$\alpha(Z\alpha)^2 E_F$ Binding Corrections to Hyperfine Splitting in Hydrogenic Atoms

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A perturbative expansion of the electron's Dirac Coulomb propagator around a nonrelativistic form is used to evaluate the one-loop nonrecoil corrections to ground-state hyperfine splitting in hydrogenic atoms. A contribution previously estimated as $(\alpha/\pi)(Z\alpha)^2 \times (18.36 \pm 5)E_F$ is found to be $(\alpha/\pi)(Z\alpha)^2 (15.10 \pm 0.29)E_F$. Theory and experiment are compared for muonium hyperfine splitting and consequences for the fine-structure constant are discussed.

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Recent advances in the experimental measurement of ground-state hyperfine splitting in muonium[1] and the extremely precise determination of hydrogen hyperfine splitting[2] present a challenge to theory to complete the calculation of effects that contribute at the order of one-tenth of a part per million. A major difficulty in achieving this goal is the complexity of the evaluation of the one-loop electromagnetic mass shift of an electron bound in the combined Coulomb and magnetic field of the muon or proton. While the lowest-order effect of this contribution simply modifies the Fermi splitting by the Schwinger correction, $\alpha/2\pi$, the calculation of binding corrections of relative order $\alpha(Z\alpha)$ and $\alpha(Z\alpha)^2$ is required to this accuracy. ($Z\alpha$ will be used in the following even for $Z=1$ in order to distinguish the α coming from photons emitted and reabsorbed on the electron line from α's from exchanged photons.) Although the $\alpha(Z\alpha)$ corrections can be worked out straightforwardly,[3] at the level of $(Z\alpha)^2$ infinite sums over states analogous to those encountered in the lowest-order Lamb shift[4] are encountered; it is important to have an approach that can easily handle such terms. The most recent calculation of effects of this order by Brodsky and Erickson[5] (BE), while not explicitly evaluating such sums, did evaluate large constants associated with the double and single logarithms of $Z\alpha$ that come in at this order. They found

$$\Delta E = [\alpha(Z\alpha)^2 E_F/\pi][-\tfrac{2}{3}\ln^2(Z\alpha)^{-2} + (\tfrac{37}{72} + \tfrac{4}{15} - \tfrac{8}{3}\ln 2)\ln(Z\alpha)^{-2} + C], \quad C = 18.36 \pm 5. \tag{1}$$

It is the purpose of this paper to reduce this 0.6 ppm uncertainty by a direct evaluation of ΔE along the lines of an approach previously applied to the Lamb shift.[6] The result of this work can be expressed as

$$C = 15.10 \pm 0.29. \tag{2}$$

While consistent with the previous calculation, this new evaluation of C has an error sufficiently small that the major uncertainties in the theoretical prediction for muonium are the uncertainties in the muon mass (0.30 ppm) and the fine-structure constant (0.22 ppm). In hydrogen, the uncertainties in the proton size (0.9 ppm) and polarizability ($\lesssim 3$ ppm) continue to dominate.[7]

Since a detailed description of the calculation will be given elsewhere, I mention here only the most important points. Part of the calculation is a direct repetition of the Lamb-shift calculation, with the exception that one of the external Coulomb wave functions, ψ_C, is replaced with a wave-function perturbation, ψ_m, where ψ_m is the change induced in the Coulomb wave function by the dipole magnetic field of the nucleus:

$$\Delta E_{LS} = -ie^2 \int \frac{d^4k}{(2\pi)^4}\frac{1}{k^2}\int d^3p\, d^3p' [\bar{\psi}_m(\vec{p})\gamma_\mu S_C(\vec{p}-\vec{k}, \vec{p}'-\vec{k}; E-k_0)\gamma^\mu \psi_C(p') + \bar{\psi}_C(p)\gamma_\mu S_C(\vec{p}-\vec{k}, \vec{p}'-\vec{k}; E-k_0)\gamma^\mu \psi_m(\vec{p}')]. \tag{3}$$

