78(5): Spin Orbit Interaction from Fermion Equation

We refer to:

P. Novak, "Calculation of Spin-Orbit Coupling"
Institute of Physics, Czech Republic.

The fermion equation is:

$$\left(\hat{E} - c\,\underline{\sigma}\cdot\hat{\underline{p}}\right)\phi^R = mc^2\phi^L \quad -(1)$$

$$\left(\hat{E} + c\,\underline{\sigma}\cdot\hat{\underline{p}}\right)\phi^L = mc^2\phi^R \quad -(2)$$

In the presence of a potential V:

$$V = -e\phi \quad -(3)$$

then:

$$\left(\hat{E} - V - c\,\underline{\sigma}\cdot\hat{\underline{p}}\right)\phi^R = mc^2\phi^L \quad -(4)$$

$$\left(\hat{E} - V + c\,\underline{\sigma}\cdot\hat{\underline{p}}\right)\phi^L = mc^2\phi^R \quad -(5)$$

As in UFT 173 make the transformations:

$$\phi^R = \frac{1}{\sqrt{2}}\left(\phi^R_S + \phi^L_S\right) \quad -(6)$$

$$\phi^L = \frac{1}{\sqrt{2}}\left(\phi^R_S - \phi^L_S\right) \quad -(7)$$

to obtain:

$$\left(E - V - mc^2\right)\phi^R_S = c\,\underline{\sigma}\cdot\hat{\underline{p}}\,\phi^L_S \quad -(8)$$

$$\left(E - V + mc^2\right)\phi^L_S = c\,\underline{\sigma}\cdot\hat{\underline{p}}\,\phi^R_S \quad -(9)$$

Now write

$$\epsilon = E - mc^2 \quad -(10)$$

$$\phi^R_S = \Phi, \quad \phi^L_S = \chi \quad -(11)$$

to obtain:

$$c\,\underline{\sigma}\cdot\underline{p}\,\chi = (\epsilon - V)\,\Phi \quad -(12)$$

$$c\,\underline{\sigma}\cdot\underline{p}\,\Phi = \left(\epsilon - V + 2mc^2\right)\chi \quad -(13)$$

2) These are Novak's eqns. (4) and (5), which have therefore been derived from ECE theory

From eq. (13):

$$\chi = \frac{c\,\underline{\sigma}\cdot\underline{\hat{p}}\,\underline{\Phi}}{\epsilon - V + 2mc^2} . \quad -(14)$$

So in eq. (12):

$$\epsilon\,\underline{\Phi} = V\underline{\Phi} + c^2\,\underline{\sigma}\cdot\underline{\hat{p}}\left(\frac{\underline{\sigma}\cdot\underline{\hat{p}}\,\underline{\Phi}}{\epsilon - V + 2mc^2}\right) \quad -(15)$$

$$= V\underline{\Phi} + \frac{1}{2m}\,\underline{\sigma}\cdot\underline{\hat{p}}\left(\frac{\underline{\sigma}\cdot\underline{\hat{p}}\,\underline{\Phi}}{1 + \frac{\epsilon - V}{2mc^2}}\right) \quad -(16)$$

This is Novak's eq. (6).

Now use:

$$\left(1 + \frac{\epsilon - V}{2mc^2}\right)^{-1} \sim 1 - \left(\frac{\epsilon - V}{2mc^2}\right) \quad -(17)$$

$$\text{if} \quad \epsilon - V << 2mc^2 \quad -(18)$$

Therefore:

$$\epsilon\,\underline{\Phi} = V\underline{\Phi} + \frac{1}{2m}\,\underline{\sigma}\cdot\underline{\hat{p}}\left(\left(1 - \left(\frac{\epsilon - V}{2mc^2}\right)\right)\underline{\sigma}\cdot\underline{\hat{p}}\,\underline{\Phi}\right) \quad -(19)$$

where

$$\hat{p} = -i\hbar\underline{\nabla} \quad -(20)$$

3) Eq. (19) is:

$$\epsilon \underline{\Phi} = V \underline{\Phi} + \frac{1}{2m} \underline{\sigma} \cdot \underline{\hat{p}}\, \underline{\sigma} \cdot \underline{\hat{p}}\, \underline{\Phi} - \frac{1}{4m^2c^2} \underline{\sigma} \cdot \underline{\hat{p}} \left(\epsilon\, \underline{\sigma} \cdot \underline{\hat{p}}\, \underline{\Phi} \right)$$

$$+ \frac{1}{4m^2c^2} \underline{\sigma} \cdot \underline{\hat{p}} \left(V \underline{\sigma} \cdot \underline{\hat{p}}\, \underline{\Phi} \right) \quad -(21)$$

