Finite nuclear mass correction to the hyperfine splitting in hydrogenic systems: HPQED

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Dirac equation and QED

Infinitely heavy nucleus with the charge density $\rho_C(r)$, and with a single electron

- (stationary) Dirac equation

  $(\vec{\alpha}\cdot\vec{p} + \beta\, m + V_C)\psi = E\,\psi$

  where the Coulomb potential includes the finite nuclear charge distribution ρ

  $V_C(r) = -Z\,\alpha\,\int d^3r' \frac{1}{4\,\pi\,r'}\,\rho_C(|\vec{r}-\vec{r}'|)$

- electron self-energy

$$E_{\rm self} = \langle\bar{\phi}|\Sigma_{\rm rad}(E_D)|\phi\rangle$$

  where

$$\Sigma_{\rm rad}(E) = e^2\int\frac{d^4k}{(2\,\pi)^4\,i}\,\frac{1}{k^2}\,\gamma^\mu\,e^{-i\,\vec{k}\cdot\vec{r}}\,S_F(E+\omega)\,\gamma_\mu\,e^{i\,\vec{k}\cdot\vec{r}}$$

- vacuum polarization potential for a finite size nucleus

$$V_{\rm vp}(r) = \int d^3r'\;V_{\rm pvp}(|\vec{r}-\vec{r}\,'|)\,\rho_C(r')\,,$$

  and the corresponding vacuum polarization correction

$$E_{\rm vp} = \langle\phi|\,V_{\rm vp}|\phi\rangle\,.$$

- They can be calculated numerically with an arbitrary precision, but it does not say us how much they depend on the nuclear size

Finite nuclear size effects

$Z\,\alpha$ expansion for the finite nuclear size contribution:

$E_{\rm fs} = E^{(4)}_{\rm fs} + E^{(5)}_{\rm fs} + E^{(6)}_{\rm fs} + \ldots$, where $\Psi(n) = \Gamma'(n)/\Gamma(n)$

$$
\begin{aligned}
E^{(4)}_{\rm fs} &= \frac{2\,\pi}{3}\,\phi^2(0)\,Z\,\alpha\,r_C^2 \\
E^{(5)}_{\rm fs} &= -\,\frac{\pi}{3}\,\phi^2(0)\,(Z\,\alpha)^2\,m\,r_F^3 \\
E^{(6)}_{\rm fns}(nS) &= -\,(Z\,\alpha)^6\,m^3\,r_C^2\,\frac{2}{3\,n^3}\left[\frac{9}{4n^2} - 3 - \frac{1}{n} + 2\,\gamma - \ln\frac{n}{2} + \Psi(n) + \ln(m\,r_{C2}\,Z\,\alpha)\right] \\
&\quad + (Z\,\alpha)^6\,m^5\,r_C^4\,\frac{4}{9\,n^3}\left[-\frac{1}{n} + 2 + 2\,\gamma - \ln\frac{n}{2} + \Psi(n) + \ln(m\,r_{C1}\,Z\,\alpha)\right] \\
&\quad + (Z\,\alpha)^6\,m^5\,r_{CC}^4\,\frac{1}{15\,n^5} - 1.43113\,\frac{\alpha\,(Z\,\alpha)^5}{n^3}\,m^3\,r_C^2\,, \\
E^{(6)}_{\rm fns}(nP_{1/2}) &= (Z\,\alpha)^6\,m\left(\frac{m^2\,r_C^2}{6} + \frac{m^4\,r_{CC}^4}{45}\right)\frac{1}{n^3}\left(1 - \frac{1}{n^2}\right), \\
E^{(6)}_{\rm fns}(nP_{3/2}) &= (Z\,\alpha)^6\,m^5\,r_{CC}^4\,\frac{1}{45\,n^3}\left(1 - \frac{1}{n^2}\right), \\
E^{(6)}_{\rm fns}(nL_J) &= 0 \text{ for } L > 1\,,
\end{aligned}
$$

$$
r_C^2 = \int d^3r\,\rho(r)\,r^2, \qquad r_F^3 = \int d^3r_1 \int d^3r_2\;\rho(r_1)\,\rho(r_2)\,|\vec r_1 - \vec r_2|^3, \qquad r_{CC}^4 = \int d^3r\,\rho(r)\,r^4
$$

Corrections to the infinite nuclear mass limit

which are relevant to the nuclear radii determination

1. finite nuclear mass corrections: $\rightarrow$ pure recoil corrections
   the nuclear charge density in the momentum space $\rho = \rho(\vec{q}\,^2 - q_0^2)$,
2. the electron self-energy and vacuum polarization,
   combined with the finite nuclear mass $\rightarrow$ radiative recoil correction
3. the nuclear self-energy vs the mean square charge radius
4. nuclear polarizability effects: important for muonic atoms
5. the hyperfine structure with finite nuclear mass and size
   for the Zemach radius r_Z determination.

