QED theory of hyperfine structure

Krzysztof Pachucki

University of Warsaw

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QED theory of compound particles

- Proton radius puzzle: how come r_p from (electronic) H differs by 4% from that of μH ?
- High precision test of the lepton universality by comparison of hfs in eH and μH, and as well as in other systems
- QED of point particles with the anomalous magnetic moment is not renormalizable
- Nontrivial QED expansion the for finite size particles
- One can not separate QED from the nuclear structure effects in hfs
- Little progress in accurate calculation of nuclear structure effects for nuclei $\neq p$
- Cancellation between elastic and inelastic contributions
- Several misconceptions and missing contributions: (inelastic) three photon exchange

Measurements of atomic properties

Measurement of transition frequencies can be very accurate [Garching, 2013]

- $\nu(1S-2S)_{\mathrm{H}} = 2466\,061\,413\,187\,018(11)\ \mathrm{Hz}$
- sensitive to the nuclear size and to the nuclear polarizability
- from $\nu(1S-2S)_{\mathrm{H-D}}$: $r_d^2 - r_p^2 = 3.820\,07(65)\ \mathrm{fm}^2$

Another example: hydrogen(-like) hyperfine splitting:

- $\nu(H) = 1\,420\,405\,751.768(1)$ Hz, $\frac{\nu_{\mathrm{exp}}-\nu_{QED}}{\nu_F} = -33$ ppm
- $\nu(D) = 327\,384\,352.522\,2(17)$ Hz, $\frac{\nu_{\mathrm{exp}}-\nu_{QED}}{\nu_F} = 138$ ppm
- $\nu(^3\mathrm{He}^+) = -8\,665\,649\,867(10)$ Hz, $\frac{\nu_{\mathrm{exp}}-\nu_{QED}}{\nu_F} = -213$ ppm

Proton charge radius puzzle

- $\delta_{\rm fs} E = (2\,\pi\,\alpha/3)\,\phi^2(0)\,\langle r_p^2\rangle$
- $H(2S-4P)$ by Maisenbacher *et al*, Garching (2017), $r_p = 0.8335(95)$ fm, (in agreement with μH)
- $H(1S-3S)$ by Fleurbaey *et al*, Paris (2018), $r_p = 0.877(13)$ fm, (in agreement with the previous eH)
- $H(1S-3S)$ by Matveev *et al*, Garching, announced on PSAS (2018), $r_p =$ ... fm, (in agreement with μH)
- If the hydrogen spectroscopy gets into an agreement with μH, what is the impact on interpretation of e-p scattering data and on hfs predictions ?

QED theory of hfs in H

- $E_{\rm hfs} = E_{\rm hfs}(\alpha, m/M, r_E, g_N, \ldots)$
- power expansion in α at constant values of nuclear parameters (which in principle depend on α)
- $E_{\rm hfs}(\alpha) = E^{(4)} + E^{(5)} + E^{(6)} + E^{(7)} + o(\alpha^8)$
- $E^{(4)}$ corresponds to 1γ, $E^{(5)}$ corresponds to 2γ, $E^{(6)}$ corresponds to $3 - \infty, \gamma$, and so on
- a convenient collection of expansion terms involve α and $Z\,\alpha$, to distinguish exchange from self-energy photons

