L71-Hyperfine structure

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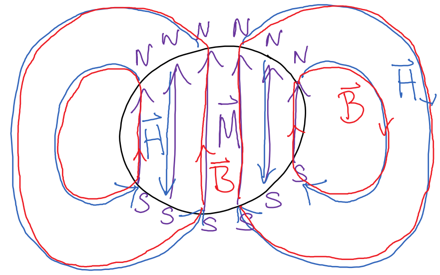
* Dipole energy: $H' = -\vec{\mu}_e \cdot \vec{B}$

- Zeeman effect: $\vec{B}_{ext}$ external field
- fine structure spin-orbit coupling: $\vec{B} = \frac{\mu_0 I}{2r} = \frac{1}{4\pi\epsilon_0} \frac{e}{mc^2 r^3} \vec{L}$
- hyperfine structure:

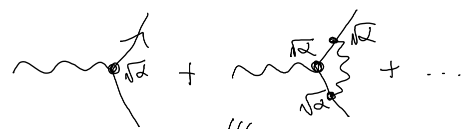
$$\vec{H}_{ext} = -\nabla U = \frac{\vec{\mu}\cdot\vec{r}}{4\pi r^3} \qquad \vec{H}_{int} = -\frac{1}{3}\vec{M}$$

$$\vec{B} = \frac{\mu_0}{4\pi}\left(3\hat{r}\,\hat{r}\cdot\vec{\mu} - \vec{\mu}\right) + \frac{2}{3}\mu_0\,\vec{\mu}\,\delta^3(\vec{r})$$



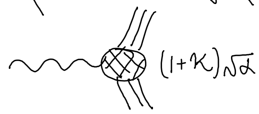
* Magnetic moment $\vec{\mu}_{e,p}$ of the electron & proton:

$$\mu_e = g_e \mu_B \vec{S}/\hbar \quad g_e = 2.00232 \approx 2\Big[1 + \underbrace{\tfrac{\alpha}{2\pi}}_{a} + O(\alpha^2)\Big] =$$



$$\mu_p = g_p \mu_N \vec{I}/\hbar \quad g_p = 5.59 \quad \text{ie} \quad \mu_p = \tfrac{1}{2} g_p \mu_N = \underbrace{2.79}_{1+\kappa_p}\mu_N$$

nuclear spin



$\mu_B = \frac{e\hbar}{2m_e}$ Bohr magneton, $\mu_N = \frac{e\hbar}{2m_p}$ Nuclear magneton

* spin-spin coupling:

$$H'_{hf} = -\mu_e \cdot \vec{B} = +g_e \mu_B/\hbar\, \vec{S} \cdot g_p \mu_N/\hbar \left[\frac{\mu_0}{4\pi}\left(3\hat{r}\,\hat{r}\cdot\vec{I} - \vec{I}\right) + \frac{2\mu_0}{3}\vec{I}\,\delta^3(\vec{r})\right]$$

$$= \frac{\mu_0 g_e g_p e^2}{16\pi m_e m_p}\left\{\underbrace{\left(3\,\vec{S}\cdot\hat{r}\,\hat{r}\cdot\vec{I} - \vec{S}\cdot\vec{I}\right)}_{\text{dipole field.}} + \underbrace{\frac{8\pi}{3}\,\vec{S}\cdot\vec{I}\,\delta^3(\vec{r})}_{\text{contact term}}\right\}$$

$$E^1_{hf} = \langle H'_{hf} \rangle$$

integrates to 0 over the sphere when $l=0$

also $|\psi_{100}(0)|^2 = \frac{1}{\pi a^3}$

$$= \frac{\mu_0 g_e g_p e^2}{6\pi m_e m_p a^3}\langle \vec{S}\cdot\vec{I}\rangle$$

looks familiar!

$$a = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = \frac{4\pi\hbar^2}{\mu_0 m_e c^2 e^2}$$

