QM Fine Structure of H Feb 6

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

We have the followting terms in our Hamiltonian
$H = mc^2$ ~$10^6 eV$
$+\frac{p^2}{2m} - \frac{e^2}{r}$~$10eV$
$+H_k + H_D + H_{soc}$~ $\alpha^2 mc^2 10^{-2}$eV
$+ \ldots$ higher order in α

Spin Orbit Coupling(SOC) term

$H_{soc} = \frac{1}{2}\frac{e^2}{m^2c^2}\frac{1}{r^3}\vec{L}\cdot\vec{S}$
where does this come from?

Derivation

Consider an e^- of charge $-e$ in motion around a nucleus of $+Ze$
In addition to Columb interaction, a subtile relativitive effect $\rightarrow$ SOC.
In the rest frame of the e^- , the moving nucleus leads to a B field.
$\vec{B} = -\frac{1}{c}\vec{v} * \vec{E}$
This leands to a Zeeman interaction
$H_{soc} = -\vec{\mu}\cdot\vec{B}$ whtere $\vec{\mu}$ is the magnetic moment of the e^- , and $\vec{\mu} = -g\mu_B\vec{S}/\hbar$ where g~2 ,
$\mu_B = \frac{e\hbar}{mc}, \vec{S} = \frac{1}{2}$
$\vec{E} = -\Lambda\phi = \frac{\vec{r}}{r}\frac{d\phi}{dr}$
$\Rightarrow H_{soc} = -\frac{e}{mc^2}\vec{S}\cdot(\vec{v} * \vec{r})\frac{1}{r}\frac{d\phi}{dr}$, $\phi(r) = -\frac{Ze}{r} \rightarrow \frac{d\phi}{dr} = \frac{Ze}{r^2}$. Also we have $\vec{L} = \vec{r} * m\vec{v} *$
$\Rightarrow H_{soc} = (\frac{1}{2})\frac{Ze^2}{m^2c^2}\frac{1}{r^3}\vec{L}\cdot\vec{S}$
Note that the $\frac{1}{2}$ comes from the none-intertial frame of the electron.

Scaling of SOC with Z

$\frac{\hbar^2}{ma^2} \approx \frac{Ze^2}{a^2} \Rightarrow a \approx \frac{1}{Z}a_0$
$\langle\frac{1}{r^3}\rangle \approx \frac{1}{a^3} \approx \frac{z^3}{a_0^3}$. 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, $H_{soc} \approx \frac{e^2}{m^2c^2}\frac{\hbar^3}{a_0^3} \approx \alpha^4 mc^2$. 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.

$H_k = \frac{-p^4}{8m^3c^2}$ 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

$E_1^k == \frac{1}{8m^3c^2} < p^4 >_{nlm}$

tricks to evaluate matrix element.

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

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

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

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 $\langle\frac{1}{r}\rangle = \frac{1}{n^2a_0}$

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

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

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 fhe $l = 1$ block can split into a 2x2 block and 4x4 block.

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

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

whre $j = l \pm s$

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