Nonrecoil, point nucleus QED

- $E_{\rm hfs}(\alpha, Z\,\alpha) = E_{\rm hfs}(Z\,\alpha) + \alpha\,E^{(1)}_{\rm hfs}(Z\,\alpha) + \alpha^2\,E^{(2)}_{\rm hfs}(Z\,\alpha) + O(\alpha^3)$
- $E_F = \frac{8}{3}\,(Z\,\alpha)^4\,(1+\kappa)\,\frac{\mu^3}{m\,M}\,c^2$, for both $s = 1/2$.
- The electrom magnetic moment anomaly to all orders $\delta E_{\rm hfs} = a_e\,E_F$
- $E_{\rm hfs} = \langle\bar\psi|e\,\vec\gamma\cdot\vec A_I|\psi\rangle = E_F\left(1 + \frac{3}{2}\,(Z\,\alpha)^2 + \frac{17}{8}\,(Z\,\alpha)^4 + \ldots\right)$
- $E^{(1)}_{\rm hfs} = e^2\,\int\frac{d^4k}{(2\,\pi)^4\,i}\,\frac{1}{k^2}\delta_{\rm hfs}\langle\bar\psi|\gamma^\mu\,\frac{1}{\not p - \not k - \gamma^0\,V - m}\gamma_\mu|\psi\rangle$
  $E^{(1)}_{\rm hfs} = E_F\left[\alpha\,(Z\,\alpha)\,(\ln 2 - \frac{13}{4}) + \alpha\,(Z\,\alpha)^2\ldots\right]$, beyond amm
- $E^{(2)}_{\rm hfs} = E_F\,\alpha^2\,(Z\,\alpha)\ldots$, beyond amm
- all α^3 corrections (in external field approximation) are known

Nonrecoil, finite size nucleus

- $\vec{A}_I$ and V includes finite nuclear size (elastic formfactors only) and all initial formulas hold
- The leading order (in α) correction is given by the Zemach radius $\delta_Z E^{(5)} = -2\,(Z\,\alpha)\,m\,r_Z\,E_F$, where $r_Z = \int d^3r\,d^3r'\,\rho_E(r)\,\rho_M(r')\,|\vec{r}-\vec{r}'|$
- $O(Z\,\alpha)^3$ finite size correction are obtained numerically (Indelicato)
- radiative finite size corrections $\sim E_F\,\alpha\,(Z\,\alpha)\ldots$ (KP, Eides, Martynenko)

Recoil, finite size, nuclear polarizability

- Complete treatment of the two-photon exchange $\sim (Z\,\alpha)\,E_F$:
  $\delta E = \delta_Z E + \delta_R E + \delta_{\rm pol} E = \Delta\, E_F$, for μH:
  $\Delta = -6201(20) ppm$ (Tomalak 2017), (many works, next talks)

- three photon exchange with recoil

$$\delta E = (Z\,\alpha)^2\,\frac{\mu^2}{m\,M}\,\tilde{E}_F\,\Big\{\Big[2\,(1+\kappa)+\frac{7\,\kappa^2}{4}\Big]\,\ln(Z\,\alpha)^{-1} - \Big[8\,(1+\kappa)-\frac{\kappa\,(12-11\,\kappa)}{4}\Big]\,\ln 2+\frac{65}{18}+\frac{\kappa\,(11+31\,\kappa)}{36}\Big\}$$

- radiative recoil $\sim \alpha\,(Z\,\alpha)\,\frac{m}{M}\,E_F$ only estimations for H: $10^{-7}\,E_F$

- three photon inelastic contribution and the radiative loop on the nucleon line are unknown for H and μ H, needs to be estimated !
- lack of correct calculation of nuclear polarizability correction to hfs in μD !

Hyperfine splitting with compound nucleus

$$E_{\rm F} = -\frac{2}{3}\,\langle\psi|\vec{\mu}\cdot\vec{\mu}_e\,\delta^3(r)|\psi\rangle = \frac{Z\,e^2}{6}\,\frac{\psi^2(0)}{M\,m}\,g\,\vec{S}\cdot\vec{\sigma}$$

For deuterium

$$\frac{(\nu_{\rm exp}-\nu_{\rm QED})}{\nu_{\rm F}} = 138\,{\rm ppm},$$

Zemach correction

$$\frac{\delta E_{\rm Zemach}}{E_{\rm hfs}} = \frac{2\,\alpha\,m}{\pi^2}\int\frac{d^3k}{k^4}\left[\frac{G_E(-k^2)\,G_M(-k^2)}{1+\kappa}-1\right] = -2\,\alpha\,m\,r_{\rm Z}$$

does not properly accounts for the nuclear size effect, except for hydrogen . . .

