Lecture # 9

Hyperfine structure & isotope shifts

So far we considered the proton to be a mass M_p charge $q = |-e|$ particle. But - it's a spin-$\frac{1}{2}$ particle

Consider interactions between $\vec{I}$ and $\vec{S}$

$$\vec{M}_N = g_I \mu_N \vec{I}/\hbar$$

- $\vec{M}_N$: magnetic moment of nucleus
- g_I: Landé factor
- μ_N: nuclear magneton
- $\vec{I}$: spin of proton
- $\vec{S}$: spin of the electron

$$\mu_N = \frac{e\hbar}{2M_p} = \frac{m}{M_p}\mu_B$$

M_p: mass of proton; μ_B: Bohr magneton; $\frac{m}{M_p} = \frac{1}{1836.15}$

Consider

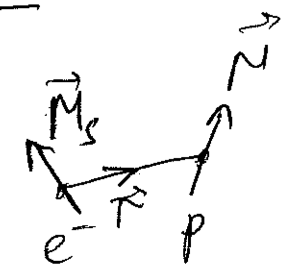
$$H = \underbrace{H_0}_{\text{only Coulomb interaction}} + H'_{fine} + H'_{hyperfine}$$

for hydrogenic atoms with $Z\alpha \ll 1$

$$H'_{hyperfine} = H'_{MD} + H'_{EQ} = \frac{\mu_0}{4\pi}\frac{2}{\hbar^2} g_I \mu_B \mu_N \frac{1}{r^3} \cdot$$

H'_{MD}: magnetic dipole; H'_{EQ}: electric quadrupole

$$\cdot \underbrace{\left[\vec{L}\cdot\vec{I} - \vec{S}\cdot\vec{I} + 3\,\frac{(\vec{S}\cdot\vec{r})(\vec{I}\cdot\vec{r})}{r^2} \right]}_{\text{for } l\neq 0\ (r\neq 0)} -$$



$$- \underbrace{\frac{\mu_0}{4\pi}\,\frac{2}{\hbar^2}\, g_I\, \mu_B \mu_N \cdot \frac{8\pi}{3}\,\delta(\vec{r})\,\vec{S}\cdot\vec{I}}_{\text{for } l=0} \;+ \Big] \leftarrow H'_{MD}$$

Fermi Contact interaction

$\vec{J} = \vec{L} + \vec{S}$

$\vec{I} \equiv \frac{\vec{I}}{\hbar}$ → here dimensionless

$$+ B\, \frac{\frac{3}{2}\,\vec{I}\cdot\vec{J}\left(2\vec{I}\cdot\vec{J}+1\right) - \vec{I}^2\vec{J}^2}{2I(2I-1)(2j-1)} \Big) \leftarrow H'_{EQ}$$

electrostatic potential created by electron s nucleus

$$Q\left\langle \frac{\partial^2 V_e}{\partial z^2}\right\rangle = Q\left\langle j, m=j \left| \frac{\partial^2 V_e}{\partial z^2} \right| j, m_j = j\right\rangle = -\left\langle j j \left| \frac{3z^2 - r^2}{r^5} \right| \ldots \right\rangle$$

→ 0 for s-states

quadrupole moment of nucleus $\quad Q_{ij} = \sum_p 3 x_{pi} x_{pj} - \delta_{ij} R_p^2$ (p ← protons in the nucleus)

$$Q = \langle I, M_I = I \,|\, Q_{zz} \,|\, I, M_I = I \rangle \quad [10^{-24}\,\mathrm{cm}^2]$$

barn

measure of deviation from spherical charge distribution

(Deuterium ⇒ deuteron ($1n + 1p$) ⇒ 0.0028 barns)

Start from H'_{MD} ⇒ find energy corrections ⇒

at $l \neq 0$ $\quad H'_{MD} = \frac{\mu_0}{4\pi}\,\frac{2}{\hbar^2}\, g_I \mu_B \mu_N \frac{1}{r^3}\,\vec{G}\cdot\vec{I}$,

$$\vec{G} = \vec{L} - \vec{S} + 3\,\frac{(\vec{S}\cdot\vec{r})\,\vec{r}}{r^2}$$

States $\Rightarrow$ $|\gamma l s j m_j I M_I\rangle$ $\leftarrow$ "unperturbed" states of $H_0 + H_{fine}'$ 3

other numbers (e.g. n) — electron — nucleus

$\{\vec{L}^2, \vec{S}^2, \vec{J}^2, J_z, \vec{I}^2, I_z\}$

$\vec{J} = \vec{L} + \vec{S}$

$\Delta E = \langle | H_{HD}' |$.

