Finite nuclear mass and size corrections in hydrogenic systems: HPQED

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Two-body systems in QED

- Bound state energy of the hydrogenic system depends on the mass ratio, the nuclear charge number Z and α

$$E = E(m/M, Z\,\alpha, \alpha)$$

  There is no Hamiltonian that gives E for an arbitrary mass ratio, or/and an arbitrary α.

- QED tells us that we can expand in α at constant $Z\,\alpha$

$$E(m/M, Z\,\alpha, \alpha) = E^{(0)}(m/M, Z\,\alpha) + \alpha\, E^{(1)}(m/M, Z\,\alpha) + \alpha^2\, E^{(2)}(m/M, Z\,\alpha) + \ldots$$

  where powers of α correspond to the number of QED loops.

- We still do not know the exact form of $E^{(i)}(m/M, Z\,\alpha)$

  $\rightarrow$ another expansion is needed.

- Expansion in $Z\,\alpha$: NRQED

- Expansion in the mass ratio: HPQED

NRQED

- For light systems, we expand in $Z\,\alpha$ keeping the mass ratio arbitrary

$$E^{(i)}(m/M, Z\,\alpha) = E^{(i,2)}(m/M) + E^{(i,4)}(m/M) + E^{(i,5)}(m/M) + \ldots$$

  where $E^{(i,n)} \sim (Z\,\alpha)^n$, and some expansion terms may involve $\ln(Z\,\alpha)$.

- It is convenient to combine both expansions in α and $Z\,\alpha$ into one: $E^{(i)} \sim \alpha^i$
- $E^{(2)}$ is an eigenvalue of the nonrelativistic Hamiltonian

$$H = \frac{\vec{p}^{\,2}}{2\,\mu} - \frac{Z\,\alpha}{r}$$

  with the nonrelativistic wave function ϕ

- $E^{(4)}$ is an expectation value $= \langle\phi|H^{(4)}|\phi\rangle$ with the same nonrelativistic wave function ϕ
- $E^{(5)}$ includes leading QED and the Salpeter correction: $E^{(5)} = \langle\phi|H^{(5)}|\phi\rangle$
- Complete $E^{(6)}$ is quite long and has been obtained in analytic form very recently: Adkins 2023
- $E^{(7)}$ is known in only in the nonrecoil limit
- This NRQED approach can be extended to any light few electron atoms (ions).

HPQED

- For heavier systems, the expansion in m/M is preferable

$$E^{(i)}(m/M, Z\alpha) = E^{(i,0)}(Z\alpha) + E^{(i,1)}(Z\alpha) + E^{(i,2)}(Z\alpha) + \ldots$$

  where $E^{(i,n)} \sim (m/M)^n$

- For finite size nuclei this expansion is analytic and thus does not involve $\ln(m/M)$
- This approach we call the heavy particle QED (HPQED) expansion
- One solves the Dirac equation in the infinite nuclear mass limit $\rightarrow \phi$ and

$$G(E) = \frac{1}{E - H_D},$$

- all $(m/M)^i$ corrections can be expressed in terms of ϕ and the Green function $G(E)$!!!

Infinite nuclear mass limit

Let's consider an arbitrary (but infinitely heavy) nucleus with a single electron or muon, and assume that nucleus is described by the charge density $\rho_C(r)$, then

- (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

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

  It can be solved numerically with an arbitrary precision, but it does not as much how the Dirac energy depends on the nuclear size

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

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

  $E^{(4)}_{\rm fs} = \frac{2\,\pi}{3}\,\phi^2(0)\,Z\,\alpha\,r_C^2$, and $r_C^2 = \int d^3r\,\rho(r)\,r^2$

  $E^{(5)}_{\rm fs} = -\frac{\pi}{3}\,\phi^2(0)\,(Z\,\alpha)^2\,m\,r_F^3$, and $r_F^3 = \int d^3r_1 \int d^3r_2\,\rho(r_1)\,\rho(r_2)\,|\vec{r}_1-\vec{r}_2|^3$

Elastic three-photon exchange

In the infinite nuclear mass limit (Friar formula + the radiative correction)

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

where $r_{CC}^4 = \langle r^4 \rangle$ and the effective nuclear charge radii r_{C1} and r_{C2} encode the high-momentum contributions and are expected to be of the order of r_C.

