Testing fundamental interactions with the hyperfine splitting in light atomic systems

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Fundamentals

Hyperfine splitting comes from interaction between the electron and the nuclear spin

$$E_{\mathrm{F}} = -\frac{2}{3}\langle\psi|\vec{\mu}\cdot\vec{\mu}_e\,\delta^3(r)|\psi\rangle$$

- In the ground electronic state it is governed by a short range interaction
- Thus, it is very sensitive to the nuclear charge and magnetic moment distribution
- But it is also sensitive to the nuclear (vector) polarizability
- Measurements of HFS can be extremely precise: 14 digits for H, D
- QED theory can also be quite precise: about 8, 9 significant digits
- Any discrepancy with theoretical predictions will signal an unknown nuclear structure effect, or of a yet unknown short range spin-dependent interaction
- Looking for such discrepancies is our primary goal, the most known example is HFS in $\mu^+ e^-$

Simplified theory for hydrogenic systems

- According to the Dirac equation: $E_{\rm hfs} = -\langle\psi|e\,\vec{\alpha}\cdot\vec{A}|\psi\rangle$, where $e\,\vec{A}(\vec{r}) = \frac{e}{4\,\pi}\,\vec{\mu}\times\frac{\vec{r}}{r^3}$
- QED corrections, start with $\sim 10^{-3}$ can be accounted for very accurately
- Finite nuclear mass effects can not be accounted for by the Dirac equation
- Finite nuclear size effects can be accounted for, only approximately charge and magnetic moment form factors: $\tilde{\rho} = \tilde{\rho}(\vec{q}^2 - \omega^2)$
- The second order correction in $e\,\vec{\alpha}\cdot\vec{A}$ is singular ..., and is a good example of limitation of approaches based relativistic quantum mechanics

Relativistic QM versus QED

- the first order hyperfine interaction

$$E_{hfs} = -\langle\psi|e\,\vec{\alpha}\cdot\vec{A}|\psi\rangle$$

$$\vec{A}(\vec{r}) = \int \frac{d^3k}{(2\,\pi)^3}\, e^{i\,\vec{k}\vec{r}}\,(-i)\,\vec{\mu}\times\vec{k}\,\frac{\rho_M(k^2)}{k^2} = \frac{1}{4\,\pi}\,\vec{\mu}\times\left[\frac{\vec{r}}{r^3}\right]_{\rm fs}$$

- the second order hyperfine interaction according to relativistic quantum mechanics

$$E^{(2)}_{hfs} = e^2\left\langle\bar{\psi}\middle|\vec{\gamma}\cdot\vec{A}\,\frac{1}{\not p-\gamma^o\,V-m}\,\vec{\gamma}\cdot\vec{A}\middle|\psi\right\rangle$$

- the second order hyperfine interaction according to QED

$$\delta E = i\,e^2\int\frac{d\,\omega}{2\,\pi}\int\frac{d^3k_1}{(2\,\pi)^3}\int\frac{d^3k_2}{(2\,\pi)^3}\,\frac{\rho_M(k_1^2-\omega^2)}{\omega^2-k_1^2+i\,\epsilon}\,\frac{\rho_M(k_2^2-\omega^2)}{\omega^2-k_2^2+i\,\epsilon}$$
$$\times\left\langle\bar{\psi}\middle|\gamma^i\,e^{i\,\vec{k}_1\vec{r}}\,\frac{1}{\not p-\gamma^o\,V+\gamma^0\,\omega-m+i\,\epsilon}\,\gamma^j\,e^{-i\,\vec{k}_2\vec{r}}\middle|\psi\right\rangle$$
$$\times\left[(\vec{\mu}\times\vec{k}_1)^i\,\frac{1}{-\omega+i\,\epsilon}\,(\vec{\mu}\times\vec{k}_2)^j+(\vec{\mu}\times\vec{k}_2)^j\,\frac{1}{\omega+i\,\epsilon}\,(\vec{\mu}\times\vec{k}_1)^i\right]$$