Leading nuclear structure correction to hfs

$$\delta E_{\rm hfs} = \frac{i}{2}\int\frac{d\omega}{2\,\pi}\int\frac{d^3k}{(2\,\pi)^3}\,\frac{1}{(\omega^2-k^2)^2}\left(\delta^{ik}-\frac{k^i\,k^k}{\omega^2}\right)\left(\delta^{jl}-\frac{k^j\,k^l}{\omega^2}\right)t^{ji}\,T^{kl}\,\psi^2(0)$$

where

$$\begin{aligned} t^{ji} &= e^2\left[\langle\bar{u}(p)|\gamma^j\frac{1}{\not p-\not k-m}\,\gamma^i|u(p)\rangle+\langle\bar{u}(p)|\gamma^i\frac{1}{\not p+\not k-m}\,\gamma^j|u(p)\rangle\right] \\ &= e^2\,i\,\omega\,\epsilon^{ijk}\,\sigma^k\,\frac{2\,(\omega^2-k^2)}{(\omega^2-2\,m\,\omega-k^2)\,(\omega^2+2\,m\,\omega-k^2)} \end{aligned}$$

p is the momentum at rest, T^{kl} is the corresponding virtual Compton scattering amplitude off the nucleus.
One splits the nuclear structure correction $\delta E_{\rm hfs}$ into three parts:

$$\delta E_{\rm hfs} = \delta E_{\rm Low} + \delta E_{\rm Zemach} + \delta E_{\rm pol}\,.$$

χPT

The main idea behind this expansion is the existence of an expansion parameter in the effective nuclear Hamiltonian, namely the ratio of the characteristic momentum Q of a nucleon to its mass m_p, which is about $0.10 - 0.15$ in typical nuclei.
$\delta E_{\rm Low}$ is the leading correction to hfs of order $Z\,\alpha\,m\,r_N$, [Friar, 2005].

$$\delta E_{\rm Low} = \frac{\alpha}{16}\,\psi^2(0)\,\vec\sigma\sum_{a\neq b}\frac{e_a\,e_b}{m_b}\left\langle 4\,r_{ab}\,\vec r_{ab}\times\vec p_b + \frac{g_b}{r_{ab}}\left[\vec r_{ab}\,(\vec r_{ab}\cdot\vec\sigma_b) - 3\,\vec\sigma_b\,r_{ab}^2\right]\right\rangle$$

$\delta E_{\rm Zemach}$ is a coherent sum of Zemach radii from all nucleons

$$\delta E_{\rm Zemach} = \frac{e^2}{6}\,\frac{\psi^2(0)}{m_p\,m}\,\vec\sigma\cdot(-2\,\alpha\,m)\,\Big\langle\sum_a g_a\,\vec s_a\,r_{aZ}\Big\rangle.$$

The proton and neutron Zemach radius are 1.086(12) fm and -0.042 fm respectively.
$\delta E_{\rm pol}$ accounts for all the nuclear structure corrections, which are Q/m_p smaller than the leading $\delta E_{\rm Low}$ contribution.

