lect 14: Low energy approximation of Dirac equation

In the representation of $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$, $\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$, the plane wave solution can be written as $\psi_p(x) = N \begin{pmatrix} \chi \\ \frac{c\vec{\sigma}\cdot\vec{p}\chi}{mc^2+|E|} \end{pmatrix} e^{i(px-|E|t)/\hbar}$. (positive energy solution). The last two terms are smaller components at order of v/c. We want to derive an effective equation for the large component for the non-relativistic limit.

$$H = c\vec{\alpha}\cdot\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right) + mc^2\beta + e\Phi \quad \text{, i.e}$$

$$H = \begin{bmatrix} mc^2 + e\Phi, & c\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}\vec{A}) \\ c\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}\vec{A}) & -mc^2 + e\Phi \end{bmatrix}, \qquad \text{set } \psi(x) = \begin{pmatrix} \psi_a(x) \\ \psi_b(x) \end{pmatrix}$$

$$\Rightarrow \quad (mc^2 + e\Phi)\psi_a + c\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}\vec{A})\psi_b = E\psi_a$$

$$c\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}A)\psi_a - (mc^2 - e\Phi)\psi_b = E\psi_b .$$

define $W = E - mc^2$, $\Rightarrow$

$$e\Phi\psi_a + c\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}\vec{A})\psi_b = W\psi_a \qquad (1)$$

$$c\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}A)\psi_a = (2mc^2 + W - e\Phi)\psi_b \qquad (2)$$

from (2) $\Rightarrow$

$$\psi_b = \frac{1}{2mc^2 + W - e\phi} c\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}A)\psi_a$$

Zero-th order approx $\quad \psi_b \approx \frac{1}{2mc^2}\, c\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}A)\,\psi_a$

$$\Rightarrow \frac{1}{2m}\left[\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}A)\right]^2 \psi_a + e\Phi\,\psi_a = W\psi_a$$

$$\Rightarrow H_{\text{non-rel}} = \frac{1}{2m}\left[\vec{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}A)\right]^2 + e\Phi \quad \leftarrow \text{Pauli equation}$$

$$\boxed{H_{\text{non-rel}} = \underbrace{\frac{1}{2m}(-i\hbar\nabla - \frac{e}{c}A)^2}_{\text{orbital coupling}} - \underbrace{\frac{e\hbar}{2mc}\vec{\sigma}\cdot(\nabla\times\vec{A})}_{\text{zeeman term.}} + e\Phi}$$

$$\boxed{\vec{\mu}_s = \frac{e\hbar}{2mc}\vec{\sigma}} \qquad g = 2$$

§ First order approximation — spin-orbit coupling

$$\psi_b = \frac{1}{2mc}\left(1 + \frac{V-W}{2mc^2}\right)\vec{\sigma}\cdot\vec{p}\,\psi_a\,, \quad \text{where } V = e\Phi$$

↑ next order

for simplicity, we neglect $\vec{A}$ here.

$$\Rightarrow \left[\frac{1}{2m}(\vec{\sigma}\cdot\vec{p})^2 + \frac{1}{4m^2c^2}(\vec{\sigma}\cdot\vec{p})(V-W)(\vec{\sigma}\cdot\vec{p}) + V\right]\Psi_a = W\Psi_a$$

The normalization of ψ_a is not a const at $(\frac{1}{mc})^2$ level

$$\int d^3x\, \psi^\dagger(x,t)\psi(x,t) = \int d^3x\, \psi_a^{T*}(x,t)\psi_a(x,t) + \frac{1}{(2mc)^2}\int d^3x\, \psi_a^{T*}(x,t)\,\underbrace{\hat{p}^2}_{\text{momentum operator}}\psi_a(x,t)$$

up to $(mc)^{-2}$ level

we define $\psi_s \propto \left(1+\frac{1}{8m^2c^2}\hat{p}^2\right)\Psi_a$ is the normalized wavefunction,

or $\psi_a \propto \left(1-\frac{1}{8m^2c^2}\hat{p}^2\right)\psi_s$ ← Schrödinger equation

$$\Rightarrow \left\{\frac{\hat{p}^2}{2m}+\frac{1}{4m^2c^2}(\vec{\sigma}\cdot\hat{p})(V-W)(\vec{\sigma}\cdot\hat{p})+V\right\}\left(1-\frac{\hat{p}^2}{8m^2c^2}\right)\psi_s$$