- use the same trick and couple nuclear & atomic spin

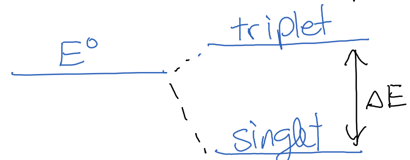
$(\vec{F} = \vec{I} + \vec{J})^2$ note if $L=0$ then $\vec{J} = \vec{S}$

$$F(F+1) = I(I+1) + S(S+1) + 2\vec{S}\cdot\vec{I}/\hbar^2$$

$I = 1/2$ $\quad F = \begin{cases} 1 & \text{triplet} \quad \uparrow\uparrow,\ \frac{1}{\sqrt{2}}(\uparrow\downarrow+\downarrow\uparrow),\ \downarrow\downarrow \\ 0 & \text{singlet} \quad \frac{1}{\sqrt{2}}(\uparrow\downarrow-\downarrow\uparrow) \end{cases}$ $\quad \frac{\vec{S}\cdot\vec{I}}{\hbar^2} = \begin{cases} \frac{1}{4} \\ -\frac{3}{4} \end{cases}$

$S = 1/2$

thus $E^1_{hf} = \underbrace{\frac{2\hbar^4 g_e g_p}{3 m_e^2 m_p c^2 \cdot a^4}} \begin{cases} 1/4 & F=1 \\ -3/4 & F=0 \end{cases}$



$\Delta E_{hf} = 5.88\,\mu\text{eV} \qquad \nu = \frac{\Delta E_{hf}}{h} \approx 1420\text{ MHz} \qquad \lambda = 21.106\text{ cm}$

Microwave.

Observed from intragalactic atomic hydrogen by Purcel in 1951, and opened up the field of radio astronomy.

Ewan, H. I.; Purcell, E. M. (September 1951). "Observation of a line in the galactic radio spectrum", *Nature*. **168** (4270): 356

* Zeeman splitting of hyperfine structure:

Including an external magnetic field, the perturbation is.

$$H'_{hf} + H'_Z = \Delta E_{hf}\frac{\vec{S}\cdot\vec{I}}{\hbar^2} + \big(\cancel{g_e\mu_B\vec{L}}_{\,l=0} + g_s\mu_B\vec{S} + \cancel{g_I\mu_N\vec{I}}\big)\cdot\vec{B}/\hbar$$

$\mu_N \approx \mu_B \cdot \frac{m_e}{m_p}$ 1836x smaller!

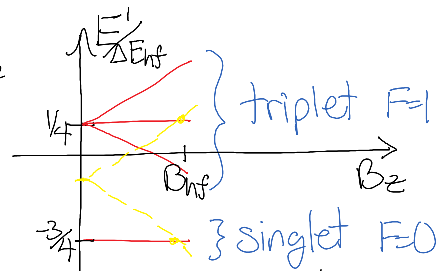
The 2 surviving terms are comparable at $B_{hf} = \frac{\Delta E_{hf}}{g_s\mu_B}$

a) for $B < B_{hf}$, H'_{hf} dominates, and F, m_F are good quantum #'s,

$$\langle H'_Z\rangle = \left\langle g_s\mu_B\frac{\vec{S}\cdot\vec{F}}{\vec{F}\cdot\vec{F}}\,\vec{F}\cdot\vec{B}/\hbar\right\rangle = \underbrace{g_s\cdot\tfrac{1}{2}}_{g_F\approx 1}\,\mu_B m_F B_z$$

using $\cancel{\vec{I}^2} = (\vec{F}-\vec{S})^2 = F^2 - 2\vec{F}\cdot\vec{S} + \cancel{\vec{S}^2}$ $\qquad I^2 = S^2 = 3/4\,\hbar^2$

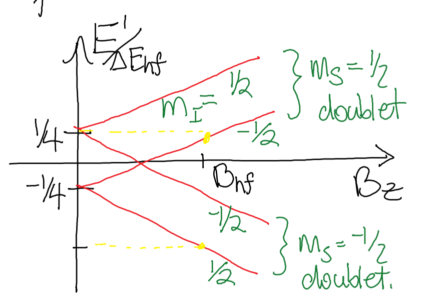
thus $E' = \Delta E_{hf}\cdot\begin{Bmatrix} 1/4 & F=1 \\ -3/4 & F=0 \end{Bmatrix} + \mu_B m_F B_z$