Corrections to the infinite nuclear mass limit

which are relevant to the nuclear radii determination,
to be calculated without $Z\alpha$ expansion

1. finite nuclear mass corrections: $\rightarrow$ pure recoil corrections

   the nuclear charge density in the momentum space $\rho = \rho(\vec{q}^{\,2} - q_0^2)$, as a consequence the e-N Breit interaction becomes modified

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 corrections for the Zemach radius r_Z determination, for example in μH.

1: Nonperturbative pure recoil corrections

- The use of the reduced mass in the Dirac equation is forbidden: for example the relativistic recoil correction to the ground hydrogenic state is $= 0$
- 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:

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

  and derives a formula for each $E^{(i)}$

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

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

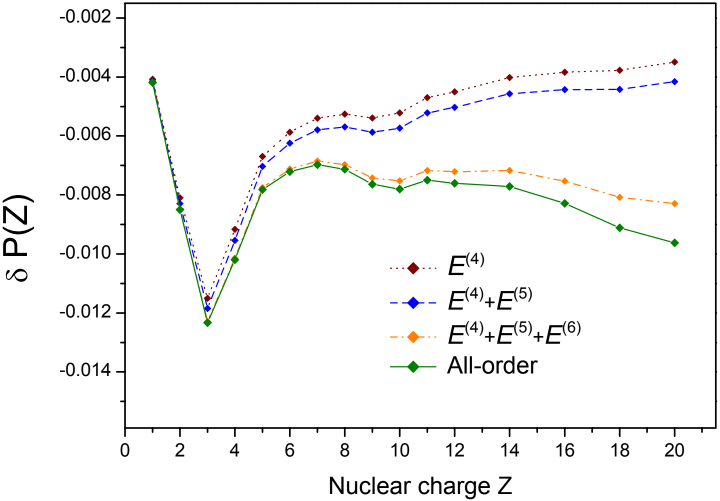
where

- $G(E) = [E - H_D(1-i\epsilon)]^{-1}$ 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 !
- the recoil fns: $\delta E_{\rm rec,fns} = -\frac{m}{M}\,\phi^2(0)\,(Z\,\alpha)^2\left[\frac{7}{6} - 2\,\gamma - 2\,\ln(m\,\tilde{r})\right] r_C^2$ important in muonic atoms

1: Numerical results for the finite size recoil



where

$\delta P = E_{\rm recfs}/[(m^2/M)(Z\alpha)^5/\pi]$ and $E^{(6)}_{\rm recfs} \approx -\frac{m^3}{M}\,(Z\alpha)^6\, r_C$ for electronic atoms

1: Second order pure recoil correction

For the scalar nucleus

$$E^{(2)} = \langle\phi|\Sigma^{(1)}(E_D)\,\frac{1}{(E_D - H_D)'}\,\Sigma^{(1)}(E_D)|\phi\rangle + \left(\frac{d}{dE}\bigg|_{E=E_D}\langle\phi|\Sigma^{(1)}(E)|\phi\rangle\right)\langle\phi|\Sigma^{(1)}(E_D)|\phi\rangle + \langle\phi|\Sigma^{(2)}(E_D)|\phi\rangle$$

where

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

$$\Sigma^{(2)}(E) = \left(\frac{i}{M}\int_s \frac{d\omega_1}{2\,\pi}\right)\left(\frac{i}{M}\int_s \frac{d\omega_2}{2\,\pi}\right) \Big[D^j(\omega_1)\, G(E_D+\omega_1)\, D^k(\omega_2)\, G(E_D+\omega_1+\omega_2)\, D^j(\omega_1)\, G(E_D+\omega_2)\, D^k(\omega_2) + D^j(\omega_1)\, G(E_D+\omega_1)\, D^k(\omega_2)\, G(E_D+\omega_1+\omega_2)\, D^k(\omega_2)\, G(E_D+\omega_1)\, D^j(\omega_1)\Big]\,.$$

This second order recoil correction has not yet been calculated,
but can be important for muonic atoms !

