Hydrogen in a magnetic field

The effect of a small magnetic field is smaller than the fine-structure splitting so we can solve the problem in two steps

(1) Find the fine structure
(2) perturb the fine structure due to the field

This weak field regime is called the Zeeman regime.

When $\vec{H}$ is large, the fine structure is small compared to the energy shifts due to the field (called the Paschen-Back regime)

We will solve the general case and then extract the limiting behavior.

The orbital magnetic moment of the electron is

$$\vec{\mu}_{orb} = -\mu_0 \vec{L}$$

$$\mu_0 = \frac{e\hbar}{2mc} = \text{Bohr magneton} = 0.579 \times 10^{-8}\ \text{eV/gauss}$$

The spin magnetic moment is

$$\mu_{spin} = -2\mu_0 \vec{S}$$

It is the extra factor of 2 that makes life difficult.

$$\hat{V}_{mag} = \mu_0 \vec{H} \cdot (\vec{L} + 2\vec{S}) = \mu_0 \vec{H} \cdot (\vec{J} + \vec{S})$$

choose the z direction along $\vec{H}$ $\quad \vec{H} = H\vec{e}_z$

Then S^2, L^2 L_z and S_z commute with $\hat{V}_{mag}$

But L_z and S_z do not separately commute with $\hat{V}_{\text{Fine structure}}$

only the sum does.

This implies the field will mix states and we do not know the parallel ~~~~ directions in the degenerate subspace.

One important note: $\hat{L}_z + 2\hat{S}_z$ is an even parity operator, so it cannot connect states with different parity
$\Rightarrow$ l must be the same or differ by a multiple of 2 as $l+1$ is different parity from l.
This reduces a lot of our work.

We have eight degenerate energy levels $2P_{3/2}$ $2P_{1/2}$ $2S_{1/2}$
$\qquad 4 \quad 2 \quad 2$

Because of the parity argument, the $2S_{1/2}$ state cannot connect to $2P_{3/2}$ or $2P_{1/2}$ $\Rightarrow$ S is a $\parallel$ direction.
Similarly $2P_{3/2}$ $m = \pm 3/2$ cannot couple since J_z is a good quantum number since $\hat{L}_z + \hat{S}_z$ commutes with $\hat{H}$
So only $2P_{3/2}$ $m = 1/2$ and $2P_{1/2}$ $m = 1/2$ couple
and $2P_{3/2}$ $m = -1/2$ and $2P_{1/2}$ $m = -1/2$

Hence we reduce from an 8×8 subspace to four 1×1 subspaces

$2P_{3/2}\ m=3/2 \qquad 2P_{3/2}\ m=-3/2 \qquad 2S_{1/2}\ m=1/2 \qquad 2S_{1/2}\ m=-\frac{1}{2}$

and two 2×2 subspaces

$2P_{3/2}\ m=1/2 \qquad 2P_{1/2}\ m=1/2$

$2P_{3/2}\ m=-1/2 \qquad 2P_{1/2}\ m=-1/2$

First examine the 1×1 subspaces which can be analyzed with non degenerate PT

$$\Delta E_{mag} = \langle n l j m | J_z + S_z | n l j m \rangle \mu_0 H$$

$$= \mu_0 H \left(m + \langle n l j m | S_z | n l j m \rangle \right)$$

The radial part of the overlap is 1

the angular momentum is tricky - need to change basis

from $s l j m$ to $l m_l s m_s$

$$\langle s l j m | S_z | s l j m \rangle = \sum_{m_l m_s} \langle s l j m | l m_l s m_s \rangle \langle l m_l s m_s | S_z | s l j m \rangle$$

$$= \sum_{m_l m_s} m_s \left| \langle s l j m | l m_l s m_s \rangle \right|^2$$

Clebsch-Gordon Coefficient

use ~~table derived in class~~

$$\cancel{= \frac{1}{2} \sum_{m_l} \left(\frac{l+m_l+1}{2l+1} - \frac{l-m_l+1}{2l+1} \right) \quad \text{for } j = l+\frac{1}{2}}$$

$$\cancel{= \frac{1}{2} \sum_{m_l} \left(\frac{l-m_l}{2l+1} - \frac{l+m_l}{2l+1} \right) \quad \text{for } j = l-\frac{1}{2}}$$