1: Nonperturbative pure recoil corrections

- There is no generalization of the Dirac equation to the two-body system with arbitrary masses in the form of a differential equation
- There is no a Hamiltonian that describes relativistic two-body system
- One expands the the binding energy in powers of the electron nuclear mass ratio:

  $$E(m/M, Z\,\alpha) = E^{(0)} + \frac{m}{M}\,E^{(1)} + \left(\frac{m}{M}\right)^2 E^{(2)} + \dots$$

  and derives a formula for each $E^{(i)}$ using the QED theory
- An approach to derive these formulas is the HPQED

1: Leading order pure recoil corrections

Exact nonperturbative formula (a'la Shabaev) for the leading m/M pure recoil corrections with including the finite nuclear size

Important: the elastic contribution in the two-photon exchange should be consistent with this pure recoil correction

$$E^{(1)} = \langle\phi|\Sigma^{(1)}(E_D)|\phi\rangle$$

$$\Sigma^{(1)}(E) = \frac{i}{M}\int_s \frac{d\omega}{2\,\pi}\, D^j(\omega)\, G(E+\omega)\, D^j(\omega)$$

where

- $G(E) = [E - H_D(1 - i\epsilon)]^{-1}$ is the Dirac-Coulomb Green function
- $D^j(\omega) = -4\pi Z\alpha\,\alpha^i\, G_T^{ij}(\omega,\vec{r})$, and α^i are the Dirac matrices.
- Photon propagator in the temporal gauge

$$G_T^{ij}(\omega,\vec{r}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, \frac{\rho(\vec{k}^2-\omega^2)}{\omega^2-\vec{k}^2}\left(\delta^{ij} - \frac{k^i\,k^j}{\omega^2}\right).$$

- Breit interactions is modified by the finite nuclear size !
- numerical calculations & Vladimir Yerokkhin

Expansion in $Z\,\alpha$

- for a point nucleus

$$E_{\rm rec} = \frac{m^2 - E_D^2}{2\,M} + E^{(5)}_{\rm rec} + E^{(6)}_{\rm rec} + \ldots$$

$$E^{(5)}_{\rm rec} = -\frac{7}{6\,\pi}\,\frac{(Z\,\alpha)^2}{M\,m}\left\langle\frac{1}{r^3}\right\rangle - \frac{8}{3\,\pi}\,\frac{Z\,\alpha}{M\,m}\left\langle\vec p\,(H_0 - E_0)\,\ln\left[\frac{2\,(H_0 - E_0)}{m\,(Z\,\alpha)^2}\right]\vec p\right\rangle + \left(\frac{62}{9} - \frac{2}{3}\,\ln(Z\,\alpha)\right)\frac{(Z\,\alpha)^2}{m\,M}\,\langle\delta^{(3)}(r)\rangle$$

$$E^{(6)}_{\rm rec} = \frac{(Z\,\alpha)^2}{2\,M\,m^2}\,\langle\phi|\frac{\vec L^2}{r^4}|\phi\rangle + \left(4\,\ln 2 - \frac{7}{2}\right)\frac{(Z\,\alpha)^3}{M\,m}\,\langle\pi\,\delta^3(r)\rangle$$

- for the finite size nucleus (instead of r_F^3)

$$\delta E_{\rm rec,fns} = -\frac{m}{M}\,\phi^2(0)\,(Z\,\alpha)^2\left[\frac{7}{6} - 2\,\gamma - 2\,\ln(m\,\tilde r)\right] r_C^2 + \ldots$$

important in muonic atoms

HPQED formalism

- Hamiltonian of the nucleus:

$$H_{\rm nuc} = \frac{\vec{\Pi}^2}{2\,M} + q\,A^0 - \frac{q}{2\,M}\,g\,\vec{I}\cdot\vec{B} - \frac{q\,\delta_I}{8\,M^2}\,\vec{\nabla}\cdot\vec{E} - \frac{q}{4\,M^2}\,(g-1)\,\vec{I}\cdot[\vec{E}\times\vec{\Pi} - \vec{\Pi}\times\vec{E}] + \ldots$$

  where $\vec{\Pi} = \vec{P} - q\,\vec{A}$, $q = -Z\,e$, $\delta_0 = 0$, $\delta_{1/2} = 1$.

