OPTI 570 LECTURE NOV 25

Relativistic motion of the electron

energy: $E = c\sqrt{p^2 + m^2c^2}$

3 primary effects

1. **Relativistic**:
   - 0^{th} order energy: mc^2 - rest mass energy
   - 1^{st} order: $\frac{p^2}{2m}$ - already
   - 2^{nd} order: $-\frac{p^4}{8m^3c^2}$ - perturbation term

2. **Darwin term**: $\frac{\pi^2 q^2 \hbar^2}{2m^2c^2}\,\delta(\vec{R})$

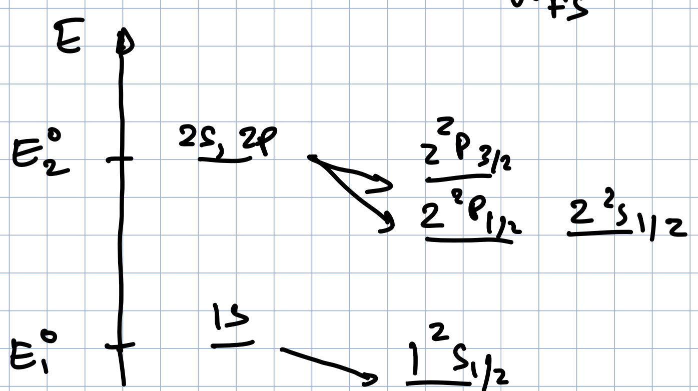
   non-zero for $L=0$ state

3. **Spin-orbit coupling**

$$\frac{q^2}{2m^2c^2R^3}\,\vec{L}\cdot\vec{S}$$

Hamiltonian - fine structure

$$H = mc^2 + \underbrace{\underbrace{\frac{p^2}{2m} - \frac{q^2}{R}}_{H_0} - \underbrace{\frac{p^4}{8m^3c^2}}_{W_{rel}} + \underbrace{\frac{\pi^2 q^2\hbar^2}{2m^2c^2}\,\delta(R)}_{W_D} + \underbrace{\frac{q^2}{2m^2c^2R^3}\,\vec{L}\cdot\vec{S}}_{W_{SO}}}_{W_{FS}}$$



What is magnitude of W

$$E_I = \frac{q^2}{2a_0} = 13.6\,eV, \quad E_n = -\frac{E_I}{n^2}, \quad n = 1, 2, 3 \ldots$$

$$a_0 = \frac{\hbar^2}{mq^2}$$

$$\Rightarrow E_I = \frac{1}{2} mc^2 \alpha^2 \qquad \alpha = \frac{q^2}{\hbar c} \simeq \frac{1}{137}$$

$$\Rightarrow E_I \sim \alpha^2 \cdot E_0$$

$$\alpha^2 \simeq \frac{1}{137^2} \ll 1 \Rightarrow E_n^0 \ll mc^2$$

$$W_{rel} \simeq \alpha^4 \cdot E_0 \simeq \alpha^2 E_I$$

<u>Hydrogen fine structure</u>

$$\{|n\,l\,m_l\rangle \otimes \{|s = \tfrac{1}{2}, m_s\rangle\}$$

$$|\pm\rangle_z$$

$$\{\underbrace{|100\rangle|+\rangle, |100\rangle|-\rangle}_{1s \text{ states}}, \underbrace{|200\rangle|+\rangle, |200\rangle|-\rangle}_{2s \text{ state}}, \underbrace{|211\rangle|+\rangle, |211\rangle|-\rangle \ldots}_{2p \text{ states}}\}$$

