The Spin Orbit Hamiltonian in Space.

With reference to Note 330(1), the spin orbit hamiltonian is:

$$H_{so}\phi = \frac{1}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,U\,\underline{\sigma}\cdot\underline{p}\,\phi \quad -(1)$$

the conventional Dirac theory, where p is the relativistic momentum, m the mass of the electron and $-$:

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

Eq (1) is obtained from:

$$E^2 = p^2c^2 + m^2c^4 \quad -(3)$$

so:

$$(E - mc^2)(E + mc^2) = p^2c^2 \quad -(4)$$

and

$$E - mc^2 = \frac{p^2c^2}{E + mc^2} \quad -(5)$$

i.e., using:

$$H = E + U \quad -(6)$$

$$H - U - mc^2 = \frac{p^2c^2}{H - U + mc^2} \quad -(7)$$

and

$$H = \frac{p^2c^2}{H - U + mc^2} + U + mc^2 \quad -(8)$$

Dirac used the approximations:

$$U \ll E \quad -(9)$$

and

$$H \sim E \sim mc^2 \quad -(10)$$

so

$$H = \frac{p^2c^2}{2mc^2 - U} + U + mc^2 \quad -(11)$$

$$= \frac{p^2}{2m}\left(1 - \frac{U}{2mc^2}\right)^{-1} + mc^2 + U$$

Using eqs. (9) and (10):

$$U << 2mc^2 \quad -(12)$$

so

$$H \sim \frac{p^2}{2m}\left(1 + \frac{U}{2mc^2}\right) + mc^2 + U \quad -(13)$$

Introducing the SU(2) basis:

$$H = \frac{p^2}{2m} + \underline{\sigma}\cdot\underline{p}\,\frac{U}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p} + mc^2 + U \quad -(14)$$

so eq. (14) defines the spin orbit hamiltonian, Q.E.D.
As in Note 422(4) Eq. (14) in m space becomes:

$$H = \frac{1}{2m}\,\underline{\sigma}\cdot\underline{p}\,\frac{1}{m(r)^{1/2}}\,\underline{\sigma}\cdot\underline{p} \quad -(15)$$

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

so the spin orbit term in m space is:

$$H_{so} = \frac{1}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,\frac{U}{m(r)^{1/2}}\,\underline{\sigma}\cdot\underline{p} \quad -(16)$$

First develop eq. (1) as in Note 330(1):

$$H_{so}\,\phi = -\frac{i\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\left(U\,\underline{\sigma}\cdot\underline{p}\,\phi\right) \quad -(17)$$

where:

$$\underline{\nabla}\left(U\,\underline{\sigma}\cdot\underline{p}\,\phi\right) = \underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\right)\left(U\phi\right) + \underline{\sigma}\cdot\underline{p}\,\underline{\nabla}\left(U\phi\right) \quad -(18)$$

so

$$H_{so}\,\phi = \frac{-i\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\left(U\phi\right)\underline{\sigma}\cdot\underline{p}\right) + \cdots \quad -(19)$$

) in which:

$$\underline{\nabla}(U\phi) = (\underline{\nabla}\phi)\overline{U} + (\underline{\nabla}U)\phi \quad -(20)$$

so:

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

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

$$= -\frac{ie\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\phi\,\underline{\sigma}\cdot\underline{p}\,\phi + \cdots \quad -(21)$$

Here:

$$\underline{E} = -\underline{\nabla}\phi \quad -(22)$$

So:

$$H_{SO}\phi = \frac{ie\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p}\,\phi \quad -(23)$$

where

$$\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p} = \underline{E}\cdot\underline{p} + i\underline{\sigma}\cdot\underline{E}\times\underline{p} \quad -(24)$$

So:

$$\mathrm{Re}\,H_{SO}\phi = -\frac{e\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\times\underline{p}\,\phi \quad -(25)$$

If Coulombic interaction is used:

$$\underline{E} = -\underline{\nabla}\phi = -\frac{e}{4\pi\epsilon_0 r^3}\,\underline{r} \quad -(26)$$

So

$$\mathrm{Re}\,H_{SO}\phi = \frac{e^2\hbar}{16\pi\epsilon_0 m^2c^2r^3}\,\underline{\sigma}\cdot\underline{r}\times\underline{p}\,\phi \quad -(27)$$

