Lecture: 7b Applications of Perturbation Theory: Hyperfine Interaction and Zeeman Effect

In addition to the Coulomb interaction between the proton and electron that leads to the Hydrogen atom, there are perturbations due to magnetic effects. Specifically, the electron and proton are both spin ½ particles with an intrinsic mag. moment

- electron: $\hat{\vec{\mu}}_e = \gamma_e \hat{\vec{S}}$ ($\vec{S}$ = spin angular momentum of electron $s = 1/2$)

$$\gamma_e = \text{gyromagnetic ratio} = -g_e \frac{\mu_B}{\hbar}, \quad g_e = 2$$

$$\mu_e = \frac{e\hbar}{2m_e c} = \text{Bohr magneton} = h\left(1.4 \text{ MHz}/\text{Gauss}\right)$$

- proton $\hat{\vec{\mu}}_p = \gamma_p \hat{\vec{I}}$ ($\hat{\vec{I}}$ = nuclear spin = ½ for proton)

$$\gamma_p = g_p \frac{\mu_N}{\hbar}, \quad g_p \hat{=} 5.6$$

$$\mu_N = \frac{e\hbar}{2m_p c} = \left(\frac{m_e}{m_p}\right)\mu_B = \text{Nuclear magneton} = h\left(0.7 \text{ Hz}/\text{Gauss}\right)$$

In the frame of the electron it sees a magnetic field due to its orbit. This leads to electron spin-orbit coupling, which together with relativistic corrections to kinetic energy leads to fine-structure

Effects arising due to the nuclear spin $\Rightarrow$ hyperfine structure since $\mu_N \ll \mu_B$

Estimation of size of effects

Atomic units $a_0 = \dfrac{\hbar^2}{me^2}$ (Bohr radius)

$$E_0 = \frac{e^2}{a_0} = 2\,\mathbb{R} \quad (\text{"Hartree"})$$

Characteristic electron speed $\dfrac{v}{c} = \alpha = \dfrac{e^2}{\hbar c} = \dfrac{1}{137}$ (Fine Structure const.)

Recall $\alpha a_0 = \lambda\!\!\!^{-}_c = \dfrac{\hbar}{mc}$ (Compton wavelength)

$\alpha \lambda\!\!\!^{-}_c = \dfrac{e^2}{mc^2}$ (classical electron radius)

$$E_0 = \alpha^2 mc^2$$

Note $\mu_B \sim \left(\dfrac{e^2}{\hbar c}\right)\left(\dfrac{\hbar^2}{m_e e^2}\right) e = \alpha e a_0$

Fine structure energy $\sim \mu_B B = \mu_B \left(\dfrac{v}{c} \mathcal{E}\right)$

$$= \mu_B\left(\alpha \frac{e}{a_0^2}\right) = (\alpha e a_0)\left(\alpha \frac{e}{a_0^2}\right) = \alpha^2 \frac{e^2}{a_0}$$

$$= \alpha^2 E_0$$

Hyperfine structure energy $\sim \mu_N B = \left(\dfrac{m_e}{m_p}\right) \mu_B B$

$$= \left(\frac{m_e}{m_p}\right) \alpha^2 E_0$$

$m_e = 0.511$ MeV

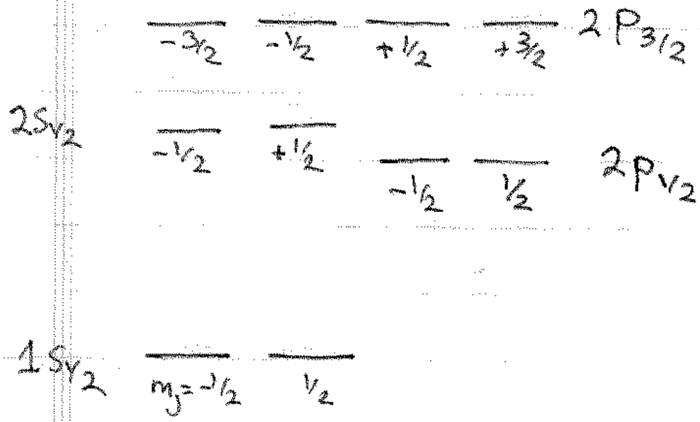
$m_p = 940$ GeV

$\dfrac{m_e}{m_p} \cong .5 \times 10^{-3}$

The total Hamiltonian is the sum:

$$\hat{H} = \underbrace{\hat{H}_{coul} + \hat{H}_{FS}}_{\hat{H}_0} + \underbrace{\hat{H}_{HF}}_{\hat{H}_1}$$

The spectrum of $\hat{H}_0$ for $n=1$ and $n=2$ appears as



- Spectroscopic labels
  $n\,l\,j$
- "Good quantum number"
  $j\ m_j\ ;\ l\ s$

Coupled representation for orbital + spin electron ang. mom $\vec{J} = \vec{L} + \vec{S}$