- First order correction

$$E^{(1)} = \left\langle \Psi \left| \frac{(\vec{P} - q\,\vec{A})^2}{2\,M} \right| \Psi \right\rangle_{\rm QED}$$

- How to interpret the derivative over Coulomb center ?

$$\hat{\psi}(x) = \sum_s^{+} a_s \phi_s(\vec{x})\,e^{-i\,E_s t} + \sum_s^{-} b_s \phi_s(\vec{x})\,e^{-i\,E_s t}\,,$$

$$\vec{\nabla}_R = -\int d^3r\,\hat{\psi}^+(\vec{r})\,\vec{\partial}_r\,\hat{\psi}(\vec{r}) + \vec{\partial}_R$$

- as a test

$$\vec{\nabla}_R\hat{\psi}(0,\vec{x}) = -\int d^3r\,\hat{\psi}^+(\vec{r})\,\vec{\partial}_r\,\hat{\psi}(\vec{r})\;\hat{\psi}(0,\vec{x}) - \vec{\partial}_x\hat{\psi}(0,\vec{x}) = 0\,,$$

- Important observation: $\vec{\Pi}$ in the Coulomb gauge $\to$ $-q\,\vec{A}$ in the temporal gauge.

2: Radiative recoil correction

combined with the finite nuclear size

$$E_{\rm vprec} = \delta_{\rm vp}\,\frac{i}{M}\int_s \frac{d\omega}{2\,\pi}\,\langle\phi|D^j(\omega)\,G(E_D+\omega)\,D^j(\omega)|\phi\rangle$$

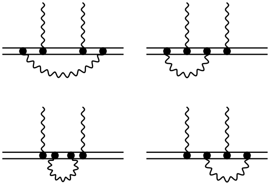
Vacuum polarization can effectively be implemented by modification of $\rho(-k^2)$ and is important for muonic atoms.

$$E_{\rm selfrec} = \langle\phi|\Sigma_{\rm radrec}(E_D)|\phi\rangle + 2\,\langle\phi|\Sigma_{\rm rad}(E_D)\,\frac{1}{(E_D-H_D)'}\,\Sigma_{\rm rec}(E_D)|\phi\rangle$$
$$+\,\langle\phi|\Sigma'_{\rm rad}(E_D)|\phi\rangle\,\langle\phi|\Sigma_{\rm rec}(E_D)|\phi\rangle + \langle\phi|\Sigma'_{\rm rec}(E_D)|\phi\rangle\,\langle\phi|\Sigma_{\rm rad}(E_D)|\phi\rangle$$

$$\Sigma_{\rm radrec}(E) = \frac{i}{M}\int_s \frac{d\omega'}{2\,\pi}\,e^2\int\frac{d^4k}{(2\,\pi)^4\,i}\,\frac{1}{k^2}$$
$$\times\Big[\alpha^\mu\,e^{-i\,\vec{k}\cdot\vec{r}}\,G(E+\omega)\,D^j(\omega')\,G(E+\omega+\omega')\,{}^j(\omega')\,G(E+\omega)\,\alpha_\mu\,e^{i\,\vec{k}\cdot\vec{r}}$$
$$+\,D^j(\omega')\,G(E+\omega')\,\alpha^\mu\,e^{-i\,\vec{k}\cdot\vec{r}}\,G(E+\omega+\omega')\,\alpha_\mu\,e^{i\,\vec{k}\cdot\vec{r}}\,G(E+\omega')\,D^j(\omega')$$
$$+\,\alpha^\mu\,e^{-i\,\vec{k}\cdot\vec{r}}\,G(E+\omega)\,D^j(\omega')\,G(E+\omega+\omega')\,\alpha_\mu\,e^{i\,\vec{k}\cdot\vec{r}}\,G(E+\omega')\,D^j(\omega')$$
$$+\,D^j(\omega')\,G(E+\omega')\,\alpha^\mu\,e^{-i\,\vec{k}\cdot\vec{r}}\,G(E+\omega+\omega')\,D^j(\omega')\,G(E+\omega)\,\alpha_\mu\,e^{i\,\vec{k}\cdot\vec{r}}\Big]$$

It has not yet been calculated numerically, and is known only within $Z\,\alpha$ expansion.

