



QM Fine Structure of H Feb 6

We have Fine structure constant $\frac{e^2}{\hbar c} \approx \frac{1}{127} \ll 1$

We have the following terms in our Hamiltonian

$$H = mc^2 \sim 10^6 \text{ eV}$$

$$+ \frac{p^2}{2m} - \frac{e^2}{r} \sim 10 \text{ eV}$$

$$+ H_k + H_D + H_{soc} \sim \alpha^2 mc^2 10^{-2} \text{ eV}$$

+ ... higher order in α

Spin Orbit Coupling(SOC) term

$$H_{soc} = \frac{1}{2} \frac{e^2}{m^2 c^2} \frac{1}{r^3} \vec{L} \cdot \vec{S}$$

where does this come from?

Derivation

Consider an e^- of charge $-e$ in motion around a nucleus of $+Ze$

In addition to Coulomb interaction, a subtle relativistic effect \rightarrow SOC.

In the rest frame of the e^- , the moving nucleus leads to a B field.

$$\vec{B} = -\frac{1}{c} \vec{v} \times \vec{E}$$

This leads to a Zeeman interaction

$$H_{soc} = -\vec{\mu} \cdot \vec{B} \text{ where } \vec{\mu} \text{ is the magnetic moment of the } e^-, \text{ and } \vec{\mu} = -g\mu_B \vec{S}/\hbar \text{ where } g \sim 2,$$

$$\mu_B = \frac{e\hbar}{mc}, \vec{S} = \frac{1}{2}$$

$$\vec{E} = -\nabla\phi = \frac{\vec{r}}{r} \frac{d\phi}{dr}$$

$$\Rightarrow H_{soc} = -\frac{e}{mc^2} \vec{S} \cdot (\vec{v} \times \vec{r}) \frac{1}{r} \frac{d\phi}{dr}, \phi(r) = -\frac{Ze}{r} \rightarrow \frac{d\phi}{dr} = \frac{Ze}{r^2}. \text{ Also we have } \vec{L} = \vec{r} \times m\vec{v}$$

$$\Rightarrow H_{soc} = \left(\frac{1}{2}\right) \frac{Ze^2}{m^2 c^2} \frac{1}{r^3} \vec{L} \cdot \vec{S}$$

Note that the $\frac{1}{2}$ comes from the non-inertial frame of the electron.

Scaling of SOC with Z

$$\frac{\hbar^2}{ma^2} \approx \frac{Ze^2}{a^2} \Rightarrow a \approx \frac{1}{Z} a_0$$

$$\left\langle \frac{1}{r^3} \right\rangle \approx \frac{1}{a^3} \approx \frac{z^3}{a_0^3}. \text{ Therefore, } H_{soc} \propto Z^4$$

Note that this scaling is a crude approximation of only one electron. Nevertheless, H_{soc} increases rapidly with Z

for Hydrogen atom

$L \approx \hbar$, $S \approx \hbar$. Therefore, $H_{soc} \approx \frac{e^2}{m^2 c^2} \frac{\hbar^3}{a_0^3} \approx \alpha^4 m c^2$. Check $\frac{H_{soc}}{H_0} \approx \alpha^2$

(Detail in HW#4) Sketch of Fine Structure Peterb.

$n = 1, l = 0, H_{soc} = 0$, we then start looking at $n = 2$ level.

$H_k = \frac{-p^4}{8m^3 c^2}$ term is rotational invariant as $p^4 = (p \cdot p)^2$

This means H_k is already diagonal in the eigenbasis $|nlm\rangle$ of H_0

$$E_1^k = \frac{1}{8m^3 c^2} \langle p^4 \rangle_{nlm}$$

tricks to evaluate matrix element.

$$H_0 = \frac{p^2}{2m} - \frac{e^2}{r}$$

$$p^4 = 4m^2 (H_0^2 + \frac{2e^2}{r} H_0 + \frac{e^4}{r^2})$$

$$E_k^1 = -\frac{1}{2mc^2} (E_n^0)^2 + 2e^2 E_n^0 \langle \frac{1}{r} \rangle_{nlm} + e^4 \langle \frac{1}{r^2} \rangle_{nlm}$$

for $\langle \frac{1}{r} \rangle$ we use virial theorem. $E = \frac{1}{2} \langle V \rangle = \frac{-e^2}{2} \langle \frac{1}{r} \rangle$. Therefore $\langle \frac{1}{r} \rangle = \frac{1}{n^2 a_0}$

$$e^4 \langle \frac{1}{r^2} \rangle = \frac{(E_n^0)^4 4n}{l + \frac{1}{2}} \text{ (Shankar ex17.3.4)}$$

H_{SOC} need to find the basis states that diagonalize $\vec{L} \cdot \vec{S}$

starting with $|nlm, s, m_s\rangle$ where $n = 2, s = \frac{1}{2}$, we have 8 states.

We can split the Hamiltonian to a 2x2 block for $l = 0$

and 6x6 block for $l = 1$. Where the $l = 1$ block can split into a 2x2 block and 4x4 block.

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

$$\vec{J}^2 = \vec{L}^2 + \vec{S}^2 + 2\vec{L} \cdot \vec{S}. \text{ Therefore, we can re-write } \vec{L} \cdot \vec{S} = \frac{1}{2}[j(j+1) - l(l+1) - s(s+1)]$$

where $j = l \pm s$

$|n = 2, l, m, \frac{1}{2}, m_s\rangle \rightarrow |n = 2, j, m_j, \frac{1}{2}, m_s\rangle$ (how to transform? Think Cleb-Gordan coeff)