Perturburation Hamiltonian

$$\hat{H}_{HF} = -\hat{\vec{\mu}}_e \cdot \vec{B}^{\text{(due to proton spin)}}(\vec{x}_e) - \hat{\vec{\mu}}_N \cdot \vec{B}^{\text{(due to electron motion)}}(\vec{x}_N)$$

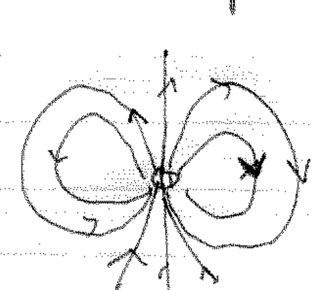
(neglect diamagnetism)

$\vec{B}$-field due to electron motion

Current loop: $\vec{B} = \dfrac{-e\,\hat{\vec{L}}}{mc\,r^3} = -2\mu_B\left(\dfrac{\hat{\boldsymbol{\ell}}}{r^3}\right)$

$\vec{B}$-field due to proton spin $\Rightarrow$ dipole field

$$\vec{B} = \vec{\nabla} \times \vec{A}, \quad \vec{A} = \vec{\mu}_N \times \frac{\vec{e}_r}{r^2}$$



$$\Rightarrow \vec{B} = \left(3\vec{\mu}_N - (\vec{\mu}_N \cdot \vec{e}_r)\vec{e}_r\right) + \frac{8\pi}{3}\vec{\mu}_N\,\delta^{(3)}(\vec{x})$$

The singularity at the origin is known as the "contact term". Physically this can be understood as the limit of a uniformly magnetized sphere whose radius shrinks to zero.

Thus we arrive at the hyperfine perturbation

$$\boxed{\hat{H}_{HF} = 2\, g_p \mu_B \mu_N \left\{ \frac{\hat{\vec{\imath}}\cdot\hat{\vec{l}}}{r^3} + \frac{3\,\hat{\vec{\imath}}\cdot\hat{\vec{s}} - (\hat{\vec{\imath}}\cdot\hat{\vec{e}}_r)(\hat{\vec{s}}\cdot\hat{\vec{e}}_r)}{r^3} + \frac{8\pi}{3}\hat{\vec{\imath}}\cdot\hat{\vec{s}}\;\delta^{(3)}(\vec{x}) \right\}}$$

<u>Hyperfine structure of $1s_{1/2}$ state of Hydrogen</u>

Without nuclear spin the $1s_{1/2}$ state is doubly degenerate

$$|1s_{1/2}, m_j = \pm 1/2\rangle = \underbrace{|n=1, l=0, m_l=0\rangle}_{|1s\rangle} \otimes \underbrace{|s=1/2, m_s=\pm 1/2\rangle}_{|\pm\rangle_e}$$

adding proton spin increases dimensionality

$i = 1/2 \Rightarrow$ Two states $\equiv |\pm\rangle_p$

Without hyperfine interaction, four degenerate states

Uncoupled representation: $|s\, m_s\rangle \otimes |i\, m_i\rangle$

$n=1$ manifold $\quad |1s\rangle \otimes \{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$

where $|++\rangle \equiv |+\rangle_e \otimes |+\rangle_p$ etc.

Now add in the hyperfine interaction

$\Longrightarrow$ Degenerate Perturbation theory.

We must diagonalize $\hat{A}_{HF}$ in 4-dim subspace

Aside: For s-state ($\ell=0$), only contact term contributes

Proof:

- $\langle 1s | \vec{\ell} | 1s \rangle = 0$ (obvious)
- $$\frac{3(\hat{\imath}\cdot\vec{e}_r)(\hat{s}\cdot\vec{e}_r) - \hat{\imath}\cdot\hat{s}}{r^3} = \hat{\imath}\cdot\left(\frac{3\vec{e}_r\vec{e}_r - \overleftrightarrow{\mathbb{1}}}{r^3}\right)\cdot\hat{s}$$

$$\frac{3\vec{e}_r\vec{e}_r - \overleftrightarrow{\mathbb{1}}}{r^3}$$ = rank-2 tensor whose angular distributions go like $Y_{2,m}(\theta,\phi)$

$$\Longrightarrow \langle 1s | \left(\frac{3\vec{e}_r\vec{e}_r - \overleftrightarrow{\mathbb{1}}}{r^3}\right) | 1s \rangle = 0$$

- Finally $\langle 1s | \delta^{(3)}(\vec{x}) | 1s \rangle = |\psi_{1s}(0)|^2 = \frac{1}{4\pi} |R_{10}(0)|^2$