$(2j+1)(2I+1)$-fold degenerate (no m_j, M_I depend.)

Introduce total ang. mom.
$\vec{F} = \vec{I} + \vec{J}$ and $|F, M_F\rangle$

$|I+j|, \ldots, |I-j|$

$|l s j m_j I M_I\rangle \Rightarrow |l s j I F M_F\rangle$ change of basis

$-F \le M_F \le F$

Then,

$\Delta E = \frac{\mu_0}{4\pi}\frac{2}{\hbar^2} g_I \mu_B \mu_N \langle l s j I F M_F | \frac{1}{r^3} \cdot$

energy correction

Wigner-Eckart: $j(j+1)\hbar^2 \langle \alpha j m | \vec{V} | \alpha j m\rangle = \langle \alpha j m | (\vec{V}\cdot\vec{J})\vec{J} | \alpha j m\rangle$

$\cdot\, \vec{G}\cdot\vec{I} \,|\, l s j I F M_F\rangle = \frac{C}{2}\left[F(F+1) - I(I+1) - j(j+1)\right]$, where $C = \frac{\mu_0}{4\pi} 2 g_I \mu_B \mu_N \frac{1}{j(j+1)\hbar^2}\cdot$

$\vec{V} =$

$\langle \vec{G}\cdot\vec{I}\rangle = \frac{1}{j(j+1)\hbar^2}\langle(\vec{G}\cdot\vec{J})(\vec{I}\cdot\vec{J})\rangle$, $\vec{L}^2$

$\langle \frac{1}{r^3}\vec{G}\vec{J}\rangle$, $l \neq 0$

expectation value

$$\vec{G}\cdot\vec{J} = \left(\vec{L} - \vec{S} + 3\frac{(\vec{S}\cdot\vec{r})\vec{r}}{r^2}\right)(\vec{L}+\vec{S}) = $$

$\nwarrow \vec{L}\cdot\vec{r} = 0$

$$= \vec{L}^2 - \vec{S}^2 + 3\frac{(\vec{S}\cdot\vec{r})^2}{r^2} = \vec{L}^2$$

$\uparrow$ show!

Then, $\left\langle \frac{1}{r^3}\vec{G}\cdot\vec{J}\right\rangle = \hbar^2 l(l+1)\underbrace{\left\langle \frac{1}{r^3}\right\rangle}_{=\frac{Z^3}{a_\mu^3 n^3 l(l+\frac{1}{2})(l+1)}}$

$l \neq 0$

$a_0\frac{m}{\mu} \to a_\mu$

At $l=0$:

$$\Delta E = \frac{\mu_0}{4\pi}\frac{2}{\hbar^2} g_I \mu_B \mu_N \frac{8\pi}{3}\langle \delta(\vec{r})\underbrace{\vec{S}\cdot\vec{I}}_{=\frac{1}{2}(\vec{F}^2 - \vec{I}^2 - \vec{S}^2)}\rangle =$$

$\leftarrow$ at $\vec{L}=0$

$$= \frac{C_0}{2}\left[F(F+1) - I(I+1) - \frac{3}{4}\right]$$

$\uparrow S(S+1)$, $S = 1/2$

$$C_0 = \frac{\mu_0}{4\pi} 2 g_I \mu_B \mu_N \frac{8\pi}{3}\langle\delta(\vec{r})\rangle$$

$$\langle\delta(\vec{r})\rangle = \int |\Psi_{n00}|^2 \delta(\vec{r})\, d\vec{r} = |\Psi_{n00}(0)|^2 = \frac{Z^3}{\pi a_\mu^3 n^3}$$