3: Nuclear self-energy



- The effective coupling constant $= Z^2\,\alpha$ can be large, for Mg: $12^2/137 > 1$!!!
- $\Delta T^{00} = \frac{q^2\,M}{p^2 - M^2}\left(\frac{4\,Z^2\alpha}{3\,\pi\,M^2}\ \ln\frac{M^2}{M^2-p^2} + \frac{2}{3}\,r_C^2\right) + (q \to -q)$
- $E(n,l) = \frac{2}{3\,n^3}\,(Z\,\alpha)^4\,\mu^3\,r_C^2\,\delta_{l0} + \frac{4\,Z\,(Z\,\alpha)^5}{3\,\pi\,n^3}\,\frac{\mu^3}{M^2}\,\left[\ln\left(\frac{M}{\mu\,(Z\,\alpha)^2}\right)\delta_{l0} - \ln k_0(n,l)\right]$
- strange artefact of the elastic approximation: anomalously large self-energy

5: HFS in the nonrecoil limit

- Hyperfine splitting for the infinitely heavy nucleus is obtained from the expectation value

$$E_{\rm hfs} = \langle \phi | V_{\rm hfs} | \phi \rangle \,.$$

where

$$V_{\rm hfs} = -\,e\,\vec{\alpha}\cdot\vec{A}_I\,,$$
$$e\,\vec{A}_I(\vec{r}) = \frac{e}{4\,\pi}\,\vec{\mu}\times\left[\frac{\vec{r}}{r^3}\right]_{\rm fs}\,,$$
$$\frac{1}{4\,\pi}\left[\frac{\vec{r}}{r^3}\right]_{\rm fs} = -\,\vec{\nabla}\int\frac{d^3q}{(2\,\pi)^3}\,\frac{\rho_M(\vec{q}^{\,2})}{\vec{q}^{\,2}}\,e^{i\,\vec{q}\,\vec{r}}\,.$$

- The finite nuclear size contribution can be expanded in $Z\,\alpha$

$\delta E_{\rm nucl} = \delta^{(1)}E_{\rm nucl} + \delta^{(2)}E_{\rm nucl} + \ldots$

- $\delta^{(1)}E_{\rm nucl} = -2\,m_r Z\alpha\, r_Z E_F$ where $r_Z = \int d^3r_1 \int d^3r_2\, \rho_M(r_1)\,\rho_E(r_2)\,|\vec{r}_1 - \vec{r}_2|$

- $\delta^{(2)}E_{\rm fns} = \frac{4}{3}E_F(mr_C Z\alpha)^2\left[-\,\frac{1}{n} + 2\gamma - \ln\frac{n}{2} + \Psi(n) + \ln(m\,\tilde{r}\,Z\alpha) + \frac{r_M^2}{4r_C^2 n^2}\right]$

Finite nuclear mass correction to the hyperfine splitting

Exact in $Z\,\alpha$ formula: $H_{\rm nuc} = \frac{\vec\Pi^2}{2\,M} - \frac{q}{2\,M}\,g\,\vec I\cdot\vec B - \frac{q}{4\,M^2}\,(g-1)\,\vec I\cdot[\vec E\times\vec\Pi - \vec\Pi\times\vec E]$