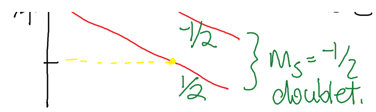
b) for $B > B_{hf}$, H'_Z dominates: M_S, M_I are good quantum numbers.

$$\langle H_{hf}\rangle = \frac{\Delta E_{hf}}{\hbar^2}\underbrace{\langle\vec{S}\rangle\cdot\langle\vec{I}\rangle}_{\text{act in different spaces}} = \Delta E_{hf}\cdot M_S\cdot M_I$$

thus $E' = \Delta E_{hf}\cdot M_S M_I + (\mu_B g_s M_s + \cancel{\mu_N g_I M_I}^{\,\text{small}})B_z$



Thus $E = \Delta E_{hf} \cdot M_S M_I + (\mu_B g_S M_S + \cancel{\mu_N} g_I M_I) B_z$



c) In the intermediate region, we must solve the full eigenvalue problem. Write out both perturbations in the same basis - either works.

Write each perturbation in matrix form in its natural basis:

$$\mathcal{H}_{hf} = \Delta E_{hf} \frac{\vec{S}\cdot\vec{I}}{\hbar} = \begin{array}{c c} & \begin{array}{cccc} |11\rangle & |10\rangle & |00\rangle & |1\text{-}1\rangle \end{array} \\ \begin{array}{c} |11\rangle \\ |10\rangle \\ |00\rangle \\ |1\text{-}1\rangle \end{array} & \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -3 & \\ & & & 1 \end{pmatrix} \end{array} \cdot \Delta E_{hf}/4 \quad \text{in the } |F, M_F\rangle \text{ basis}$$

$$\mathcal{H}_Z = g_S \mu_B \vec{S}\cdot\vec{B}/\hbar = \begin{array}{c c} & \begin{array}{cccc} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \begin{array}{c} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{array} & \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \end{array} \cdot \mu_B B_z \quad \text{in the } |M_I, M_S\rangle \text{ basis.}$$

* Transform each matrix to the other "unnatural" basis:

$|11\rangle = |\uparrow\uparrow\rangle$ are
$|1\text{-}1\rangle = |\downarrow\downarrow\rangle$ easy!

$|10\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\uparrow\downarrow\rangle)$
$|00\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

or

$|\uparrow\downarrow\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |00\rangle)$
$|\downarrow\uparrow\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |00\rangle)$

Ex. #1: $\mathcal{H}'_{hf}\underset{\text{--- }|\downarrow\uparrow\rangle}{|\uparrow\downarrow\rangle} = \mathcal{H}_{hf}\frac{1}{\sqrt{2}}(|10\rangle \underset{\text{--- (−) ---}}{+} |00\rangle) = \frac{1}{\sqrt{2}}[1\cdot|10\rangle \underset{\text{--- (+) ---}}{-3}\cdot|00\rangle]$

$= \frac{1}{\sqrt{2}}\left[1\cdot\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \underset{\text{--- (+) ---}}{-3}\cdot\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right] = \underset{(2)\cdot\text{ ---}}{-1}\cdot|\uparrow\downarrow\rangle + \underset{(-1)\cdot\text{ ---}}{2}\cdot|\downarrow\uparrow\rangle$

Ex. #2: $\mathcal{H}'_Z\underset{\text{--- }|00\rangle}{|10\rangle} = \mathcal{H}_Z\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle \underset{\text{--- (−) ---}}{+} |\downarrow\uparrow\rangle) = \frac{1}{\sqrt{2}}[-1\cdot|\uparrow\downarrow\rangle \underset{\text{--- (−) ---}}{+} 1\cdot|\uparrow\downarrow\rangle]$