$$= W\left(1-\frac{1}{8m^2c^2}\hat{p}^2\right)\psi_s$$

left & right times $\left(1-\frac{1}{8m^2c^2}\hat{p}^2\right)$, and keep to $\left(\frac{1}{mc}\right)^2$ level

$$\Rightarrow \left(1-\frac{1}{8m^2c^2}\hat{p}^2\right)\left(\frac{p^2}{2m}\left(1-\frac{\hat{p}^2}{8m^2c^2}\right)\right)] + \frac{1}{4m^2c^2}(\vec{\sigma}\cdot\hat{p})V(\vec{\sigma}\cdot\hat{p})$$

$$-\frac{1}{4m^2c^2}\left(1-\cancel{\frac{\hat{p}^2}{8m^2c^2}}\right)(\vec{\sigma}\cdot\hat{p})W(\vec{\sigma}\cdot\hat{p})\left(1-\cancel{\frac{\hat{p}^2}{8m^2c^2}}\right)$$

$$+\left(1-\frac{1}{8m^2c^2}\hat{p}^2\right)V\left(1-\frac{\hat{p}^2}{8m^2c^2}\right)] = W\left(1-\frac{1}{4m^2c^2}\hat{p}^2\right)\psi_s$$

$$\Rightarrow \left\{\frac{p^2}{2m}-\frac{\hat{p}^4}{8m^3c^2}+\frac{1}{4m^2c^2}(\vec{\sigma}\cdot\hat{p})V(\vec{\sigma}\cdot\hat{p})-\cancel{\frac{1}{4m^2c^2}(\vec{\sigma}\cdot\hat{p})W(\vec{\sigma}\cdot\hat{p})}\right.$$

$$\left.+V-\frac{1}{8m^2c^2}(V\hat{p}^2+\hat{p}^2V)\right\}\psi_s = W\psi_s - \cancel{W\frac{1}{4m^2c^2}\hat{p}^2\psi_s}$$

$$\Rightarrow \left\{\frac{\hat{p}^2}{2m}-\frac{\hat{p}^4}{8m^3c^2}+\frac{1}{4m^2c^2}(\vec{\sigma}\cdot\hat{p})V(\vec{\sigma}\cdot\hat{p})+V-\frac{1}{8m^2c^2}(V\hat{p}^2+\hat{p}^2V)\right\}\psi_s$$

$$= W\psi_s$$

$$[V, \hat{p}^2] = \hbar^2 [\nabla^2 V] + 2i\hbar (\nabla V) \cdot \hat{p}$$

$$(\vec{\sigma} \cdot \hat{p}) V = V (\vec{\sigma} \cdot \hat{p}) + \vec{\sigma} \cdot [\hat{p}, V]$$

$$(\vec{\sigma} \hat{p}) V (\vec{\sigma} \cdot \hat{p}) = V \hat{p}^2 - i\hbar [\nabla V] \cdot \hat{p} + \hbar \vec{\sigma} \cdot (\nabla V) \times \hat{p}$$

$$\Rightarrow H_{non\text{-}rel} = \frac{\hat{p}^2}{2m} - \frac{\hat{p}^4}{8m^3c^2} + \underbrace{\frac{\hbar}{4m^2c^2} \vec{\sigma} \cdot (\nabla V) \times \hat{p}}_{\text{spin-orbit coupling: } H_{so}} + \underbrace{\frac{\hbar^2}{8m^2c^2} \nabla^2 V}_{\text{Darwin term}}$$

other term cancels

$$H_{so} = \frac{\hbar}{4m^2c^2} \vec{\sigma} \cdot \frac{1}{r} \frac{dv}{dr} (\vec{r} \times \hat{p}) = \underbrace{\frac{\hbar}{4m^2c^2} \frac{1}{r} \frac{dv}{dr}}_{\text{SO-coupling coefficient.}} \vec{\sigma} \cdot \vec{L}$$

In atoms, H_{so} is more ~~importantt~~ important than $-\frac{\hat{p}^4}{8m^3c^2}$

because $\frac{\hat{p}^4}{8m^3c^2} \Big/ \frac{p^2}{2m} \propto \left(\frac{v}{c}\right)^2$

$$\frac{H_{so}}{\frac{\hat{p}^2}{2m}} \approx \frac{\hbar \nabla V / p}{m c^2} = \frac{a \cdot \nabla V}{mc^2} = \frac{E_{Bohr}}{mc^2} = \alpha \propto \frac{v}{c}$$