$$
\begin{aligned}
E_{\rm hfsrec} &= E_{\rm kin} + E_{\rm so} + E_{\rm sec}\\
E_{\rm kin} &= \frac{1}{M}\int_s \frac{d\omega}{2\,\pi}\,\frac{1}{\omega}\,\big[\langle\phi|D^j_T(\omega)\,G(E_D+\omega)\,\partial^j(V_{\rm hfs}(\omega))|\phi\rangle - \langle\phi|\partial^j(V_{\rm hfs}(\omega))\,G(E_D+\omega)\,D^j_T(\omega)|\phi\rangle\big]\\
&\quad + \delta_{\rm hfs}\,\frac{i}{M}\int_s \frac{d\omega}{2\,\pi}\,\langle\phi|D^j_T(\omega)\,G(E_D+\omega)\,D^j_T(\omega)|\phi\rangle\,,\\
E_{\rm so} &= -\,\frac{(g-1)}{M^2}\,\epsilon^{ijk}\,I^i\int_s \frac{d\,\omega}{2\,\pi}\,\omega\,\langle\phi|D^j_T(\omega)\,G(E_D+\omega)\,D^k_T(\omega)|\phi\rangle\,,\\
E_{\rm sec} &= \left(\frac{4\,\pi\,Z\,\alpha}{2\,M}\,g\right)^2\epsilon^{ijk}\,I^k\int_s \frac{d\,\omega}{2\,\pi}\,\frac{1}{\omega}\,\langle\phi|(\vec\alpha\times\vec\nabla)^i\,D(\omega)\,G(E_D+\omega)\,(\vec\alpha\times\vec\nabla)^j\,D(\omega)\,|\phi\rangle\,,
\end{aligned}
$$

where

$$V_{\rm hfs}(\omega,\vec r) = e\,\vec\mu\cdot\vec\alpha\times\vec\nabla D(\omega,r)\,,$$

such that $V_{\rm hfs}(0,r) = V_{\rm hfs}(r)$, and

$$D(\omega,r) = \int\frac{d^3k}{(2\pi)^3}\,e^{i\vec k\cdot\vec r}\,\frac{\rho(\vec k^2-\omega^2)}{\omega^2-\vec k^2}\,.$$

Recoil HFS: expansion in $Z\,\alpha$

$$\delta E_{\rm rec} = \delta^{(1)} E_{\rm rec} + \delta^{(2)} E_{\rm rec} + \ldots$$

$$\delta^{(1)} E_{\rm rec} = -\,E_F\,\frac{Z\,\alpha}{\pi}\,\frac{m}{M}\,\frac{3}{8}\,\biggl\{g\left[\gamma - \frac{7}{4} + \ln(m\,r_{M^2})\right] - 4\left[\gamma + \frac{9}{4} + \ln(m\,r_{EM})\right] - \frac{12}{g}\left[\gamma - \frac{17}{12} + \ln(m\,r_{E^2})\right]\biggr\}$$

$$\delta^{(2)} E_{\rm rec} = E_F\,(Z\,\alpha)^2\,\frac{m_{\rm r}^2}{m\,M}\,\biggl\{-\frac{\ln(Z\,\alpha)}{4}\left[-6 + \frac{7}{2}\,g + \frac{14}{g}\right] - \frac{\ln 2}{4}\left[-2 + \frac{11}{2}\,g + \frac{46}{g}\right] + \frac{1}{36}\left[-\frac{81}{2} + \frac{31}{2}\,g + \frac{279}{g}\right]\biggr\}\,.$$

$\delta^{(1)} E_{\rm rec}$ is about 10% of the leading Zemach contribution for light elements, however the elastic form-factor assumption is not necessarily a good approximation !

$\delta^{(2)} E_{\rm rec}$ is an of result of complicated calculations by Bodwin and Yennie (1988) in the point nucleus limit and has not yet been verified.

We aim to verify their result using exact formulas analytically and numerically (to all orders in $Z\,\alpha$)

HPQED

- There exists a compact formula for $(m/M)^n$ recoil correction for any n
- Hamiltonian of the nucleus:

$$H_{\rm nuc} = \frac{\vec{\Pi}^2}{2\,M} + q\,A^0 - \frac{q}{2\,M}\,g\,\vec{I}\cdot\vec{B} - \frac{q\,\delta_I}{8\,M^2}\,\vec{\nabla}\cdot\vec{E} - \frac{q}{4\,M^2}\,(g-1)\,\vec{I}\cdot[\vec{E}\times\vec{\Pi} - \vec{\Pi}\times\vec{E}] + \ldots$$

  where $\vec{\Pi} = \vec{P} - q\,\vec{A}$
- In the temporal gauge $\vec{\Pi} \to -q\,\vec{A}$
- Two-time Green function a'la Shabaev with the recoil vertex
- Potential applications: hydrogen Lamb shift and hfs, muonic atoms
- Extension to a few electron ions using $1/Z$ expansion