$= \frac{1}{\sqrt{2}}\left[-1\cdot\frac{1}{\sqrt{2}}(|10\rangle + |00\rangle) \underset{(-)}{+} 1\cdot\frac{1}{\sqrt{2}}(|10\rangle - |00\rangle)\right] = -1\cdot\underset{\text{--- }|10\rangle}{|00\rangle}$

$$\mathcal{H}' = \mathcal{H}'_{hf} + \mathcal{H}'_Z = \begin{array}{c c} & \begin{array}{cccc} |11\rangle & |10\rangle & |00\rangle & |1\text{-}1\rangle \end{array} \\ \begin{array}{c} |11\rangle \\ |10\rangle \\ |00\rangle \\ |1\text{-}1\rangle \end{array} & \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -3 & \\ & & & 1 \end{pmatrix} \end{array} \cdot \underbrace{\Delta E_{hf}/4}_{a} + \begin{array}{c c} & \begin{array}{cccc} |11\rangle & |10\rangle & |00\rangle & |1\text{-}1\rangle \end{array} \\ \begin{array}{c} |11\rangle \\ |10\rangle \\ |00\rangle \\ |1\text{-}1\rangle \end{array} & \begin{pmatrix} 1 & & & \\ & 0 & -1 & \\ & -1 & 0 & \\ & & & -1 \end{pmatrix} \end{array} \cdot \underbrace{\mu_B B_z}_{b} = \begin{array}{c c} & \begin{array}{cccc} |11\rangle & |10\rangle & |00\rangle & |1\text{-}1\rangle \end{array} \\ \begin{array}{c} |11\rangle \\ |10\rangle \\ |00\rangle \\ |1\text{-}1\rangle \end{array} & \begin{pmatrix} a+b & & & \\ & a & -b & \\ & -b & -3a & \\ & & & a-b \end{pmatrix} \end{array}$$

in the $|FM_F\rangle$ basis where $\mathcal{H}'_{hf}$ is already diagonal.

$$\mathcal{H}' = \mathcal{H}'_{hf} + \mathcal{H}'_Z = \begin{array}{c c} & \begin{array}{cccc} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \begin{array}{c} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{array} & \begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix} \end{array} \cdot \underbrace{\Delta E_{hf}/4}_{a} + \begin{array}{c c} & \begin{array}{cccc} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \begin{array}{c} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{array} & \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \end{array} \cdot \underbrace{\mu_B B_z}_{b} = \begin{array}{c c} & \begin{array}{cccc} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \begin{array}{c} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{array} & \begin{pmatrix} a+b & & & \\ & -a-b & 2a & \\ & 2a & -a+b & \\ & & & a-b \end{pmatrix} \end{array}$$

in the $|FM_F\rangle$ basis where $\mathcal{H}'_{hf}$ is already diagonal.

* Diagonalize either of these to obtain exact perturbations: we only need to diagonalize a 2x2 submatrix (boxed elements).

EIGENVALUES in $|F m_F\rangle$ basis:

$$\begin{vmatrix} a-\lambda & -b \\ -b & -3a-\lambda \end{vmatrix} = (a-\lambda)(-3a-\lambda)-(-b)(-b) = \lambda^2+2a\lambda+(-3a^2-b^2)=0$$

$$\lambda_\pm = -a \pm \sqrt{(-a)^2-(-3a^2-b^2)} = -a \pm \sqrt{4a^2+b^2}$$ hyperbola.

$$\lim_{b\to 0} \lambda_\pm = -a \pm 2a\left(1+\tfrac{1}{2}\cdot\tfrac{b^2}{4a^2}+\dots\right)$$

$\lambda_+ \to a + \tfrac{1}{4} b^2/a + \dots$

$\lambda_- \to -3a - \tfrac{1}{4} b^2/a + \dots$ parabola

$$\lim_{b\to\infty} \lambda_\pm = -a \pm b\left(1+\tfrac{1}{2}\tfrac{4a^2}{b^2}+\dots\right)$$

$\lambda_+ \to b - a + 2a^2/b + \dots$

$\lambda_- \to -b - a - 2a^2/b + \dots$

linear hf shift. flattening out.