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.

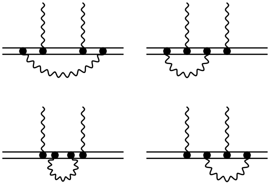
$$E_{\rm selfrec} = \langle\phi|\Sigma_{\rm radrec}(E_D)|\phi\rangle + 2\,\langle\phi|\Sigma_{\rm rad}(E_D)\,\frac{1}{(E_D-H_D)'}\,\Sigma_{\rm rec}(E_D)|\phi\rangle$$
$$+\,\langle\phi|\Sigma'_{\rm rad}(E_D)|\phi\rangle\,\langle\phi|\Sigma_{\rm rec}(E_D)|\phi\rangle + \langle\phi|\Sigma'_{\rm rec}(E_D)|\phi\rangle\,\langle\phi|\Sigma_{\rm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

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

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

3: Nuclear self-energy

How to define the nuclear charge radius in the presence of nuclear self-energy ?



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

4: TPE

Elastic nucleus approximation does not work well for muonic atoms

$$E_{\rm TPE} = E_{\rm nucl1} + E_{\rm nucl2} + E_{\rm pol} + \ldots\,,$$
$$E_{\rm nucl1} = -\frac{\pi}{3}\, m\,\alpha^2\phi^2(0)\Big[Z\,\tilde{R}_F^3(p) + (A-Z)\,\tilde{R}_F^3(n)\Big]\,,$$
$$E_{\rm nucl2} = -\frac{\pi}{3}\, m\,\alpha^2\phi^2(0)\sum_{i,j=1}^{Z}\langle\phi_N||\vec{r}_i - \vec{r}_j|^3|\phi_N\rangle\,,$$
$$E_{\rm pol} = -\frac{4\,\pi\,\alpha^2}{3}\,\phi^2(0)\int_{E_T} dE\,\sqrt{\frac{2\,\mu}{E}}\,|\langle\phi_N|\vec{d}|E\rangle|^2,$$

- Instead of the Friar radius r_F, the TPE contribution involves effective Friar radii of individual nucleons,

  $R_F^3(p) = 2.876(246)\ {\rm fm}^3,\ \ R_F^3(n) = 0.712(223)\ {\rm fm}^3,$

  the inter-proton $|\vec{r}_i - \vec{r}_j|^3$ and a kind of the electric dipole polarizability
- the difference between the elastic and the complete TPE is significant
- $E_{\rm TPE}$ requires subtraction of the point nucleus $(Z\,\alpha)^5$ contribution to be consistent with the pure recoil correction

Charge radii of light muonic atoms

Rev. Mod. Phys. 96, 015001 (2024), KP, V. Lensky, F. Hagelstein, S.S. Li Muli, S. Bacca, and R. Pohl