4) The relativistic momentum is:

$$\underline{p} = \gamma \underline{p}_0 \quad -(28)$$

where γ is the Lorentz factor, and $\underline{p}_0$ the non-relativistic momentum. Defining:

$$\underline{L} = \underline{r} \times \underline{p}_0 \quad -(29)$$

then:

$$\mathrm{Re}\, H_{SO}\, \phi = \frac{e^2 \hbar \gamma}{16\pi \epsilon_0 m^2 c^2 r^3} \underline{\sigma} \cdot \underline{L}\, \phi \quad -(30)$$

The use of γ introduces new terms as in Notes for UFT330. Usually it is approximated by:

$$\gamma \sim 1. \quad -(31)$$

Using:

$$\underline{S} = \frac{\hbar}{2} \underline{\sigma} \quad -(32)$$

the spin orbit hamiltonian is:

$$H_{SO}\, \phi = \frac{e^2}{8\pi c^2 \epsilon_0 m^2 r^3} \underline{S} \cdot \underline{L}\, \phi \quad -(33)$$

$$= \frac{e^2}{16\pi^2 c^2 \epsilon_0 m^2 r^3} \left(J(J+1) - L(L+1) - S(S+1) \right) \phi$$

The expectation value of H_{SO} is evaluated with:

$$\left\langle \frac{1}{r^3} \right\rangle = \int \phi^* \frac{1}{r^3} \phi \, d\tau \quad -(34)$$

$$= \left(\frac{Z}{a_0} \right)^3 \frac{1}{n^3 L (L+1/2)(L+1)}$$

5)

So:

$$\langle H_{so} \rangle = \frac{e^2 \hbar^2}{16\pi c^2 \epsilon_0 m^2 a_0^3} \left(\frac{J(J+1) - L(L+1) - S(S+1)}{n^3 L(L+\frac{1}{2})(L+1)} \right) \quad -(35)$$

where

$$J = L - S, \ldots, L + S \quad -(36)$$

Eq. (35) gives the fine structure of the H atom but does not give the Lamb shift as is well known. This calculation must now be repeated for eq. (16) in n space. Denote:

$$U_1 = \frac{U}{n(r)^{1/2}} \quad -(37)$$

then the relevant spin orbit term is:

$$H_{so}\phi = -\frac{i\hbar}{4m^2c^2} \underline{\sigma} \cdot (\underline{\nabla} U_1) \phi \, \underline{\sigma} \cdot \underline{p} + \ldots$$

$$= -\frac{i\hbar}{4m^2c^2} \underline{\sigma} \cdot \underline{\nabla} U_1 \, \underline{\sigma} \cdot \underline{p} \, \phi + \ldots \quad -(38)$$

so:

$$\mathrm{Re}\, H_{so}\phi = \frac{e\hbar}{4m^2c^2} \underline{\sigma} \cdot \underline{\nabla} U_1 \times \underline{p} \, \phi \quad -(39)$$

Here:

$$\underline{\nabla} U_1 = \underline{\nabla} \left(\frac{U}{n(r)^{1/2}} \right) \quad -(40)$$

$$= \frac{1}{n(r)^{1/2}} \underline{\nabla} U + U \underline{\nabla} \left(\frac{1}{n(r)^{1/2}} \right)$$

6) It follows that:

$$\mathrm{Re}\,H_{SO}\,\phi = \frac{e^2\hbar}{16\pi\epsilon_0 m^2 c^2 r^3 m(r)^{1/2}}\,\underline{\sigma}\cdot\underline{L}\,\phi \qquad -(41)$$

$$+\frac{e\hbar}{4m^2c^2}\,U\,\underline{\sigma}\cdot\underline{\nabla}\left(\frac{1}{m(r)^{1/2}}\right)\times\underline{p}\,\phi$$

$$\mathrm{Re}\,H_{SO}\,\phi = \frac{e^2\hbar}{16\pi\epsilon_0 m^2 c^2 r^3 m(r)^{1/2}}\,\underline{\sigma}\cdot\underline{L}\,\phi \qquad -(42)$$

$$= \frac{e^2}{8\pi c^2\epsilon_0 m^2 r^3 m(r)^{1/2}}\,\underline{S}\cdot\underline{L}\,\phi + \cdots$$

$$\langle H_{SO}\rangle = \frac{e^2\left(J(J+1)-L(L+1)-S(S+1)\right)}{16\pi c^2\epsilon_0 m^2}\left\langle\frac{1}{r^3 m(r)^{1/2}}\right\rangle \qquad -(43)$$

where

$$\left\langle\frac{1}{r^3 m(r)^{1/2}}\right\rangle = \int\phi^*\frac{1}{r^3 m(r)^{1/2}}\phi\,d\tau \qquad -(44)$$

This theory may already be sufficient to explain the Lamb shift, if not, the additional term in eq. (41) may be used.