- coincides with the relativistic QM after changing the order in the second term

Nuclear structure effects in hyperfine splitting

- $\delta E_{\rm nucl} = \delta^{(1)} E_{\rm nucl} + \delta^{(2)} E_{\rm nucl} + \ldots$ where
  $\delta^{(1)} E_{\rm nucl}$ is the two-photon exchange correction of order $(Z\,\alpha)\,E_F$,
  $\delta^{(2)} E_{\rm nucl}$ is the three-photon exchange correction of order $(Z\,\alpha)^2\,E_F$,
  $E_F = -\frac{2}{3}\,\psi^2(0)\,\vec{\mu}\cdot\vec{\mu}_e$
- $\delta^{(1)} E_{\rm nucl} = -2\,m_r Z\alpha\, r_Z E_F$ where
  r_Z is the Zemach radius defined by $r_Z = \int d^3 r_1 \int d^3 r_2\, \rho_M(r_1)\,\rho_E(r_2)\,|\vec{r}_1 - \vec{r}_2|$
- nuclear recoil correction (includes the second order HFS

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

Accurate QED theory of HFS

- The complete hyperfine splitting is conveniently represented as

$$E_{\rm hfs} = E_F\,(1+\delta)\,,$$

- δ represents the correction to the Fermi energy

$$\delta = \kappa + \delta^{(2)} + \delta^{(3)} + \delta^{(4)} + \delta^{(1)}_{\rm nuc} + \delta^{(1)}_{\rm rec} + \delta^{(2)}_{\rm nuc} + \delta^{(2)}_{\rm rec}\,,$$

- $\delta^{(i)}$, $\delta^{(i)}_{\rm nuc}$, and $\delta^{(i)}_{\rm rec}$ are the QED, nuclear, and recoil corrections of order α^i
- coefficients $\delta^{(i)}$ can be calculated for 1-, 2-, and 3-electron atoms and ions very accurately using NRQED theory
- What is left, are unknown nuclear polarizability effects

Contributions to HFS in $^3\mathrm{He}^+$ ion

Term	Value	$\times E_F$ [kHz]
1	1	−8 656 527.892 (7)
κ	0.001 159 65	−10 038.6
$\delta^{(2)}$	0.000 127 07	−1 100.0
$\delta^{(3)}$	−0.000 019 49	168.7
$\delta^{(4)}$	−0.000 000 75	6.5
$\delta^{(1)}_{\mathrm{rec}}$	−0.000 012 17 (60)	105.4 (5.3)
$\delta^{(2+)}_{\mathrm{nuc}}$	−0.000 002 89(3)	25.0
$\delta^{(2)}_{\mathrm{rec}}$	−0.000 001 16 (18)	10.1 (1.6)
theory without $\delta^{(1)}_{\mathrm{nuc}}$	1.001 250 26 (63)	−8 667 350.8 (5.5)
experiment (Blaum:2022)	1.001 053 77	−8 665 649.865 77 (26)
$\delta^{(1)}_{\mathrm{nuc}}$	−0.000 196 49 (63)	1 701.0 (5.5)
$\widetilde{r}_Z$ this work	2.600 (8) fm	
r_Z (Blaum:2022)	2.608 (24) fm	
r_Z (Sick:2014) exp	2.528 (16) fm	
$\widetilde{r}_Z$ ($\mu\mathrm{He}^+$:2023)	2.420(16) fm	
$\widetilde{r}_Z - r_Z(\mathrm{exp})$ =	0.072 (18) fm	
$\widetilde{r}_Z(\mu\mathrm{He}^+)$ - $r_Z(\mathrm{exp})$ =	−0.108 (18) fm	

Polarizability contribution is relatively small in He^+, but ifor $\mu\mathrm{He}^+$ is of opposite sign !

Contributions to HFS in $^3\mathrm{He}$ atom in 2^3S_1 state

Using He^+ HFS

Term	$\times 10^6$	$\times E_F(\mathrm{He})$ [Hz]
$\delta^{(2)}(\mathrm{He}\text{-}\mathrm{He}^+)$	3.012 0	−20 279
$\delta^{(2+)}_{\mathrm{rec}}(\mathrm{He}\text{-}\mathrm{He}^+)$	−8.993 7 (21)	60 552 (14)
$\delta^{(3)}(\mathrm{He}\text{-}\mathrm{He}^+)$	0.184 3	−1 241
$\delta^{(4)}(\mathrm{He}\text{-}\mathrm{He}^+)$	0.005 8 (58)	−39 (39)
$\delta(\mathrm{He}\text{-}\mathrm{He}^+)$	−5.791 6 (62)	38 993 (41)
$1+\delta(\mathrm{He}^+)$, from (Schneider:2022)		−6 739 740 174
$\nu_{\mathrm{hfs,theo}}(\mathrm{He})$		−6 739 701 181 (41)
$\nu_{\mathrm{hfs,exp}}(\mathrm{He})$ (Rosner:1970)		−6 739 701 177 (16)

Perfect agreement !