$\uparrow$ $l=0$

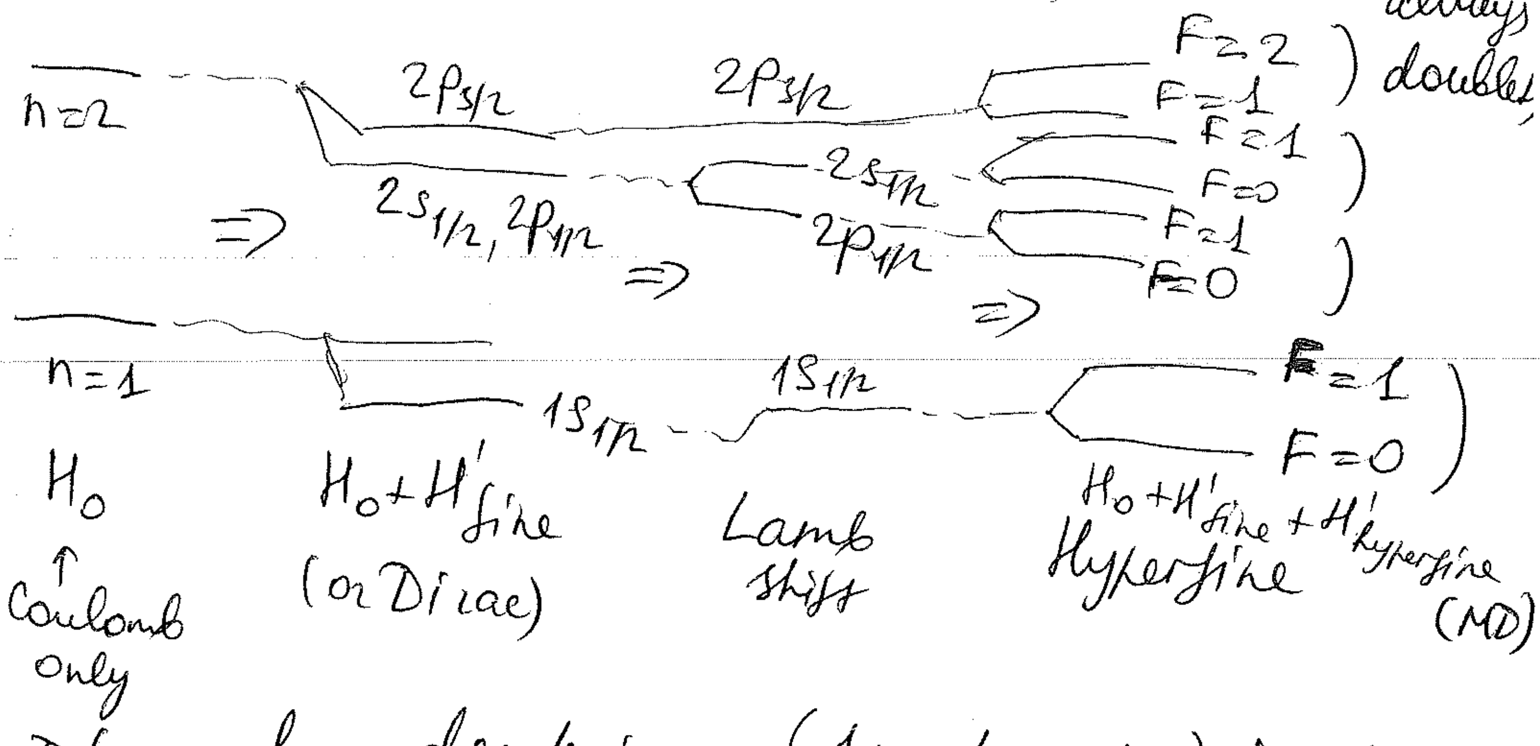
Overall (for both cases $l=0$ and $l\neq 0$) $\Rightarrow$

$$\Delta E = \frac{C}{2}\left[F(F+1) - I(I+1) - j(j+1)\right],$$

where $C = \frac{\mu_0}{4\pi} 4 g_I \mu_B \mu_N \frac{Z^3}{j(j+1)(2l+1) a_\mu^3 n^3}$

So, now energy levels depend on n, j, l, I, F $\Rightarrow$
each level with a fixed l & j $\Rightarrow$ splits further
into <u>hyperfine structure multiplet</u> $\Rightarrow F = |I-j|, \dots, I+j$

