268(8): The Complete Derivation of the Spin - Orbit Hamiltonian

The derivation starts from the definition of the relativistic momentum of special relativity:

$$\underline{p} = \gamma m \underline{v} \quad - (1)$$

Eq. (1) leads to the Einstein energy equation:

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

The interaction of an electron with an electromagnetic field is described by the minimal prescription:

$$E \rightarrow E - e\phi \quad - (3)$$

and

$$\underline{p} \rightarrow \underline{p} - e\underline{A} \quad - (4)$$

where ϕ is the scalar potential and $\underline{A}$ is the vector potential. In the absence of a magnetic field only the scalar potential need be considered. So eq. (2) becomes:

$$(E - e\phi)^2 - m^2 c^4 = c^2 p^2 \quad - (5)$$

$$= (E - e\phi - mc^2)(E - e\phi + mc^2)$$

So:

$$E - e\phi - mc^2 = \frac{c^2 p^2}{E - e\phi + mc^2} \quad - (6)$$

2) and:

$$E - mc^2 = e\phi + \frac{c^2 p^2}{E - e\phi + mc^2} \quad -(7)$$

The usual approximation made in standard physics is

$$E = \gamma mc^2 \sim mc^2. \quad -(8)$$

When looked at objectively this is a rough approximation because if literally true the left hand side of eq. (7) would vanish. In this approximation:

$$E - mc^2 \sim e\phi + \frac{c^2 p^2}{2mc^2 - e\phi} \quad -(9)$$

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

At this point a second rough approximation is made:

$$\left(1 - \frac{e\phi}{2mc^2}\right)^{-1} \sim 1 + \frac{e\phi}{2mc^2} \quad -(10)$$

which is true for

$$e\phi \ll 2mc^2. \quad -(11)$$

So with these approximations:

$$E - mc^2 = e\phi + \frac{p^2}{2m} + \frac{e\phi}{4m^2c^2}p^2 \quad -(12)$$

) At this stage the SU(2) basis is introduced:

$$E - mc^2 = e\phi + \frac{1}{2m}\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{p} + \underline{\sigma}\cdot\underline{p}\,\frac{e\phi}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}. \quad -(13)$$

In order to describe the interaction between an electron and proton, a Coulombic potential is assumed:

$$\phi = -\frac{e}{4\pi\epsilon_0 r} \quad -(14)$$

so

$$E - mc^2 = \frac{-e^2}{4\pi\epsilon_0 r} + \frac{p^2}{2m} - \frac{e^2}{16\pi\epsilon_0 m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,\frac{1}{r}\,\underline{\sigma}\cdot\underline{p} \quad -(15)$$

Here we have used:

$$\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{p} = p^2 \quad -(16)$$

The Schroedinger equation is obtained from the non relativistic hamiltonian:

$$H = E = \frac{-e^2}{4\pi\epsilon_0 r} + \frac{p^2}{2m} \quad -(17)$$

In order to reduce eq. (12) to eq. (17) we:

$$\frac{p^2}{m^2c^2} = \left(\frac{E}{mc^2}\right)^2 - 1 \quad -(18)$$

4)

so in the approximations

$$E \sim mc^2 \quad -(19)$$

and

$$e\phi \ll mc^2 \quad -(20)$$

eq. (12) reduces to:

$$E - mc^2 = \frac{1}{2}mv^2 = \frac{p^2}{2m} \quad -(21)$$

In these rough approximations eq. (15) reduces to eq. (17). Another way to look at these approximations is to write eq. (6) as:

$$E - mc^2 = e\phi + \frac{c^2p^2}{E - e\phi + mc^2} \quad -(22)$$

and using (19) and (20):

$$\boxed{E - mc^2 \sim e\phi + \frac{p^2}{2m}} \quad -(23)$$

so

$$H \sim E - mc^2 \quad -(24)$$

where H is the classical hamiltonian (17). Having established the basis of the approximation used the spin orbit term can be developed using quantization:

$$H\phi \sim (E - mc^2)\phi \qquad -(25)$$

$$= \left(-\frac{e^2}{4\pi\epsilon_0 r} + \frac{p^2}{2m} - \frac{e^2}{16\pi\epsilon_0 m^2 c^2}\, \boldsymbol{\sigma}\cdot\boldsymbol{p}\, \frac{1}{r}\, \boldsymbol{\sigma}\cdot\boldsymbol{p} \right)\phi$$