EIGENVALUES in $|m_I m_S\rangle$ basis:

$$\begin{vmatrix} -a-b-\lambda & 2a \\ 2a & -a+b-\lambda \end{vmatrix} = (-a-b-\lambda)(-a+b-\lambda)-(2a)^2 = \lambda^2+2a\lambda+(-3a^2-b^2)=0$$

this is the same charateristic equation $\Rightarrow$ same solutions.

EIGENVECTORS: in $|F m_F\rangle$ basis:

$$\begin{pmatrix} a-(-a\pm\sqrt{4a^2+b^2}) & -b \\ -b & -3a-(-a\pm\sqrt{4a^2+b^2}) \end{pmatrix}\begin{pmatrix} c_{10} \\ c_{00} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} c_{10} \\ c_{00} \end{pmatrix} = \underbrace{\begin{pmatrix} b \\ 2a\mp\sqrt{4a^2+b^2} \end{pmatrix}}_{\text{(row 1)}} = \underbrace{\begin{pmatrix} -2a\mp\sqrt{4a^2+b^2} \\ b \end{pmatrix}}_{\text{(row 2)}} \cdot \frac{2a\mp\sqrt{4a^2+b^2}}{b}$$

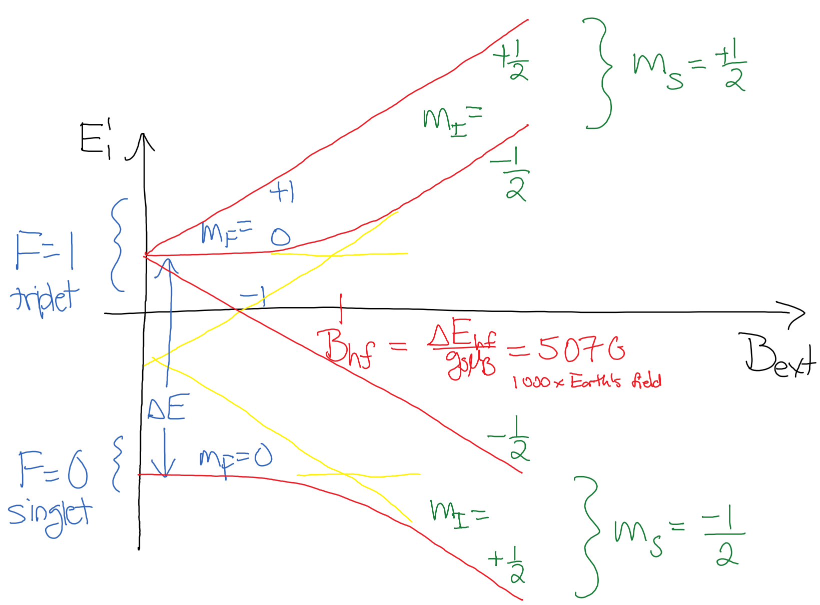
$$\begin{pmatrix} c_{10} \\ c_{00} \end{pmatrix} = N\cdot\begin{pmatrix} (-2a+b)\mp\sqrt{4a^2+b^2} \\ (2a+b)\mp\sqrt{4a^2+b^2} \end{pmatrix}$$

take sum of row 1,2. still an eigenvector, but symmetric.

$$c_{10}^2+c_{00}^2 = N^2\Big([(-2a+b)^2\mp 2(-2a+b)\sqrt{4a^2+b^2}+(4a^2+b^2)] + [(2a+b)^2\mp 2(2a+b)\sqrt{4a^2+b^2}+(4a^2+b^2)]\Big) = 1$$

$$N = \tfrac{1}{2}\left((4a^2+b^2)\mp 2b\sqrt{4a^2+b^2}\right)^{-1/2}$$

the limit is $\binom{1}{0},\binom{0}{1}$ as $b\to 0$, and $\frac{1}{\sqrt{2}}\binom{1}{1}, \frac{1}{\sqrt{2}}\binom{-1}{1}$ as $b\to\infty$



if $B \ll B_{hf}$

then F, m_F are good quantum #'s

if $B \gg B_{hf}$

then m_S, m_I are good quantum #'s.