330(1): Review of the Conventional Spin Orbit Term and effect of the New Hamiltonian

The basic classical relativistic hamiltonian is:

$$H_0 = H - mc^2 = \frac{p^2}{m(1+\gamma)} + U \quad -(1)$$

$$\sim \frac{p^2}{2m}\left(1 - \left(\frac{\langle \hat{H}_0 \rangle - U}{2mc^2}\right)\right) + U \quad -(2)$$

where

$$U = -\frac{e^2}{4\pi\epsilon_0 r} \quad -(3)$$

for the H atom ($Z = 1$).

If:

$$\gamma \rightarrow 1 \quad -(4)$$

in Eq. (1) the classical non-relativistic hamiltonian is obtained:

$$H_0 \xrightarrow[\gamma \rightarrow 1]{} \frac{p_0^2}{2m} + U \quad -(4)$$

In eq. (1) $\underline{p}$ is the relativistic momentum:

$$\underline{p} = \gamma \underline{p}_0 \quad -(5)$$

where $\underline{p}_0$ is the non-relativistic momentum of eq. (4):

$$p_0^2 = 2m(\langle H_0 \rangle - U) \quad -(6)$$

where

$$\langle \hat{H}_0 \rangle = H_0 \quad -(7)$$

2) The Lorentz factor is:

$$\gamma = \left(1 - \frac{p_0^2}{m^2c^2}\right)^{-1/2} \quad -(8)$$

The conventional Dirac approximation leads to:

$$H_{Dirac} \sim \frac{p^2}{2m}\left(1 + \frac{U}{2mc^2}\right) + U \quad -(9)$$

so from eqs. (2) and (9):

$$\boxed{H_0 = H_{Dirac} - \frac{p^2}{4m^2c^2}\langle \hat{H}_0 \rangle} \quad -(10)$$

Quantizing eq. (9) in the SU(2) basis leads to:

$$\hat{H}_{Dirac}\phi = \left(\frac{1}{2m}\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{p} + \frac{1}{4m^2c^2}\underline{\sigma}\cdot\underline{p}\,U\,\underline{\sigma}\cdot\underline{p} + U\right)\phi \quad -(11)$$

$$= \left(\frac{p^2}{2m} + U + \frac{1}{4m^2c^2}\underline{\sigma}\cdot\underline{p}\,U\,\underline{\sigma}\cdot\underline{p}\right)\phi$$

with

$$\underline{\hat{p}}\,\phi = -i\hbar\,\underline{\nabla}\phi \quad -(12)$$

Eq. (11) is the Schroedinger equation with conventional spin orbit hamiltonian:

3) $$\hat{H}_{SO}\phi = \frac{1}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,U\,\underline{\sigma}\cdot\underline{p}\,\phi \quad -(13)$$

in which $\underline{p}$ can be interpreted either as an operator or as a function. In the conventional development:

$$\hat{H}_{SO}\phi = -\frac{i\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\left(U\,\underline{\sigma}\cdot\underline{p}\,\phi\right) \quad -(14)$$

where the first $\underline{p}$ on the RHS of eq. (13) is an operator and the second $\underline{p}$ is a function. This point is very rarely mentioned in textbooks but is fundamentally important. The second fundamentally important point is that $\underline{p}$ in eq. (13) is the <u>relativistic</u> momentum. It was simply assumed by Dirac that:

$$p^\mu = i\hbar\,\partial^\mu \quad -(15)$$

where p^μ is the <u>relativistic</u> four-momentum:

$$p^\mu = \left(\frac{E}{c},\,\underline{p}\right) \quad -(16)$$

where

$$E = \gamma mc^2 \quad -(17)$$

and

$$\underline{p} = \gamma\,\underline{p}_0 = \gamma m\underline{v} \quad -(18)$$

There is no a priori theoretical justification for

4) Eq (15), it is an axiom of relativistic quantum mechanics.

Conventionally, Eq. (14) is developed with the Leibnitz theorem:

$$\underline{\nabla}\left(U\,\underline{\sigma}\cdot\underline{p}\,\phi\right) = \underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\right)\left(U\phi\right) + \underline{\sigma}\cdot\underline{p}\,\underline{\nabla}\left(U\phi\right) \quad -(19)$$

so

$$H_{so}\phi = -\frac{i\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\left(U\phi\right)\underline{\sigma}\cdot\underline{p}\right) + \cdots \quad -(20)$$

Applying the Leibnitz theorem again:

$$\underline{\nabla}\left(U\phi\right) = \left(\underline{\nabla}\phi\right)U + \left(\underline{\nabla}U\right)\phi \quad -(21)$$

So

$$H_{so}\phi = -\frac{i\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\left(\left(\underline{\nabla}U\right)\phi + U\underline{\nabla}\phi\right)\underline{\sigma}\cdot\underline{p}\right. + \cdots \quad -(22)$$