The other part of the calculation takes into account the change in the electron propagator arising from its propagating with an energy shifted by the Fermi splitting (ΔE_{p_1}), and in the presence of the nuclear

magnetic field (ΔE_{p_2}):

$$\Delta E_{p_1} = ie^2 E_F \int \frac{d^4k}{(2\pi)^4}\frac{1}{k^2}\int d^3p\, d^3q\, d^3p'\, \bar{\psi}_C(\vec{p})\gamma_\mu S_C(\vec{p}-\vec{k},\vec{q}-\vec{k};E-k_0)\gamma_0 \times S_C(\vec{q}-\vec{k},\vec{p}'-\vec{k};E-k_0)\gamma^\mu\psi_C(\vec{p}'), \tag{4a}$$

$$\Delta E_{p_2} = -ie^2\frac{ie}{8\pi^3}\int\frac{d^4k}{(2\pi)^4}\frac{1}{k^2}\int\frac{d^3p\,d^3q\,d^3q'\,d^3p'}{|\vec{q}-\vec{q}'|^2}\bar{\psi}_C(\vec{p})\gamma_\mu S_C(\vec{p}-\vec{k},\vec{q}-\vec{k};E-k_0) \times\vec{\gamma}\cdot\vec{\mu}\times(\vec{q}-\vec{q}')S_C(\vec{q}'-\vec{k},\vec{p}'-\vec{k};E-k_0)\gamma^\mu\psi_C(\vec{p}'). \tag{4b}$$

While these energy shifts are exhibited in Feynman gauge, Coulomb gauge was found most convenient for their evaluation. To evaluate the above expressions, the Dirac Coulomb propagator $S_C(x,x';E)$ is first expressed in terms of a Klein-Gordon type propagator G via

$$S_C(\vec{x},\vec{x}';E)\equiv[(E_C+Z\alpha/x)\gamma_0+i\vec{\gamma}\cdot\nabla+m]G_C(\vec{x},\vec{x}';E), \tag{5}$$

where G satisfies

$$\left(E_C{}^2-m^2+\frac{2E_CZ\alpha}{x}+\nabla^2+\left\{\frac{Z^2\alpha^2+Z\alpha\alpha_x}{x^2}\right\}\right)G(\vec{x},\vec{x}';E)=\delta^3(\vec{x}-\vec{x}'). \tag{6}$$

In the absence of the bracketed terms, G can be expressed in a form essentially equivalent to the nonrelativistic Coulomb propagator due to Schwinger[8] and Hostler.[9] This form has the advantage of separating out the parts of the propagator where the electron propagates freely or interacts once with the Coulomb field of the nucleus, and having the effect of multiple Coulomb exchanges taken into account at the cost of a single integration. It was found that the bracketed terms need to be included only as a first perturbation to the required order. With the above expressions multidimensional integrals were set up giving the energy shift, from which were subtracted terms that could be evaluated analytically as the $(\alpha/2\pi)E_F$ and $\alpha(Z\alpha)(\ln 2-\frac{13}{4})E_F$ terms, leaving an integral of $O(\alpha(Z\alpha)^2)E_F$ that was evaluated numerically.[10] No attempt was made to evaluate analytically the known logarithmic terms, those terms being part of the numerical result. By varying Z, however, consistency with a $-\frac{2}{3}\ln^2[(Z\times\alpha)^{-2}]$ was established. Because of the size of the numerical errors a separate determination of the logarithm and constant was not possible. The result presented in Eq. (2) incorporates certain terms of higher order in $Z\alpha$, a large fraction of the calculation being valid to all orders, while other terms explicitly of higher orders have not been included. These terms would have to be incorporated and the numerical error in the present calculation reduced in order to make this part of the hyperfine-splitting calculation good to less than a tenth of a kilohertz. Given the present uncertainty in the muon mass and the fine-structure constant, this extension of the calculation is not yet necessary.