To the Schroedinger hamiltonian on the right hand side of eq. (25) is added <u>the spin - orbit hamiltonian</u>:

$$\boxed{H_{so}\phi = -\frac{e^2}{16\pi\epsilon_0 m^2 c^2}\, \boldsymbol{\sigma}\cdot\boldsymbol{p}\, \frac{1}{r}\, \boldsymbol{\sigma}\cdot\boldsymbol{p}\, \phi} \qquad -(26)$$

This term is a direct consequence of special relativity and gives many important results. Several new results have been found in recent UFT papers. The Schroedinger quantization rule is:

$$\boldsymbol{p}\,\phi = -i\hbar\,\boldsymbol{\nabla}\phi \qquad -(27)$$

So:

$$H_{so}\phi = \frac{ie^2\hbar}{16\pi\epsilon_0 m^2 c^2}\, \boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\left(\frac{1}{r}\, \boldsymbol{\sigma}\cdot\boldsymbol{p}\, \phi \right) \qquad -(28)$$

Note carefully that the first $\boldsymbol{p}$ in eq. (26) is been replaced by $-i\hbar\boldsymbol{\nabla}$, but the second remains classical. There is no a priori

6) reasoning for this choice. It gives the data however to high precision. This choice was first made by Dirac or shortly after 1928 by others.

<u>Note</u> that $\underline{\nabla}$ <u>acts on everything included in the bracket</u>. So the Leibniz Theorem must be used:

$$\underline{\nabla}\left(\frac{1}{r}\,\underline{\sigma}\cdot\underline{p}\,\phi\right) = \left(\underline{\nabla}\left(\frac{1}{r}\right)\right)\left(\underline{\sigma}\cdot\underline{p}\,\phi\right) + \ldots \qquad -(29)$$

$$= \left(\underline{\nabla}\left(\frac{1}{r}\right)\right)\left(\underline{\sigma}\cdot\underline{p}\,\phi\right) + \frac{1}{r}\,\underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\,\phi\right)$$

in which:

$$\underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\,\phi\right) = \left(\underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\right)\right)\phi + \underline{\sigma}\cdot\underline{p}\,\underline{\nabla}\phi \qquad -(\overset{30}{\cancel{24}})$$

by another application of the Leibniz Theorem. These terms have all been developed in recent UFT papers. The usual spin-orbit term is the first term on the right ~~hand~~ side of Eq. (29):

$$\boxed{H_{SO}\,\phi = \frac{i e^2 \hbar}{16\pi\epsilon_0 m^2 c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\left(\frac{1}{r}\right)\right)\underline{\sigma}\cdot\underline{p}\,\phi} \qquad -(\overset{31}{\cancel{25}})$$

This looks at first sight to be pure imaginary

) and therefore unphysical, but by use of Pauli algebra it can be shown as follows to contain a real valued and physical component.

Firstly the gradient is evaluated:

$$\underline{\nabla}\left(\frac{1}{r}\right) = \frac{\partial}{\partial r}\left(\frac{1}{r}\right)\underline{e}_r \quad -(\cancel{26}\ 32)$$

because the potential ϕ is radial. So:

$$\underline{\nabla}\left(\frac{1}{r}\right) = -\frac{1}{r^2}\underline{e}_r \quad -(\cancel{27}\ 33)$$

where

$$\underline{e}_r = \underset{\sim}{r}/r \quad -(\cancel{28}\ 34)$$

so

$$\underline{\nabla}\left(\frac{1}{r}\right) = -\frac{\underline{r}}{r^3} \quad -(\cancel{29}\ 35)$$

From eqs. ($\cancel{25}$ 31) and ($\cancel{29}$ 35):

$$H_{SO}\,\psi = -\frac{i e^2 \hbar}{16\pi\epsilon_0 m^2 c^2 r^3}\,\underline{\sigma}\cdot\underline{r}\ \underline{\sigma}\cdot\underline{p}\ \psi \quad -(\cancel{30}\ 36)$$

Pauli algebra means that:

$$\underline{\sigma}\cdot\underline{r}\ \underline{\sigma}\cdot\underline{p} = \underline{r}\cdot\underline{p} + i\,\underline{\sigma}\cdot\underline{r}\times\underline{p}. \quad -(37)$$

The classical angular momentum is:

$$\underline{L} = \underline{r}\times\underline{p} \quad -(38)$$

8) so the real and physical part of Eq. (36) is:

$$H_{SO}\phi = \frac{e^2\hbar}{16\pi\epsilon_0 m^2c^2}\left(\frac{\underline{\sigma}\cdot\underline{L}}{r^3}\right)\phi \quad -(\cancel{33}\ 39)$$