Order	Correction	μH	μD	μ^3He$^+$	μ^4He$^+$
$(Z\alpha)^5$	TPE	0.029 2(25)	1.979(20)	16.38(31)	9.76(40)
$\alpha^2(Z\alpha)^4$	Coulomb distortion	0.0	−0.261	−1.010	−0.536
$(Z\alpha)^6$	3PE	−0.001 3(3)	0.002 2(9)	−0.214(214)	−0.165(165)
$\alpha(Z\alpha)^5$	eVP$^{(1)}$ with TPE	0.000 6(1)	0.027 5(4)	0.266(24)	0.158(12)
$\alpha(Z\alpha)^5$	μSE$^{(1)}$ + μVP$^{(1)}$ with TPE	0.000 4	0.002 6(3)	0.077(8)	0.059(6)
E_{QED}	point nucleus	206.034 4(3)	228.774 0(3)	1644.348(8)	1668.491(7)
$\mathcal{C}\, r_C^2$	finite size	$-5.2259\, r_p^2$	$-6.1074\, r_d^2$	$-103.383\, r_h^2$	$-106.209\, r_\alpha^2$
E_{NS}	nuclear structure	0.028 9(25)	1.750 3(200)	15.499(378)	9.276(433)
E_L(exp)	experiment[1]	202.370 6(23)	202.878 5(34)	1258.598(48)	1378.521(48)
r_C	this work	0.840 60(39)	2.127 58(78)	1.970 07(94)	1.678 6(12)
r_C	previous[a]	0.840 87(39)	2.125 62(78)	1.970 07(94)	1.678 24(83)

[1] Presented in Antognini *et al (2013), Pohl* et al *(2016), Shuhmann* et al *(:2023), Krauth* et al *(2021)*

electronic vs muonic isotope shifts

Deuteron-proton charge radii difference: perfect agreement

$$r_d^2 - r_p^2|_{\rm muonic} = 3.820\,0(7)_{\rm exp}(30)_{\rm theo}\ {\rm fm}^2$$
$$r_d^2 - r_p^2|_{\rm electronic} = 3.820\,7(3)\ {\rm fm}^2\,.$$

Helion-alpha charge radii diference: 3.6 σ disagreement !!!

$$r_h^2 - r_\alpha^2|_{\rm muonic} = 1.063\,6(6)_{\rm exp}(30)_{\rm theo}\ {\rm fm}^2\ \text{(CREMA, 2023)}$$
$$r_h^2 - r_\alpha^2|_{\rm electronic} = 1.075\,7(15)\ {\rm fm}^2\ \text{(Eikema, 2023)}$$

Remarks

- the result for TPE and 3PE in μHe needs to be confirmed
- the finite nuclear mass effects has to be accounted for
- the main limitation in muonic atoms comes from inelastic TPE and 3PE
- the radiative recoil correction has been calculated only approximately
- for heavier muonic atoms: the exact in $Z\,\alpha$ approach, HPQED, will be more suited

5: HFS Fundamentals

Hyperfine splitting (HFS) comes from interaction between the electron (muon) 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 HFS is governed by a short range interaction
- Thus, it is very sensitive to the nuclear charge and magnetic moment distribution
- Measurements of HFS can be extremely precise: 14 digits for H, D
- QED theory can also be quite precise: about 8, 9 significant digits
- Discrepancy with theoretical predictions will signal existence of the nuclear inelastic effects

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 $r_Z = \int d^3r_1 \int d^3r_2\,\rho_M(r_1)\,\rho_E(r_2)\,|\vec r_1 - \vec r_2|$
- $\delta^{(2)}E_{\rm fns} = \frac{4}{3}E_F(mr_C Z\alpha)^2\left[-\frac{1}{n} + 2\gamma - \ln\frac{n}{2} + \Psi(n) + \ln(m\,\tilde r\,Z\alpha) + \frac{r_M^2}{4r_C^2 n^2}\right]$

Relativistic QM versus QED for the second order correction

- 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

$$\delta E = i\, e^2 \int \frac{d\,\omega}{2\,\pi} \int \frac{d^3 k_1}{(2\,\pi)^3} \int \frac{d^3 k_2}{(2\,\pi)^3} \frac{\rho_M(k_1^2 - \omega^2)}{\omega^2 - k_1^2 + i\,\epsilon} \frac{\rho_M(k_2^2 - \omega^2)}{\omega^2 - k_2^2 + i\,\epsilon}$$

$$\times \left\langle \bar{\psi} \middle| \gamma^i\, e^{i\,\vec{k}_1 \vec{r}} \frac{1}{\not{p} - \gamma^o\, V + \gamma^0\,\omega - m + i\,\epsilon} \gamma^j\, e^{-i\,\vec{k}_2 \vec{r}} \middle| \psi \right\rangle$$

$$\times \left[(\vec{\mu}\times\vec{k}_1)^i \frac{1}{-\omega + i\,\epsilon} (\vec{\mu}\times\vec{k}_2)^j + (\vec{\mu}\times\vec{k}_2)^j \frac{1}{\omega + i\,\epsilon} (\vec{\mu}\times\vec{k}_1)^i \right]$$