The theoretical prediction of muonium hyperfine splitting can be expressed in the form

$$\Delta\nu=\tfrac{16}{3}\alpha^2cR_\infty(\mu_\mu/\mu_B{}^e)(1+m_e/m_\mu)^{-3}[1+\tfrac{3}{2}(Z\alpha)^2+a_e+\epsilon_1+\epsilon_2+\epsilon_3+\sigma_1-\delta_\mu{}'],$$

$$\epsilon_1=\alpha(Z\alpha)(\ln 2-\tfrac{5}{2}),\quad \epsilon_2=-[8\alpha(Z\alpha)^2/3\pi]\ln Z\alpha[\ln Z\alpha-\ln 4+\tfrac{281}{480}],$$

$$\epsilon_3=[\alpha(Z\alpha)^2/\pi]C_1,\quad \sigma_1=[\alpha^2(Z\alpha)/\pi]D_1, \tag{7}$$

$$\delta_\mu{}'=\frac{3Z\alpha}{\pi}\frac{m_em_\mu}{m_\mu{}^2-m_e{}^2}\ln\left(\frac{m_\mu}{m_e}\right)+(Z\alpha)^2\frac{m_em_\mu}{(m_e+m_\mu)^2}\left[2\ln(Z\alpha)+8\ln 2-3\frac{11}{18}\right] +\frac{\alpha(Z\alpha)}{\pi^2}\frac{m_e}{m_\mu}\left[2\ln^2\left(\frac{m_\mu}{m_e}\right)-\frac{31}{12}\ln\left(\frac{m_\mu}{m_e}\right)+\frac{28}{9}+\frac{\pi^2}{3}-1.9-Q_1\right].$$

The result of this calculation and the one reported in the preceding Letter[11] is the refinement of the constants C_1 and Q_1, and results in the new prediction

$$\Delta\nu_{hfs}=4\,463\,304.5(1.6)(0.2)(1)\ \text{kHz}, \tag{8}$$

to be compared with the experimental value[1]

$$\Delta\nu_{exp}=4\,463\,302.88(16)\ \text{kHz}. \tag{9}$$

The first error indicated arises from the combined uncertainties in the muon mass and the fine-structure constant, and is now the largest source of error. The second is the uncertainty arising from numerical evaluations of the integrals. The last error is an estimate of the effect of the last term that remains uncalculated at this order, σ_1, which includes the first binding correction to the two-loop anomaly. The result is in agreement with experiment, but a more precise measurement of the muon mass may reveal a discrepancy.

An alternative approach is to use muonium hfs to infer a value for the fine-structure constant. I find

$$\alpha_{\mathrm{hfs}}^{-1} = 137.035\,988(20),$$

$$\alpha_{g-2}^{-1} = 137.035\,993(10),$$

$$\alpha_{\mathrm{J}}^{-1} = 137.035\,963(15),$$

$$\alpha_{\mathrm{H}}^{-1} = 137.035\,968(23),$$

where the inferred values from electron $g-2$,[12] the ac Josephson effect,[13] and the quantum Hall effect[14] are also given for comparison. It is interesting that the two values obtained from QED theory are in close agreement, but further experimental progress must be made before any conclusions can be drawn.

My comments on hydrogen hyperfine splitting can be brief: While the present result lowers the theoretical prediction by 0.4 kHz, several effects of comparable size must be taken into account before comparison with experiment can be made. The recent calculations[15] of $\alpha^2 E_F m_e/m_\mu$ terms remain to be extended to hydrogen, and can be expected to contribute at a level of several tenths of a part per million. The effect of the finite size of the proton, which has an uncertainty of 0.9 ppm, needs further work, especially considering recent results indicating a larger root mean square charge radius for the proton.[16] A further contribution from the polarizability of the proton can also contribute up to 3 ppm[17]: Recent experimental advances[7] will help determine this term more precisely. Given the large uncertainties in the proton structure, the main use of completing the pure QED calculations in hydrogen hyperfine splitting will be not to compare theory and experiment, but rather to provide another source of information on proton electromagnetic radius and polarizability.

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