Novak makes the non-relativistic approximation:

$$T = \epsilon = E - mc^2 = (\gamma - 1) mc^2 \quad -(22)$$

$$\rightarrow \frac{p^2}{2m}$$

for

$$v \ll c. \quad -(23)$$

So:

$$\epsilon \underline{\Phi} = V \underline{\Phi} + \frac{\hat{p}^2}{2m} \underline{\Phi} - \frac{\hat{p}^4}{8m^3c^2} \underline{\Phi} \quad -(24)$$

$$+ \frac{1}{4m^2c^2} \underline{\sigma} \cdot \underline{\hat{p}} \left(V \underline{\sigma} \cdot \underline{\hat{p}}\, \underline{\Phi} \right)$$

where we have used:

$$\underline{\sigma} \cdot \underline{\hat{p}}\, \underline{\sigma} \cdot \underline{\hat{p}} = \hat{p}^2 \quad -(25)$$

The Schroedinger equation is the approximation:

$$\epsilon \underline{\Phi} = \left(V + \frac{\hat{p}^2}{2m} \right) \underline{\Phi} = \hat{H} \underline{\Phi} \quad -(26)$$

The third term on the RHS of eq. (24) is known as the mass term.

4) The fourth term on the RHS of eq. (24) gives the spin-orbit interaction term and the Darwin term.

This term is:

$$\frac{\underline{\sigma} \cdot \hat{\underline{p}}}{4m^2c^2} \left(V \underline{\sigma} \cdot \hat{\underline{p}}\, \Phi \right) = -\frac{i\hbar}{4m^2c^2} \underline{\sigma} \cdot \underline{\nabla} \left(V \underline{\sigma} \cdot \hat{\underline{p}}\, \Phi \right) \quad -(27)$$

The RHS is expanded using the Leibniz Theorem, so

$$RHS = -\frac{i\hbar}{4m^2c^2} \left(\underline{\sigma} \cdot \underline{\nabla} V \underline{\sigma} \cdot \hat{\underline{p}}\, \Phi + V (\underline{\sigma} \cdot \underline{\nabla})(\underline{\sigma} \cdot \hat{\underline{p}}\, \Phi) \right) \quad -(28)$$

The electric field is defined as:

$$V = e\phi \,;\; e\underline{E} = -\underline{\nabla} V, \quad -(29)$$

so:

$$RHS = \frac{i\hbar e}{4m^2c^2} \left(\underline{\sigma} \cdot \underline{E}\, \underline{\sigma} \cdot \hat{\underline{p}}\, \Phi + V (\underline{\sigma} \cdot \underline{\nabla})(\underline{\sigma} \cdot \hat{\underline{p}}\, \Phi) \right) \quad -(30)$$

By Pauli algebra:

$$\underline{\sigma} \cdot \underline{E}\, \underline{\sigma} \cdot \hat{\underline{p}} = \underline{E} \cdot \hat{\underline{p}} + i \underline{\sigma} \cdot \underline{E} \times \hat{\underline{p}} \quad -(31)$$

Therefore:

$$RHS = -\frac{e\hbar}{4m^2c^2} \underline{\sigma} \cdot \underline{E} \times \hat{\underline{p}} - \frac{\hbar^2}{4m^2c^2} \underline{\nabla} V \underline{\nabla} \Phi - \frac{\hbar^2 V}{4m^2c^2} \nabla^2 \Phi \quad -(32)$$

5) Eq. (21) is therefore:

$$\hat{H}\,\underline{\Phi} = \epsilon\,\underline{\Phi} \quad -(33)$$

where:

$$\hat{H} = e\phi + \frac{\hat{p}^2}{2m} - \frac{\hat{p}^4}{8m^3c^2} - \frac{e\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\times\underline{\hat{p}}$$

$$-\frac{\hbar^2}{4m^2c^2}\,\underline{\nabla}\,V\,\underline{\nabla} - \frac{\hbar^2\,V\,\nabla^2}{4m^2c^2} \quad -(34)$$

The fourth term is the spin-orbit coupling term, the fifth term is the Darwin term, and the sixth term is a relativistic correction of $\hat{p}^2/(2m)$.