- coincides with the relativistic QM after changing the order (in the second term)
- $\rightarrow$ use of the Breit interaction in the second order (or on the SCF level) is doubtful.

Finite nuclear mass correction to the hyperfine splitting

Exact in $Z\,\alpha$ formula: $E_{\rm hfsrec} = E_{\rm kin} + E_{\rm so} + E_{\rm sec}$

$$E_{\rm kin} = \frac{1}{M}\int_s \frac{d\omega}{2\,\pi}\,\frac{1}{\omega}\,\Big[\langle\phi|D_T^j(\omega)\,G(E_D+\omega)\,\partial^j(V_{\rm hfs}(\omega))|\phi\rangle - \langle\phi|\partial^j(V_{\rm hfs}(\omega))\,G(E_D+\omega)\,D_T^j(\omega)|\phi\rangle\Big]$$

$$+\,\delta_{\rm hfs}\,\frac{i}{M}\int_s \frac{d\omega}{2\,\pi}\,\langle\phi|D_T^j(\omega)\,G(E_D+\omega)\,D_T^j(\omega)|\phi\rangle\,,$$

$$E_{\rm so} = -\,\frac{(g-1)}{M^2}\,\epsilon^{ijk}\,I^i\int_s \frac{d\,\omega}{2\,\pi}\,\omega\,\langle\phi|D_T^j(\omega)\,G(E_D+\omega)\,D_T^k(\omega)|\phi\rangle\,,$$

$$E_{\rm sec} = \left(\frac{4\,\pi\,Z\,\alpha}{2\,M}\,g\right)^2\epsilon^{ijk}\,I^k\int_s \frac{d\,\omega}{2\,\pi}\,\frac{1}{\omega}\,\langle\phi|(\vec\alpha\times\vec\nabla)^i\,D(\omega)\,G(E_D+\omega)\,(\vec\alpha\times\vec\nabla)^j\,D(\omega)\,|\phi\rangle\,,$$

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 $Z\alpha$

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

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

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

$\delta^{(1)} E_{\rm rec}$ 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 $Z\alpha$)

Accurate QED theory of HFS in light atoms (ions)

- 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

Discrepancies in μD hfs

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

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

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

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

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

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

- the difference

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

- Nuclear structure effects in hfs are not well understood,
  arXiv:2311.13585 is claiming an agreement without considering 3PE.

Contributions to HFS in $^3\text{He}^+$ 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
$\delta^{(1)}_{\text{rec}}$	−0.000 012 17 (60)	105.4 (5.3)
$\delta^{(2+)}_{\text{nuc}}$	−0.000 002 89(3)	25.0
$\delta^{(2)}_{\text{rec}}$	−0.000 001 16 (18)	10.1 (1.6)
theory without $\delta^{(1)}_{\text{nuc}}$	1.001 250 26 (63)	−8 667 350.8 (5.5)
experiment (Blaum:2022)	1.001 053 77	−8 665 649.865 77 (26)
$\delta^{(1)}_{\text{nuc}}$	−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	
$\widetilde{r}_Z$ (μHe$^+$:2023)	2.420(16) fm	
$\widetilde{r}_Z - r_Z$(exp) =	0.072 (18) fm	
$\widetilde{r}_Z$(μHe$^+$) - r_Z(exp) =	−0.108 (18) fm	

Polarizability contribution is relatively small in He$^+$, but for μHe$^+$ is of opposite sign !

More accurate picture of nuclear structure effects in HFS

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

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

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

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

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

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.