<u>(H)-atom</u> $\Rightarrow I = \frac{1}{2}$, $F = j + \frac{1}{2}, j - \frac{1}{2}$

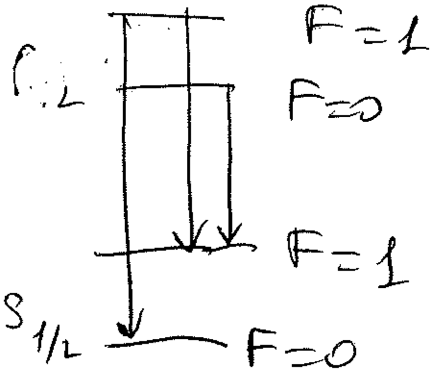


If we have deuterium $(1p + 1n + 1e)$ instead
of (H) $\Rightarrow I = 1 \Rightarrow F = j+1, j, |j-1| \Rightarrow$
doublets for $j = \frac{1}{2}$ and triplets for other j's

hyperfine separation $\Rightarrow \Delta E(F) - \Delta E(F-1) = \frac{C}{2} \cdot [F(F+1) - (F-1)F] = CF \Rightarrow \uparrow$ as $F \uparrow \Leftarrow$ interval rule

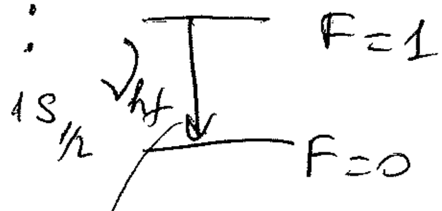
Selection rules $\Rightarrow$ $\Delta l = \pm 1$

$\Delta j = 0, \pm 1$, $\Delta F = 0, \pm 1$ except $F=0 \to F=0$



Using hyperfine transitions $\Rightarrow$ determine spin I of the nucleus

(H)-atom:



disallowed in electric dipole approx, but allowed in magnetic dipole approx.

$\Rightarrow$ $\nu_{hf} \simeq 1420\,MHz$

$\Downarrow$

$\lambda_{hf} = 21\,cm$

$\Downarrow$

this line is used in radioastronomy

$\Downarrow$

map concentration of atomic (H) in our galaxy

Note: levels are $(2F+1)$-deg.

$\Downarrow$

can remove degeneracy by external magnetic field

Now... what about ΔE_{EQ}? $\Rightarrow$

$$\Delta E_{EQ} = \langle jIFM_F | H'_{EQ} | jIFM_F \rangle = \frac{B}{4} \cdot \frac{\frac{3}{2}K(K+1) - 2I(I+1)j(j+1)}{I(2I-1)\,j(2j-1)}$$

, where $K = F(F+1) - I(I+1) - j(j+1)$

So, ΔE_{EQ} has a different behavior on F,
compared to ΔE_{MD} $\Rightarrow$ departure from the interval rule
$(E(F)-E(F-1) = CF)$
However $\rightarrow$ still have $2F+1$ - degeneracy.

<u>Note</u> that if $I = \frac{1}{2} \Rightarrow Q = 0 \Rightarrow \Delta E_{EQ} = 0$

e.g. proton

Isotope shifts

$\rightarrow$ due to mass effect $\Rightarrow \mu \leftrightarrow m$ ($\frac{Mm}{M+m}$)
(nuclear mass is finite)

$\rightarrow$ volume effect
(distribution of nuclear charge within a finite volume)

radius of the nucleus $R = r_0 A^{1/3}$ (instead of a point charge)

r_0 = 1,2 fm; A = mass number of the nucleus

$$\Delta E = \frac{Ze^2}{4\pi\varepsilon_0} \frac{2}{5} R^2 \frac{Z^4}{a_\mu^3 n^3}$$ for $l = 0$ and ≈ 0 for $l \neq 0$

most important for low n and higher Z

Also, more important for muonic atoms

$$\Rightarrow a_\mu \approx \frac{a_0 m}{m_\mu} \approx \frac{a_0}{200}$$

nucleus — μ^-: $q = -e$, $m_\mu = 200m$

$\frac{m_\mu M}{m_\mu + M} \approx m_\mu$ — not a great approxim. (much worse than for e^-)