

FINE STRUCTURE

from P.A. Dirac to Pauli...

• $H_{\text{Dirac}} = c \vec{\alpha} \cdot \vec{p} + \beta mc^2$

$$\begin{cases} \alpha_i^2 = \beta^2 = 1 & i=1,2,3 \\ \{\alpha_i, \beta\} = 0 \\ \{\alpha_i, \alpha_j\} = 0 \quad (i \neq j) \end{cases}$$

$\downarrow H\psi = E\psi \Rightarrow \psi \equiv \begin{pmatrix} \chi \\ \eta \end{pmatrix}$

• $c(\vec{\sigma} \cdot \vec{p})\eta = (E - mc^2)\chi$ $\chi \equiv \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}, \eta \equiv \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}$ $\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$ $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

• $c(\vec{\sigma} \cdot \vec{p})\chi = (E + mc^2)\eta$

$\Rightarrow \chi = \frac{2c}{v} \eta \Rightarrow \boxed{\eta \text{ small compared to } \chi}$

Solve for χ .

... $E'\chi = \frac{(\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{p})}{2m} \chi$

But let's add magnetic & electric fields!

$\vec{\sigma} \cdot (c\vec{p} - q\vec{A})\eta + (mc^2 + q\phi)\chi = E\chi$ — (a)

$\vec{\sigma} \cdot (c\vec{p} - q\vec{A})\chi + (q\phi - mc^2)\eta = E\eta$ — (b)

\downarrow

$$\boxed{(E' - q\phi) = \frac{(\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{p})}{2m} \chi} \quad \text{--- (2)}$$

$(\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{p}) = p^2 + i\vec{\sigma} \cdot (\vec{p} \times \vec{p})$ $K = \left\{ \frac{2mc^2}{E' + 2mc^2 - q\phi} \right\}$

• $(\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{p}) = \left(\vec{p} - \frac{q\vec{A}}{c}\right)^2 - \frac{iq}{c} \vec{\sigma} \cdot (\vec{A} \times \vec{p} + \vec{p} \times \vec{A})$

$(\vec{p} \times \vec{A}) \stackrel{L}{=} -i\hbar(\vec{\nabla} \times \vec{A}) = -\vec{A} \times \vec{p}$

$= \left(\vec{p} - \frac{q\vec{A}}{c}\right)^2 - \frac{q\hbar}{c} \vec{\sigma} \cdot (\vec{\nabla} \times \vec{A})$

so for $K=1$, $(E' - q\phi) = \frac{(\vec{\sigma} \cdot \vec{p})^2}{2m} \chi = \left\{ \left(\vec{p} - \frac{q\vec{A}}{c}\right)^2 - \frac{q\hbar}{2mc} \vec{\sigma} \cdot (\vec{\nabla} \times \vec{A}) \right\} \chi$ — (3)

$K = \left(\frac{1}{1 + \frac{E' - q\phi}{2mc^2}} \right) = 1 - \left(\frac{E' - q\phi}{2mc^2} \right) + \dots$ — (4)

$$(E' - q\phi) \chi = \frac{1}{2m} \left((\vec{\sigma} \cdot \vec{\pi})^2 - (\vec{\sigma} \cdot \vec{\pi}) \frac{(E' - q\phi)}{2mc^2} (\vec{\sigma} \cdot \vec{\pi}) \right) \quad (*)$$

But crap :/ doesn't explain Fine structure yet...

!! "Foldy - Wouthuysen Transformation" enter...

$$\psi = \Omega \chi, \quad \chi = \Omega^{-1} \psi. \quad \# \eta\text{-eliminated} \quad \nabla : 0 ?$$

$$\boxed{\Omega^{-1} = 1 + \frac{(\vec{\sigma} \cdot \vec{\pi})^2}{8m^2c^2}} \rightsquigarrow \text{order of } v^2/c^2 \dots$$