Interaction of nucleus with the electromagnetic field

Universal interaction Hamiltonian

$$
\begin{aligned}
H_{\rm int} \;=\;& \frac{\vec\Pi^{\,2}}{2\,M} + Z\,e\,A^0 - \frac{Z\,e}{2\,M}\,g\,\vec S\cdot\vec B + \frac{Z\,e}{4\,M^2}\,(g-1)\,\vec S\cdot(\vec\Pi\times\vec E - \vec E\times\vec\Pi) \\
& -\biggl[\sum_a \frac{e_a}{2\,m_a}\,(\vec l_a + g_a\,\vec s_a) - \frac{Z\,e}{2\,M}\,g\,\vec S\biggr]\cdot\vec B \\
& -\sum_a e_a\,\vec x_a\biggl(\vec E + \frac{1}{2\,M}\,\vec\Pi\times\vec B - \frac{1}{2\,M}\,\vec B\times\vec\Pi\biggr) \\
& +\sum_a\biggl\{-\frac{e_a}{2}\,(x_a^i\,x_a^j - x_a^2\,\delta^{ij}/3)\,E^i_{,j} - \biggl[\frac{e_a}{2\,m_a}(g_a-1) - \frac{Z\,e}{2\,M}\biggr]\vec s_a\times\vec x_a\cdot\partial_t\vec E \\
& -\frac{e_a}{6\,m_a}\,(l_a^j\,x_a^i + x_a^i\,l_a^j)\,B^j_{,i} - \frac{e_a}{2\,m_a}\,g_a\,x_a^i\,s_a^j\,B^j_{,i} + \frac{Z\,e}{6\,M}\,(\vec l_a\times\vec x_a - \vec x_a\times\vec l_a)\cdot\partial_t\vec E\biggr\}
\end{aligned}
$$

does not depend on the internal nucleon interactions

Vector polarizability

We will identify the antisymmetric part of T^{ij} with the vector polarizability

$$\alpha^{ij} = (T^{ij} - T^{ji})/2.$$

For small photon momenta the elastic part of the vector polarizability is

$$\alpha^{ij} = i\,\epsilon^{ijk}\,\frac{(Z\,e)^2}{M^2\,\omega}\left[\omega^2\,S^k\,(g-1) - \vec{k}^2\,S^k\,g/2 - k^k\,(\vec{k}\cdot\vec{S})\,g\,(g-2)/4\right]$$

and the corresponding correction to the hyperfine splitting $\delta E_{\rm hfs}$ is

$$\delta E_{\rm hfs} = e^2\,(Z\,e)^2\,\psi^2(0)\,\frac{\vec{\sigma}\cdot\vec{S}}{M^2}\,\frac{1}{64\,\pi^2}\left[\ln\left(\frac{2\,\Lambda}{m}\right)(g^2-4\,g-12)+\frac{1}{6}\,(g^2+124\,g+4)\right]. \tag{1}$$

Other contributions are obtained from $H_{\rm int}$

Vector polarizability correction to hfs

$$
\begin{aligned}
\delta E_{\rm pol} &= \frac{e^2}{64\,\pi^2}\,\psi^2(0)\,\sigma^k\biggl\{-12\,i\,\epsilon^{ijk}\,\langle D^i\,\mathrm{Ln}\,D^j\rangle \\
&+4\,i\,\epsilon^{ijk}\,\langle(\mu^i-\langle\mu^i\rangle)\,\mathrm{Ln}\,(\mu^j-\langle\mu^j\rangle)\rangle-\frac{3\,i}{M^2}\,\epsilon^{ijk}\,\langle Q^{i\,l}\,\mathrm{Ln}\,Q^{j\,l}\rangle \\
&+\frac{4\,i}{M}\sum_a\biggl[\frac{e_a}{m_a}\Bigl(\frac{g_a}{3}+1\Bigr)+\frac{Z\,e}{M}\biggr]\langle Q^i\,\mathrm{Ln}\,x_a^i\,s_a^k-\mathrm{h.c.}\rangle \\
&+\frac{2\,i}{M}\sum_a\biggl[\frac{e_a}{m_a}+\frac{3\,Z\,e}{4\,M}\biggr]\,\langle Q^i\,\mathrm{Ln}\,(l_a^k\,x_a^i+x_a^i\,l_a^k)-\mathrm{h.c.}\rangle \\
&-\frac{16}{M^2}\,\epsilon^{ijk}\langle D^i\,\mathrm{Ln}\,Q^j\rangle-\frac{14}{M^2}\,\langle\vec D\times\vec Q\rangle^k+\Bigl(\frac{Z\,e}{M}\Bigr)^2 S^k\biggl[\frac{3}{2}\,g^2+26\,g-10\biggr] \\
&-\sum_a\Bigl(\frac{e_a}{m_a}\Bigr)^2\langle s_a^k\rangle\,\biggl[\frac{3}{2}\,g_a^2+26\,g_a-10\biggr]\biggr\}+\sum_a\frac{e^2}{6\,m\,m_a}\,\psi^2(0)\,\vec\sigma\langle\vec s_a\rangle\,\delta g_a,
\end{aligned}
$$