$$\cancel{= \frac{1}{2} \sum_{m_l=-l}^{l} \frac{2m_l}{2l+1}}$$

We already showed
$$|l+\tfrac{1}{2}, m\rangle = \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\,|m_l = m-\tfrac{1}{2}\ m_s = \tfrac{1}{2}\rangle + \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\,|m_l = m+\tfrac{1}{2}\ m_s = -\tfrac{1}{2}\rangle$$
$$|l-\tfrac{1}{2}, m\rangle = -\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\,|m_l = m-\tfrac{1}{2}, m_s = \tfrac{1}{2}\rangle + \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\,|m_l = m+\tfrac{1}{2}, m_s = \tfrac{1}{2}\rangle$$

so for $j = l+\frac{1}{2}$ (only two m_l terms contribute to each sum)

$$= \frac{1}{2}\,\frac{l+m+\frac{1}{2}}{2l+1} - \frac{1}{2}\,\frac{l-m+\frac{1}{2}}{2l+1} = \frac{m}{2l+1}$$

for $j = l-\frac{1}{2}$ (only two m_l terms contribute)
$$= \frac{1}{2}\,\frac{l-m+\frac{1}{2}}{2l+1} + \frac{1}{2}\,\frac{l+m+\frac{1}{2}}{2l+1} = -\frac{m}{2l+1}$$

so $\langle s\, l\, j\, m | s_z | s\, l\, j\, m\rangle = \pm \frac{m}{2l+1}$ for $j = l \pm \frac{1}{2}$

$$\Delta E_{mag} = \mu_0 H \left(m \pm \frac{m}{2l+1}\right) = \mu_0 H m \left(\frac{2l+1\pm 1}{2l+1}\right)$$

recall $\Delta E_{FS} = E_n^0 \frac{\alpha^2}{n^2}\left[\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right]$

so $\Delta E\,(2P_{3/2}\ m = \pm 3/2) = E_2^0 \frac{\alpha^2}{4}\left[\frac{1}{4}\right] \pm \mu_0 H \frac{3}{2}\cdot\frac{4}{3}$
$$= \boxed{E_2^0 \frac{\alpha^2}{16} \pm 2\mu_0 H}$$

$\Delta E\,(2S_{1/2}\ m = \pm 1/2) = E_2^0 \frac{\alpha^2}{4}\left[\frac{5}{4}\right] \pm \mu_0 H \frac{1}{2}\cdot 2$
$$= \boxed{E_2^0 \frac{5}{16}\alpha^2 \pm \mu_0 H}$$

now onto the 2x2 cases

The diagonal FS matrix elements are

$$\alpha^2 \frac{E_2^0}{4}\left[\frac{2}{2}-\frac{3}{4}\right] = \frac{E_2^0}{16}\alpha^2 \qquad j=3/2$$

$$\alpha^2 \frac{E_2^0}{4}\left[\frac{2}{1}-\frac{3}{4}\right] = \frac{5}{16}E_2^0\alpha^2 \qquad j=1/2$$

The diagonal magnetic matrix elements are

$$\mu_0 H m \frac{2l+1\pm1}{2l+1} = \begin{cases} \pm\frac{2}{3}\mu_0 H & j=3/2 \text{ since } \pm\frac{1}{2}*\frac{4}{3} \\ \pm\frac{1}{3}\mu_0 H & j=1/2 \text{ since } \pm\frac{1}{2}*\frac{2}{3} \end{cases}$$

The off diagonal are

$$\langle P_{1/2}\, m | S_z | P_{3/2}\, m\rangle = \sum_{m_l m_s} \langle s=\tfrac{1}{2}\; l=1\; j=\tfrac{1}{2}\; m | S_z | s=\tfrac{1}{2}\; l=1\; m_l\, m_s\rangle$$

$$* \langle s=\tfrac{1}{2}\; l=1\; m_l\, m_s | s=\tfrac{1}{2}\; l=1\; j=3/2\; m\rangle$$

$$= \sum_{m_l m_s} m_s \langle s=\tfrac{1}{2}\; l=1\; j=\tfrac{1}{2}\; m | s=\tfrac{1}{2}\; l=1\, m_l m_s\rangle\langle s=\tfrac{1}{2}\; l=1\; m_l m_s | s=\tfrac{1}{2}\; l=1\; j=3/2\rangle$$

only two m_l values contribute

$$= \frac{1}{2}\left(-\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\right) - \frac{1}{2}\left(\sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\right)$$

$$= -\frac{1}{2}\frac{1}{2l+1}\sqrt{(l+\tfrac{1}{2})^2-m^2} * 2 \qquad \text{for } m=\pm 1/2,\ l=1$$

we get

$$= -\frac{1}{3}\sqrt{\frac{9}{4}-\frac{1}{4}} = -\frac{\sqrt{2}}{3} \qquad \text{for } m=\pm 1/2$$