$l = 1, \; m_l = -1, 0, 1$

$s = \frac{1}{2} \quad m_s = \pm\frac{1}{2}$

$$H_0 \to -E_I \begin{pmatrix} 1 & 0 & & & & & & & & \\ 0 & 1 & & 0 & & & \phi & & & \\ 0 & 0 & \frac{1}{4} & 0 & & & & & & \\ 0 & 0 & 0 & \frac{1}{4} & & & & & & \\ & & & & \frac{1}{4} & 0 & 0 & 0 & & \\ & & & & & \frac{1}{4} & 0 & 0 & \phi & \\ & \phi & & & & & \frac{1}{4} & 0 & & \\ & & & & & & & \frac{1}{4} & & \\ & & & & & \phi & & & \frac{1}{4} & \\ & & & & & & & & & \frac{1}{4} \end{pmatrix}$$

$$W_{D,rel} = W_D + W_{rel}$$

$$\langle n' \ell' m_\ell' | W_{D,rel} | n \ell m_\ell \rangle \langle m_s | m_s' \rangle$$

$$W_{D,rel} \to -\frac{\alpha^2}{4} E_I \left(\begin{array}{c|c|c} \underbrace{\begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix}}_{1s} & \multicolumn{2}{c}{\text{non-zero}} \\ \hline \text{non-zero} & \underbrace{\begin{matrix} \frac{5}{16} & 0 \\ 0 & \frac{5}{16} \end{matrix}}_{2s} & \phi \\ \hline & \phi & \underbrace{\begin{matrix} \frac{7}{48} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{7}{48} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{7}{48} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{7}{48} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{7}{48} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{7}{48} \end{matrix}}_{2p} \end{array} \right)$$

→ energies modified by eigenvalues of each block.

→ $W_{D,rel.}$ breaks degeneracy of 2s and 2p

\+ Spin-orbit coupling

$$W_{so} = \frac{q^2}{2m^2c^2R^3} \vec{L} \cdot \vec{S}$$

$L = 0 \Rightarrow W_{so} = 0$ only $L = 1$

$\bar{J} = \bar{L} + \bar{S} \Rightarrow J^2 = L^2 + S^2 + 2\bar{L}\cdot\bar{S}$

$$\bar{L}\cdot\bar{S} = \frac{1}{2}(J^2 - L^2 - S^2)$$

$$W_{so} = \frac{1}{2} \frac{q^2}{2m^2c^2} \cdot \underbrace{\frac{1}{R^3}}_{\text{radial integral}} \cdot \underbrace{(J^2 - L^2 - S^2)}_{\text{angular integral}}$$

$$\langle n' = 2, \ell' = 1, s' = \tfrac{1}{2}, m_\ell', m_s' | W_{so} | n = 2, \ell = 1, s = \tfrac{1}{2}, m_\ell, m_s \rangle =$$

$$= \frac{1}{2}\,\underbrace{\frac{q^2}{2m^2c^2}}\,\underbrace{\langle n'=2, l'=1 \,|\, \frac{1}{R^3} \,|\, n=2, l=1\rangle}\,\underbrace{\langle l'=1, s'=\tfrac{1}{2}, m_l' m_s' \,|\, J^2 - L^2 - S^2 \,|\, l=1, s=\tfrac{1}{2}, m_l, m_s\rangle}$$

$$\xi_{2p} \equiv \frac{1}{48\hbar^2}\, mc^2\alpha^4 = \frac{E_I\,\alpha^2}{24\hbar^2}$$

$$W_{so}^{(2p)} \to \frac{\alpha^2 E_I}{48}\;
\begin{array}{c}
\begin{array}{cccccc} |211\rangle|+\rangle & |211\rangle|-\rangle & \cdot & \cdot & \cdot & \cdot \end{array}\\
\begin{pmatrix}
1 & & & & & \\
 & -1 & \sqrt{2} & & & \\
 & \sqrt{2} & 0 & & & \\
 & & & 0 & \sqrt{2} & \\
 & & & \sqrt{2} & -1 & \\
 & & & & & 1
\end{pmatrix}
\end{array}$$

$L = 1,\ S = \frac{1}{2} \Rightarrow J = \frac{3}{2} \quad m_J = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$