Putting it all together, in the 1s manifold, after averaging over the spatial wave function

$$\hat{H}_{HF} = A\,\hat{\imath}\cdot\hat{s}$$ in 1s, acting in

space spanned by $\{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$

where $A = \frac{8\pi}{3}|\psi_{1s}(0)|^2\, 2\, g_P \mu_B \mu_N$

$$= \frac{4}{3} g_P \frac{m_e}{m_p} \alpha^4 m_e c^2$$

$$= h\,(1.42 \text{ GHz})$$

Diagonalizing $\hat{H}_{HF} = A\,\hat{\vec{I}}\cdot\hat{\vec{S}}$

Consider "coupled representation" of total angular momentum (electron + nuclear spin)

$$\vec{F} \equiv \vec{I} + \vec{J} \qquad\qquad \vec{J} \equiv \vec{L} + \vec{S}$$

Here, for s-state $\vec{L} = 0 \Rightarrow \vec{F} = \vec{I} + \vec{S}$

Coupled representation: Common eigenstates of

$$\hat{F}^2, \hat{F}_z, \hat{J}^2, \hat{I}^2$$

or $\hat{F}^2, \hat{F}_z, \hat{S}^2, \hat{I}^2$

Denote $|F, M_F\rangle$ (magnitude $S = I = 1/2$ understood)

$$\hat{F}^2 |F, M_F\rangle = F(F+1)\,|F, M_F\rangle$$
$$\hat{F}_z\,|F, M_F\rangle = M_F\,|F, M_F\rangle \qquad -F \leq M_F \leq +F$$

Now: $\hat{\vec{F}}^2 = \vec{I}^2 + \vec{J}^2 + 2\hat{\vec{I}}\cdot\hat{\vec{J}} = \hat{\vec{I}}^2 + \hat{\vec{S}}^2 + 2\hat{\vec{I}}\cdot\hat{\vec{S}}$

$$\Rightarrow \hat{\vec{I}}\cdot\hat{\vec{S}} = \frac{1}{2}\left(\hat{\vec{F}}^2 - \hat{\vec{I}}^2 - \hat{\vec{S}}^2\right) = \frac{1}{2}\left(\hat{\vec{F}}^2 - I(I+1) - S(S+1)\right)$$

$$\hat{\vec{I}}\cdot\hat{\vec{S}} = \frac{1}{2}\left(\hat{\vec{F}}^2 - \frac{3}{2}\right)$$

$\Rightarrow$ Coupled representation are the eigenstates of $\hat{\vec{I}}\cdot\hat{\vec{S}}$!

Eigenvalues: $\boxed{\frac{A}{2}\left(F(F+1) - \frac{3}{2}\right)}$

Coupled representation adding electron spin $s = 1/2$ to proton spin $I = 1/2$

Total possibles: $F_{max} = s + I = 1$ "Triplet"
$F_{min} = |s - I| = 0$ "Singlet"

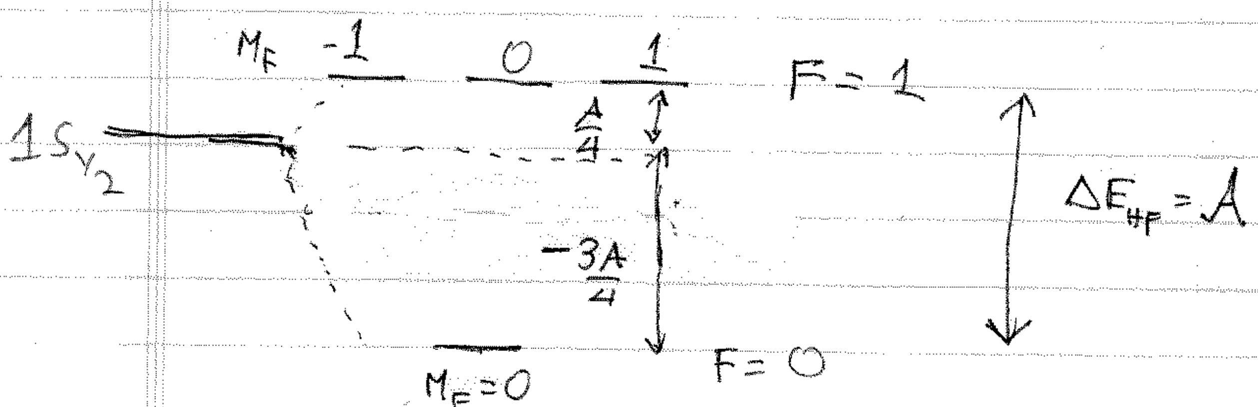
Triplet manifold

$$|F=1, M_F = \pm 1\rangle = |\pm\rangle_e \otimes |\pm\rangle_p$$

$$|F=1, M_F = 0\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle_e|-\rangle_p + |-\rangle_e|+\rangle_p\right)$$

Singlet: $|F=0, M_F=0\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle_e|-\rangle_p - |-\rangle_e|+\rangle_p\right)$

$\Rightarrow$ Hyperfine ground state of Hydrogen



The Hyperfine splitting of the ground state of Hydrogen is a very important transition in physics

$$\Delta E_{HF} \Rightarrow \text{Radio freq transition} = 21\text{ cm}$$

All of radio astronomy depends on observing this line.