now do $\Omega^{-1} \{ \text{Eqn } (*) \} \Omega^{-1} \psi$

$$\begin{aligned} \Omega^{-1} (E' - q\phi) \Omega^{-1} \psi &= \frac{\Omega^{-1}}{2m} \left\{ (\vec{\sigma} \cdot \vec{\pi})^2 - (\vec{\sigma} \cdot \vec{\pi}) \frac{(E' - q\phi)}{2mc^2} (\vec{\sigma} \cdot \vec{\pi}) \right\} \Omega^{-1} \psi \\ &\downarrow \\ &= (E' - q\phi) \psi - \frac{(\vec{\sigma} \cdot \vec{\pi})^2 (E' - q\phi) \psi}{8m^2c^2} - \frac{(E' - q\phi) (\vec{\sigma} \cdot \vec{\pi})^2 \psi}{8m^2c^2} + \dots \\ &\quad \downarrow \quad \quad \quad \downarrow \\ &= \left[\frac{(\vec{\sigma} \cdot \vec{\pi})^2}{2m} - \frac{(\vec{\sigma} \cdot \vec{\pi})^4}{8m^3c^2} + \dots \right] \psi \quad \left\{ \text{up to } O(v^2/c^2) \right\} \\ &= \frac{(\vec{\sigma} \cdot \vec{\pi}) (E' - q\phi) (\vec{\sigma} \cdot \vec{\pi})}{4m^2c^2} \psi + \dots \end{aligned}$$

Thus,

$$(E' - q\phi) \psi = \left\{ \frac{(\vec{\sigma} \cdot \vec{\pi})^2}{2m} - \frac{(\vec{\sigma} \cdot \vec{\pi})^4}{8m^3c^2} + \frac{(\vec{\sigma} \cdot \vec{\pi})^2 (E' - q\phi)}{8m^2c^2} + \frac{(E' - q\phi) (\vec{\sigma} \cdot \vec{\pi})^2}{8m^2c^2} - \frac{(\vec{\sigma} \cdot \vec{\pi}) (E' - q\phi) (\vec{\sigma} \cdot \vec{\pi})}{4m^2c^2} \right\} \psi$$

• Simplifying further using: $(\vec{r} \cdot \vec{\pi})(E' - q\phi) - (E' - q\phi)(\vec{r} \cdot \vec{\pi}) = i\hbar q (\vec{r} \cdot \nabla \phi)$

• $(\vec{r} \cdot \vec{\pi})(\vec{r} \cdot \nabla \phi) - (\vec{r} \cdot \nabla \phi)(\vec{r} \cdot \vec{\pi})$
 $= -i\hbar \vec{r} \cdot \nabla \phi + 2i(\vec{r} \cdot \vec{\pi}) \times \nabla \phi$

• $(\vec{\sigma} \cdot \vec{\pi})^2 (E' - q\phi) - (E' - q\phi)(\vec{\sigma} \cdot \vec{\pi})^2$
 $= q\hbar^2 (\vec{\sigma} \cdot \nabla \phi) - 2\hbar (\vec{r} \cdot \vec{\pi}) \times \nabla \phi + 2(\vec{r} \cdot \vec{\pi})(E' - q\phi) \cdot (\vec{r} \cdot \vec{\pi})$

$(E' - q\phi)\psi = \frac{1}{2m} \left\{ (\vec{\sigma} \cdot \vec{\pi})^2 - \frac{(\vec{\sigma} \cdot \vec{\pi})^4}{4m^2 c^2} + \frac{q\hbar^2 (\vec{\sigma} \cdot \nabla \phi)}{4m^2 c^2} - \frac{q\hbar (\vec{r} \cdot \vec{\pi}) \times \nabla \phi}{2m c^2} \right\} \psi$

$A = 0$

~~$H = \frac{\hat{p}^2}{2m} + V - \frac{\hat{p}^4}{8m^3 c^2} + \frac{e^2}{2m^2 c^2} \frac{\vec{L} \cdot \vec{S}}{r} + \frac{\pi}{2} \frac{e^2 \hbar^2}{m^2 c^2} \delta(r)$~~

$H = \underbrace{\frac{\hat{p}^2}{2m} + V}_{H^{(0)}} - \underbrace{\frac{\hat{p}^4}{8m^3 c^2}}_{\delta H_{rel}} + \underbrace{\frac{1}{2m^2 c^2} \frac{1}{r} \frac{dV}{dr} \vec{S} \cdot \vec{L}}_{\delta H_{SO}} + \underbrace{\frac{\hbar^2}{8m^2 c^2} \nabla^2 V}_{\delta H_{Darwin}}$

$H = \underbrace{\frac{\hat{p}^2}{2m} + V}_{H^{(0)}} - \underbrace{\frac{\hat{p}^4}{8m^3 c^2}}_{\delta H_{rel}} + \underbrace{\frac{e^2}{2m^2 c^2} \frac{\vec{S} \cdot \vec{L}}{r^3}}_{\delta H_{spin-orbital}} + \underbrace{\frac{\pi}{2} \frac{e^2 \hbar^2}{m^2 c^2} \delta(r)}_{\delta H_{Darwin}}$