So off diagonal elements are $-\mu_0 H \frac{\sqrt{2}}{3}$

The matrix is

$$\det\begin{pmatrix} \frac{\alpha^2 E_2^0}{16} \pm \frac{2}{3}\mu_0 H - \varepsilon & -\mu_0 H\frac{\sqrt{2}}{3} \\ -\mu_0 H\frac{\sqrt{2}}{3} & \frac{5\alpha^2 E_2^0}{16} \pm \frac{1}{3}\mu_0 H - \varepsilon \end{pmatrix} = 0$$

$$\varepsilon^2 - \varepsilon\left(\tfrac{3}{8}\alpha^2 E_2^0 \pm \mu_0 H\right) + \tfrac{5}{256}\alpha^4 (E_2^0)^2 \pm \tfrac{11}{48}\alpha^2 E_2^0 \mu_0 H = 0$$

these signs correspond to the two roots

$$\varepsilon = \tfrac{3}{16}\alpha^2 E_2^0 \pm \tfrac{1}{2}\mu_0 H \pm \tfrac{1}{2}\sqrt{\tfrac{1}{16}\alpha^4 (E_2^0)^2 \mp \tfrac{1}{6}\alpha^2 E_2^0 \mu_0 H + \mu_0^2 H^2}$$

these signs correspond to $m_j = \pm\frac{1}{2}$

$$\Delta E\left(^2P_{3/2} \,\&\, ^2P_{1/2},\ m_j = \tfrac{1}{2}\right) = \tfrac{3}{16}\alpha^2 E_2^0 + \tfrac{1}{2}\mu_0 H \pm \tfrac{1}{2}\sqrt{\tfrac{1}{16}\alpha^4 (E_2^0)^2 - \tfrac{1}{6}\alpha^2 E_2^0 \mu_0 H + \mu_0^2 H^2}$$

$$\Delta E\left(^2P_{3/2} \,\&\, ^2P_{1/2},\ m_j = -\tfrac{1}{2}\right) = \tfrac{3}{16}\alpha^2 E_2^0 - \tfrac{1}{2}\mu_0 H \pm \tfrac{1}{2}\sqrt{\tfrac{1}{16}\alpha^4 (E_2^0)^2 + \tfrac{1}{6}\alpha^2 E_2^0 \mu_0 H + \mu_0^2 H^2}$$

Small H limit — $m_j = +\frac{1}{2}$: $\frac{3}{16}\alpha^2 E_2^0 \pm \frac{1}{8}\alpha^2 E_2^0 + \frac{1}{2}\mu_0 H \pm \frac{1}{8}\alpha^2 E_2^0 \cdot \left(-\frac{16}{6}\frac{\mu_0 H}{\alpha^2 E_2^0}\right)\frac{1}{2}$

$$\tfrac{5}{16}\alpha^2 E_2^0 + \tfrac{1}{3}\mu_0 H$$

$$\tfrac{1}{16}\alpha^2 E_2^0 + \tfrac{2}{3}\mu_0 H$$

$m_j = -\frac{1}{2}$: $\frac{3}{16}\alpha^2 E_2^0 \pm \frac{1}{8}\alpha^2 E_2^0 - \frac{1}{2}\mu_0 H \pm \frac{1}{8}\alpha^2 E_2^0 \left(\frac{16}{6}\frac{\mu_0 H}{\alpha^2 E_2^0}\right)\frac{1}{2}$

$$\tfrac{5}{16}\alpha^2 E_2^0 - \tfrac{1}{3}\mu_0 H$$

$$\tfrac{1}{16}\alpha^2 E_2^0 - \tfrac{2}{3}\mu_0 H$$

which can be read of the above matrix with H small

large H limit: ~~Both $m_j = \pm\frac{1}{2}$~~

$m_j = +\frac{1}{2}$ $\quad \frac{1}{2}\mu_0 H \pm \frac{1}{2}\mu_0 H = \begin{cases}\mu_0 H \\ 0\end{cases}$

$m_j = -\frac{1}{2}$ $\quad -\frac{1}{2}\mu_0 H \pm \frac{1}{2}\mu_0 H = \begin{cases}-\mu_0 H \\ 0\end{cases}$

which is $j_z + s_z$ when we think of j_z and s_z as independent.