$J = \frac{1}{2} \quad m_J = -\frac{1}{2}, \frac{1}{2}$

TAM basis: $\{ |\frac{3}{2},\frac{3}{2}\rangle, |\frac{3}{2},\frac{1}{2}\rangle, |\frac{1}{2},\frac{1}{2}\rangle, |\frac{3}{2},-\frac{1}{2}\rangle, |\frac{1}{2},-\frac{1}{2}\rangle, |\frac{3}{2},-\frac{3}{2}\rangle$

$J^2 - L^2 - S^2$

$J = \frac{3}{2}$: $\frac{3}{2}\cdot\frac{5}{2}\hbar^2 - 1\cdot 2\cdot\hbar^2 - \frac{1}{2}\cdot\frac{3}{2}\cdot\hbar^2 = \hbar^2$

$J = \frac{1}{2}$: $-2\hbar^2$

$$W_{so}^{(2p)} \to \frac{\alpha^2}{48} E_I \begin{pmatrix} 1 & & & & & \\ & 1 & & & \phi & \\ & & -2 & & & \\ & & & 1 & & \\ & \phi & & & -2 & \\ & & & & & 1 \end{pmatrix}$$

$$W_{so}^{(2p)}{}_{\{j,m_j\}} = M^{\dagger}\, W_{so}^{(2p)}{}_{\{m_l,m_s\}}\, M$$

$$H = \begin{pmatrix} 1 & & & & & \\ & \sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} & & & \\ & \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{3}} & & & \\ & & & \sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} & \\ & & & \sqrt{\frac{1}{3}} & -\sqrt{\frac{2}{3}} & \\ & & & & & 1 \end{pmatrix}$$

$1 \times \frac{1}{2}$ CG table

$$H = H_0 + W_{rel} + W_D + W_{SO}$$

state	$\langle H_0 \rangle$	$\langle W_D + W_{rel} \rangle$	$\langle W_{SO} \rangle$	E tot
$1^2S_{\frac{1}{2}}$	$E_1^0 = -E_I$	$E_I \frac{\alpha^2}{I} - \frac{5}{4}\frac{\alpha^2}{4} E_I = -\frac{E_I \alpha^2}{4}$	0	$E_1^0 - \frac{16}{64} \cdot E_I \alpha^2$
$2^2S_{\frac{1}{2}}$	$-\frac{E_I}{4}$	$-\frac{5}{16} \frac{E_I \alpha^2}{4}$	0	$E_2^0 - \frac{5}{64} E_I \alpha^2$
$2^2P_{\frac{1}{2}}$	$-\frac{E_I}{4}$	$-\frac{7}{48}\left(\frac{E_I}{4}\right)\alpha^2$	$-\frac{1}{6}\left(\frac{E_I}{4}\right)\alpha^2$	$E_2^0 - \frac{5}{64} E_I \alpha^2$
$2^2P_{\frac{3}{2}}$	$-\frac{E_I}{4}$	$-\frac{7}{48}\left(\frac{E_I}{4}\right)\alpha^2$	$\frac{1}{12}\left(\frac{E_I}{4}\right)\alpha^2$	$E_2^0 - \frac{1}{64} E_I \alpha^2$

General form of hydrogen fine structure

$$E_{n,J} \simeq E_n^0 \left[1 + \frac{\alpha^2}{n^2} \left(\frac{n}{J + \frac{1}{2}} - \frac{3}{4} \right) \right]$$