<u>These terms all emerge from the fermion equation.</u>

In a Coulomb potential:

$$\phi = -\frac{e}{4\pi\epsilon_0 r} \quad -(35)$$

$$\underline{E} = -\frac{e^2}{4\pi\epsilon_0}\,\frac{\underline{r}}{r^3} \quad -(36)$$

so the spin orbit term is:

$$\hat{H}_{so} = \frac{e^2\hbar}{16\pi\epsilon_0 r^3 m^2c^2}\,\underline{\sigma}\cdot\underline{r}\times\underline{\hat{p}} \quad -(37)$$

$$= \frac{e^2\hbar}{16\pi\epsilon_0 r^3 m^2c^2}\,\underline{\sigma}\cdot\underline{\hat{L}} \quad -(38)$$

6) where $\underline{\hat{L}}$ is the orbital angular momentum operator.

The spin angular momentum is defined as an operator

$$\underline{\hat{S}} = \frac{1}{2}\hbar\,\underline{\hat{\sigma}} \quad -(39)$$

So:

$$\boxed{\hat{H}_{SO} = \frac{e^2}{8\pi\epsilon_0 r^3 m^2 c^2}\,\underline{\hat{S}}\cdot\underline{\hat{L}}} \quad -(40)$$

Therefore the relativistic hamiltonian (34) is:

$$\boxed{\begin{aligned}\hat{H} = V - \frac{\hbar^2}{2m}\left(1 + \frac{V}{2m^2c^2}\right)\nabla^2 + \frac{\hbar^4}{8m^3c^2}\nabla^4 \\ + \frac{e^2}{8\pi\epsilon_0 r^3 m^2 c^2}\,\underline{\hat{S}}\cdot\underline{\hat{L}} - \left(\frac{\hbar^2}{4m^2c^2}\underline{\nabla} V\right)\underline{\nabla}\end{aligned}}$$

$$-(41)$$

and

$$\boxed{\hat{H}\phi = \epsilon\phi = (E - mc^2)\phi} \quad -(42)$$

The force equation is:

$$\boxed{(\hat{H} - \epsilon)\,\underline{\nabla}\phi = \underline{F}\phi} \quad -(43)$$

7)

The conventions used in this note are:

$$p^{\mu} \rightarrow p^{\mu} - eA^{\mu}, \quad - (44)$$

$$E \rightarrow E - e\phi, \quad - (45)$$

$$V = e\phi \quad - (46)$$

$$\phi = -\frac{e}{4\pi\epsilon_0 r} \quad - (47)$$

$$\underline{E} = -\underline{\nabla}\phi = -\frac{e}{4\pi\epsilon_0}\frac{\underline{r}}{r^3} \quad - (48)$$

$$e\underline{E} = -\underline{\nabla} V \quad - (49)$$

So:

$$\hat{H}_{SO} = -\frac{e\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\times\hat{\underline{p}}$$

$$= \frac{e^2}{8\pi\epsilon_0 r^3 m^2 c^2}\,\hat{\underline{S}}\cdot\hat{\underline{L}} \quad - (49)$$

which is the same as eq. (9.3.6) of Atkins, 2nd. edition, with $Z = 1$.

Note that the convention used by Atkins is different because he defines:

$$V = -\frac{e^2}{4\pi\epsilon_0 r^2} = -e\phi, \quad - (50)$$

so $$\phi = \frac{e}{4\pi\epsilon_0 r} \quad (\text{Atkins}) \quad - (51)$$

This makes no difference to the final result (49)