Contributions to HFS in $^{6,7}\mathrm{Li}^+$ ion

Term	Value ($^6\mathrm{Li}^+$)	Value ($^7\mathrm{Li}^+$)
1	1	1
κ	0.001 159 7	0.001 159 7
$\delta^{(2)}$	0.000 443 5	0.000 443 5
$\delta^{(3)}$	−0.000 032 8	−0.000 032 8
$\delta^{(4)}$	−0.000 002 1(5)	−0.000 002 1(5)
$\delta^{(1)}_{\mathrm{rec}}$	−0.000 010 3(5)	0.000 001 8 (1)
$\delta^{(2+)}_{\mathrm{nuc}}$	−0.000 004 7	−0.000 006 4
$\delta^{(2)}_{\mathrm{rec,mix}}$	0.000 002 4	0.000 006 2
$\delta^{(2)}_{\mathrm{rec,rel}}$	0.000 000 3	0.000 000 4
$\delta^{(2)}_{\mathrm{rec,rad}}$	0.000 000 0(2)	0.000 000 0
Sum	1.001 555 7(8)	1.001 570 3(5)
$1+\delta_{\mathrm{exp}}$ (Sun: 2023, Guan: 2020)	1.001 299 9(24)	1.001 197 6(29)
$\delta^{(1)}_{\mathrm{nuc}}$	−0.000 255 8(25)	−0.000 372 7(29))
this work $\widetilde{r}_Z$	2.26(2) fm	3.29(3) fm
Sun:2023	2.44(2) fm	
Xiao-Qiu Qi: 2020	2.40(16) fm	3.33(7) fm
X(iao-Qiu Qi: 2020	2.47(8) fm	3.38(3) fm
Puchalski: 2013	2.30(3) fm	3.25(3) fm

More accurate picture of nuclear structure effects in HFS

$$\delta^{(1)} E_{\rm hfs} = E_{\rm Low} + E_{\rm 1nuc} + E_{\rm pol}$$

$$E_{\rm 1nuc} = -\frac{8\,\pi}{3}\,\alpha^2\,\frac{\psi^2(0)}{m_p + m}\,\vec{s}\cdot\langle\sum_a g_a\,\vec{s}_a\,r_{aZ}\rangle$$

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

For the case of an nS state of D, Low's correction becomes

$$\delta E_{\rm Low} \approx -2\,\mu\,\alpha\,E_F\,\frac{g_n}{g_d}\langle R\rangle\,, \qquad (1)$$

where R is the distance of the proton from the center of mass, $\langle R\rangle \approx 1.63$ fm.

- It is similar to the Zemach correction, but with the important difference that the deuteron g-factor is replaced by the neutron one, but they have a opposite sign !
- The calculation by by Friar and Payne in 2005 for the $1S$ state of deuterium, $(\delta E_{\rm Low}(e{\rm D}) + \delta E_{\rm 1nucl})/E_F = 141$ ppm, is in approximate agreement with the experiment, $(E_{\rm hfs}^{\rm exp} - E_{\rm hfs}^{\rm theo})/E_F = -3$ ppm.

Discrepancies in μD hfs

- the "experimental value" of the nuclear-structure correction in μD(2S) hfs

  $\delta E_{\mathrm{nucl,exp}} = E_{\mathrm{hfs}}(\mathrm{exp}) - E_{\mathrm{hfs}}(\mathrm{point}) = 0.0966(73)$ meV

- the numerical value of the Zemach correction with $r_Z = 2.593(16)$ fm is

  $\delta E_{\mathrm{Zem}} = -0.1177(33)$ meV, opposite sign !

- including the nuclear vector polarizability and the inelastic three-photon exchange (10% effect)

  $\delta E_{\mathrm{nucl,theo}} = 0.028\,3(86)$ meV

- the difference is

  $\delta E_{\mathrm{nucl,theo}} - \delta E_{\mathrm{nucl,exp}} = 0.058\,3(113)$

- There is no a comprehensive theory for nuclear polarizability effects

Conclusions

- QED theory of HFS is sufficiently accurate to probe the nuclear structure
- the finite nuclear mass effects have to be accounted for (beyond the Dirac equation)
- the finite nuclear size effects $\tilde{\rho}(\vec{q}^2 - \omega^2)$ require inclusion of the photon exchange energy
- there is no yet a comprehensive theory for nuclear polarizability effects to HFS
- comparison to muonic atoms HFS would be very interesting μLi, μBe, μB