$\approx 5 \cdot 10^{-5}$ - Small energy shift

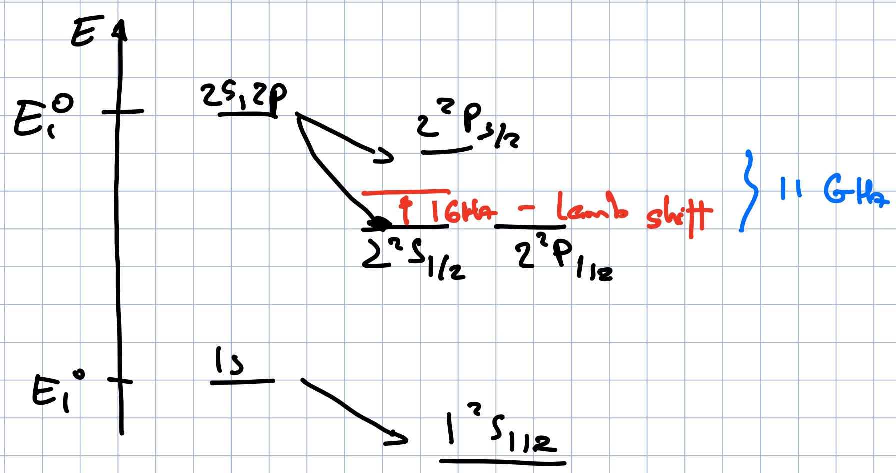
new basis:

$$H_{\text{fine structure}} |n L S J m_J\rangle = E_{n,J} | n L S J, M_J \rangle$$

Dirac equation:

$$E_{n,j} = mc^2 \left[1 + \alpha^2 \left(n - J - \frac{1}{2} + \sqrt{(J + \frac{1}{2})^2 - \alpha^2} \right)^{-2} \right]^{-\frac{1}{2}}$$

Results - energy level diagram



Hyperfine structure

ex: $n=1$ $\qquad \vec{F} = \vec{I} + \vec{J}$

$$W_{HF} = \frac{2 \cdot \tilde{\epsilon}}{\hbar^2}\left(\hat{F}^2 - \hat{I}^2 - \hat{J}^2\right) \qquad \tilde{\epsilon} \simeq \frac{\alpha^2 E_I}{500}$$

values of F ?

$I = \frac{1}{2} \quad J = \frac{1}{2}$

$F = 1, 0$

TP basis: $\{|100\rangle\} \otimes \{|\pm\rangle_z\} \otimes \{|\pm\rangle_z\}$
e^- spin $\qquad p^+$ spin

4 basis elements: $\{F, m_F\}$

$\{|1,1\rangle, |1,0\rangle, |0,0\rangle, |1-1\rangle\}$

$W_{HF} \propto F^2 - J^2 - I^2$

evals: $F^2 - \frac{1}{2}\cdot\frac{3}{2}\hbar^2 - \frac{1}{2}\cdot\frac{3}{2}\hbar^2 =$

$= F^2 - \frac{3}{2}\hbar^2$

$$W_{HF} \rightarrow \frac{2\tilde{\epsilon}}{\hbar^2}\cdot\hbar^2 \begin{pmatrix} 2-\frac{3}{2} & 0 & 0 & 0 \\ 0 & 2-\frac{3}{2} & 0 & 0 \\ 0 & 0 & 0-\frac{3}{2} & 0 \\ 0 & 0 & 0 & 2-\frac{3}{2} \end{pmatrix}$$

$$W_{HF} \to \tilde{\epsilon} \begin{pmatrix} 1 & & & \emptyset \\ & 1 & & \\ & & -3 & \\ \emptyset & & & 1 \end{pmatrix}$$

<u>$n=1$</u>

$1^2S_{1/2}$ → $F=1$, $F=0$

$$\frac{\tilde{\epsilon}}{2\pi\hbar^2} = 0.35 \text{ GHz}$$

$$-3\,\frac{\tilde{\epsilon}}{2\pi\hbar^2} = 1.06 \text{ GHz}$$

<u>$n=2$</u>

$2^2P_{3/2}$ → $F=2$, $F=1$ $\}$ 23.7 MHz

$2^2S_{1/2}$ → $F=1$, $F=0$ $\}$ 178 MHz

Lamb shift ~ 1 GHz

$2^2P_{1/2}$ → $F=1$, $F=0$ $\}$ 59 MHz.