There are several effects implied by eq. (22) but in the conventional theory the term considered is:

$$H_{so}\phi = -\frac{ie\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\left(\underline{\nabla}\phi\right)\phi\,\underline{\sigma}\cdot\underline{p} + \cdots \quad -(23)$$

where

$$U = e\phi \quad -(24)$$

5) Eq. (23) is written as:

$$H_{so}\phi = -\frac{ie\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\phi\,\underline{\sigma}\cdot\underline{p}\,\phi \quad -(25)$$

$$+ \ldots$$

In the conventional theory the electric field strength is:

$$\underline{E} = -\underline{\nabla}\phi \quad -(26)$$

so

$$H_{so}\phi = \frac{ie\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p}\,\phi \quad -(27)$$

where

$$\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p} = \underline{E}\cdot\underline{p} + i\underline{\sigma}\cdot\underline{E}\times\underline{p} \quad -(28)$$

so the real part of eq. (27) is:

$$\mathrm{Re}\,H_{so}\phi = -\frac{e\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\times\underline{p}\,\phi \quad -(29)$$

From eqs. (3), (24) and (26):

$$\underline{E} = -\underline{\nabla}\phi = -\frac{e}{4\pi\epsilon_0}\frac{\underline{r}}{r^3} \quad -(30)$$

so

$$\mathrm{Re}\,H_{so}\phi = \frac{e^2\hbar}{16\pi\epsilon_0 m^2c^2r^3}\,\underline{\sigma}\cdot\underline{r}\times\underline{p}\,\phi \quad -(31)$$

At this point in the conventional treatment

b) the relativistic momentum $\underline{p}$ is approximated by the non-relativistic momentum $\underline{p_0}$, and it is assumed that

$$\underline{L} = \underline{r} \times \underline{p} \sim \underline{r} \times \underline{p_0} \quad -(32)$$

where $\underline{L}$ is the classical orbital momentum. So:

$$\mathrm{Re}\, H_{SO}\, \phi = \frac{e^2 \hbar}{16 \pi \epsilon_0 m^2 c^2 r^3} \underline{\sigma} \cdot \underline{L}\, \phi \quad -(33)$$

This is the conventional spin orbit hamiltonian QED.

However, it should be:

$$\boxed{\mathrm{Re}\, H_{SO}\, \phi = \frac{e^2 \hbar \gamma}{16 \pi \epsilon_0 m^2 c^2 r^3} \underline{\sigma} \cdot \underline{L}\, \phi} \quad -(34)$$

The γ factor is missing in nearly all the conventional textbooks and websites, but produces a significant new term to be developed later in these notes for UFT 330.

The conventional treatment continues with eq. (33) using:

$$\hat{S} = \frac{\hbar}{2} \hat{\underline{\sigma}} \quad -(35)$$

introducing the spin quantum number. Therefore:

7)

$$H_{SO}\phi = \frac{e^2}{8\pi c^2 \epsilon_0 m^2 r^3} \hat{\underline{S}} \cdot \hat{\underline{L}} \phi \quad -(36)$$

Now introduce the total angular momentum quantum number:

$$J^2 = |(\underline{L} + \underline{S})^2| = L^2 + S^2 + 2\underline{L}\cdot\underline{S} \quad -(37)$$

So:

$$\hat{\underline{L}} \cdot \hat{\underline{S}} \phi = \frac{1}{2}\left(J(J+1) - L(L+1) - S(S+1)\right)\phi$$

and:

$$\langle H_{SO} \rangle = \frac{e^2 \left(J(J+1) - L(L+1) - S(S+1)\right)}{16\pi c^2 \epsilon_0 m^2} \left\langle \frac{1}{r^3} \right\rangle \quad -(38)$$

Finally use:

$$\left\langle \frac{1}{r^3} \right\rangle = \left(\frac{Z}{a_0}\right)^3 \frac{1}{n^3 L\left(L+\frac{1}{2}\right)(L+1)} \quad -(39)$$

where

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^4} \quad -(40)$$

i.e. the Bohr radius, and for the H atom:

$$Z = 1 \quad -(41)$$

8) Therefore, in the conventional treatment:

$$\langle H_{SO} \rangle = \frac{e^2 \hbar^2}{16\pi c^2 \epsilon_0 m^2 a_0^3} \left(\frac{J(J+1) - L(L+1) - S(S+1)}{n^3 L \left(L + \frac{1}{2}\right)(L+1)} \right) \quad -(42)$$

Using the Clebsch Gordan series:

$$J = L \pm \frac{1}{2} \quad -(43)$$

From eqs. (10) and (42) there are other terms to be added to Eq. (42) to give the complete hamiltonian expectation value:

$$\langle H \rangle = \frac{-me^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} \left(1 + \frac{\hbar^2}{4m^2c^2} \int \psi^* \nabla^2 \psi \, d\tau \right)$$

$$+ \frac{e^2 \hbar^2}{16\pi c^2 \epsilon_0 m^2 a_0^3} \left(\frac{J(J+1) - L(L+1) - S(S+1)}{n^3 L \left(L + \frac{1}{2}\right)(L+1)} \right) \quad -(44)$$