In the quantum mechanical evaluation of this hamiltonian $\underline{\sigma}\cdot\underline{L}$ is regarded as an operator product of the spin and orbital angular momentum, so the expectation value is:

$$\langle H_{SO}\rangle = \frac{e^2\hbar}{16\pi\epsilon_0 m^2c^2}\int\phi^*\frac{\hat{\underline{\sigma}}\cdot\hat{\underline{L}}}{r^3}\phi\, d\tau \quad -(\cancel{34}\ 40)$$

This is a direct result of special relativity and gives the fine structure of atomic and molecular spectroscopy to high accuracy if radiative corrections are neglected. The spin angular momentum operator is defined as:

$$\hat{\underline{S}} = \frac{\hbar}{2}\hat{\underline{\sigma}} \quad -(\cancel{35}\ 41)$$

so the Pauli matrix $\underline{\sigma}$ is regarded as an operator. The spin angular momentum has no classical counterpart, so fine structure is a phenomenon of relativistic quantum mechanics. We have:

$$\langle H_{SO} \rangle = \frac{e^2}{8\pi\epsilon_0 m^2 c^2} \int \phi^* \frac{\hat{\underline{S}} \cdot \hat{\underline{L}}}{r^3} \phi \, d\tau \quad -(\cancel{36}\ 42)$$

The evaluation of this expectation value takes place by defining the total angular momentum operator:

$$\underline{J} = \underline{L} + \underline{S} \quad -(43)$$

so

$$J^2 = L^2 + S^2 + 2 \underline{L} \cdot \underline{S} \quad -(44)$$

It follows that:

$$\underline{S} \cdot \underline{L} = \underline{L} \cdot \underline{S} = \frac{1}{2} \left(J^2 - L^2 - S^2 \right) \quad -(45)$$

where:

$$J^2 \phi = J(J+1)\phi \quad -(46)$$

$$L^2 \phi = L(L+1)\phi \quad -(47)$$

$$S^2 \phi = S(S+1)\phi \quad -(48)$$

so

$$\boxed{\hat{\underline{S}} \cdot \hat{\underline{L}} \phi = \frac{1}{2} \left(J(J+1) - L(L+1) - S(S+1) \right) \phi} \quad -(49)$$

here J, L and S are quantum numbers.

The total angular momentum quantum number is

10) defined by the Clebsch Gordan series:

$$J = L + S,\ L + S - 1,\ \ldots,\ |L - S| \quad -(50)$$

The spin quantum number takes the values:

$$S = \frac{1}{2} \text{ or } -\frac{1}{2} \quad -(51)$$

In atomic hydrogen these quantum numbers are written with lower case letters. The principal quantum number is:

$$n = 0,\ 1,\ 2,\ \ldots \quad -(52)$$

and for any given n:

$$l = 0,\ 1,\ 2,\ \ldots,\ n-1 \quad -(53)$$

with

$$j = l + s,\ l + s - 1,\ \ldots,\ |l - s|, \quad -(54)$$

$$j_Z \psi = m_j \hbar \psi \quad -(55)$$

$$m_j = j,\ j-1,\ \ldots,\ -j \quad -(56)$$

Therefore:

$$\langle H_{SO} \rangle = \frac{e^2 \hbar^2}{8\pi \epsilon_0 m^2 c^2} \left(j(j+1) - l(l+1) - s(s+1) \right) \int \psi^* \frac{1}{r^3} \psi \, d\tau \quad -(57)$$

The expectation value of $1/r^3$ is

given conventionally by :

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{r_{B0}^3} \cdot \left(n^3 \ell (\ell + 1/2)(\ell+1) \right)^{-1} \quad -(58)$$

where the Bohr radius is :

$$r_{B0} = \frac{4\pi\epsilon_0 \hbar^2}{m e^4} \quad -(59)$$

However in x theory it is evaluated in general using :

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{\alpha^3} \left\langle \left(1 + \epsilon \cos(x\phi) \right)^3 \right\rangle \quad -(60)$$

or

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{\alpha^3} \left\langle \left(1 + \epsilon \cos(x\theta) \right)^3 \right\rangle \quad -(61)$$

where

$$\alpha = \ell(\ell+1) r_{B0}, \quad -(62)$$

$$\epsilon = 1 - \frac{\ell(\ell+1)}{n^2} \quad -(63)$$

So x can be found from eqs. (58) to (63) for given quantum numbers.