where $\mathrm{Ln}=\ln[2\,(H_{\rm N}-E_{\rm N})/m]$, $\vec D=\sum_a e_a\,\vec x_a$, $\vec Q=\sum e_a\,\vec q_a/m_a$,
$Q^{ij}=\sum_a e_a\,[x_a^i\,q_a^j+q_a^i\,x_a^j-(\vec x_a\,\vec q_a+\vec q_a\,\vec x_a)\,\delta^{ij}/3]/m_a$.

Vector polarizability correction to deuterium hfs

$$\delta E_{\rm pol} = \frac{e^2}{64\,\pi^2}\,\psi^2(0)\,\sigma^k\,\biggl\{-12\,i\,\epsilon^{ijk}\,\langle e\,R^i/2\,\ln[2\,(H-E)/m]\,e\,R^j/2\rangle$$

$$-S^k\left[\frac{e\,(g_p-g_n)}{2\,m_p}\right]^2\langle\,\ln[2\,(H_S-E)/m]\,\rangle$$

$$+\frac{4\,S^k}{m_p}\left(\frac{g_p-g_n}{3}+1\right)\langle e\,R^i/2\,(H_T-E)\,\ln[2\,(H_T-E)/m]\,e\,R^i/2\rangle$$

$$+S^k\left(\frac{e}{m_p}\right)^2\left[\frac{1}{4}\left(\frac{3}{2}\,g_d^2+26\,g_d-10\right)-\frac{1}{2}\left(\frac{3}{2}\,(g_p^2+g_n^2)+26\,g_p-10\right)\right]$$

$$+\frac{e^2}{12\,m\,m_p}\,\psi^2(0)\,\vec\sigma\,\vec S\,(\delta g_p+\delta g_n),$$

where $\vec{R} = \vec{r}_p - \vec{r}_n$ and H_T and H_S are nonrelativistic proton-neutron Hamiltonians in the triplet and singlet states respectively.

Li: ground state hyperfine structure

Fermi contact interaction

$$H_{\rm hfs} = \frac{2\,g_N\,Z\,\alpha}{3\,m\,M}\,\sum_a \vec{I}\cdot\vec{\sigma}_a\,\pi\,\delta^3(r_a)\,.$$

Finite nuclear size effect:

$$H_{\rm size} = -H_{\rm hfs}\,2\,Z\,\alpha\,m\,r_Z$$

where

$$r_Z = \int d^3r\,d^3r'\,\rho_E(r)\,\rho_M(r')\,|\vec{r}-\vec{r}'|$$

Li: hyperfine structure

	^{7}Li[MHz]	^{6}Li[MHz]
$A^{(4)}$	401.654 08(21)	152.083 69(11)
$A^{(5)}_{\rm rec}$	$-0.004\,14$	$-0.001\,80$
$A^{(6)}$	0.260 08(2)	0.098 48(1)
$A^{(7)}$	$-0.010\,2(13)$	$-0.003\,9(5)$
$A_{\rm the}$ (point nucleus)	401.899 8(13)	152.176 5(5)
$A_{\rm exp}$	401.752 043 3(5)	152.136 839(2)
$(A_{\rm exp} - A_{\rm the})/A_{\rm exp}$	$-368(3)$ ppm	$-261(3)$ ppm
r_Z	3.25(3) fm	2.30(3) fm
r_E	2.390(30) fm	2.540(28) fm

significant dependence of r_Z on the isotope