also, perhaps, determine the fine-structure constant!?!
Determination of the Electron Mass

The following values may be derived from the recent carbon and oxygen-ion measurements, using the new theory:

\[
\begin{align*}
m^{(12}C^{5+}) &= 0.000\ 548\ 579\ 909\ 32(29)\ \text{u} \\
m^{(16}O^{7+}) &= 0.000\ 548\ 579\ 909\ 60(41)\ \text{u}
\end{align*}
\]

The uncertainty of the electron mass currently is almost exclusively due to the Larmor-to-cyclotron frequency; this experimental uncertainty dominates over the theoretical uncertainty due to the \(g\)-factor by more than an order of magnitude.

Consequence: The electron mass could be determined more accurately by measuring the bound-electron \(g\)-factor in carbon and/or oxygen more precisely; the current theory is not a limiting factor any more.
**Alternative Determination of the Fine-Structure Constant: Low Z**

**Recipe:** Measure the bound-electron $g$ factor in hydrogenlike $^4$He and $^{10}$Be, which are both spinless and (almost) stable, and solve for the electron mass and the fine-structure constant (same trick as for the Rydberg). The plotted uncertainty due to $\alpha$ as a function of $Z$ corresponds to the (now obsolete) value of $\alpha$ in the 2002 CODATA adjustment.


In the plot at $Z=0$: $8.6 \times 10^{-12}$

Now at $Z=0$: $1.5 \times 10^{-12}$
Recipe: Measure the bound-electron $g$ factor in hydrogenlike $^4$He and $^{10}$Be, which are both spinless and (almost) stable, and solve for the electron mass and the fine-structure constant (same trick as for the Rydberg). The plotted uncertainty due to $\alpha$ as a function of $Z$ corresponds to the (now obsolete) value of $\alpha$ in the 2002 CODATA adjustment.

Advantage: $Z^2$ enhancement, so less accuracy required for the $g$ factor:

$$g(nS) = 2 - \frac{2 (Z\alpha)^2}{3 n^2} + \left(\frac{Z\alpha}{n}\right)^4 \left(\frac{1}{2n} - \frac{2}{3}\right) + \mathcal{O}(Z\alpha)^6$$

Observation: Uncertainty due to Nuclear Charge Distribution can be eliminated in a weighted combination of hydrogenlike and boronlike ions, at high nuclear charge (use the ground-state of the boron-like ion, $1s^2\ 2s^2\ 2p^2\ ^2P_{1/2}$).

Disadvantages:
One must evaluate electron-interaction corrections in high order.
One must evaluate all two-loop diagrams nonperturbatively in $Z\alpha$.
One must evaluate even all three-loop diagrams nonperturbatively in $Z\alpha$, to a good approximation (to better than 10%).
Conclusions

- Fundamental constants currently determined on the basis of QED (2002 CODATA): fine-structure constant, Rydberg constant, the proton, deuteron and alpha particle charge radii, Bohr radius as well as the electron mass and several mass ratios (e.g., the electron-proton mass ratio).

- Completion of the hydrogen Lamb shift in eigth order for the weighted difference of $S$ states, and for arbitrary non-$S$ excited states.

- From the electron g factor, one may determine the electron mass. However, because of recent progress in two-loop binding corrections, one may also use the bound-electron g factor as an alternative access route to the fine-structure constant, which may one day lead to a least-squares adjusted value of $\alpha$, based on various measurements in hydrogenlike ions of different nuclear charge number. Both the low-$Z$ as well as the high-$Z$ regime are being discussed in that context.

- Many new ideas and possibilities...
Thank you for your attention!