332(1): Relativistic Spin Orbit Hyperfine Structure.

· This phenomena is first inferred with the traditional Dirac approximation and then developed when this approximation is not used. The Dirac approximation is first defined as follows from the Einstein energy equation:

$$E^2 = p^2c^2 + m^2c^4 \quad -(1)$$

of special relativity, now developed into ECE2. In eq. (1):

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

and

$$\underline{p} = \gamma \underline{p_0} = \gamma m v_0 \quad -(3)$$

Here

$$\underline{p_0} = m\underline{v_0} \quad -(4)$$

is the classical momentum, so $\underline{p}$ is the relativistic momentum. The factor γ is the Lorentz factor:

$$\gamma = \left(1 - \frac{v_0^2}{c^2}\right)^{-1/2} \quad -(5)$$

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

The quantity E is the relativistic total energy, m is the particle mass and c the vacuum speed of light.

Define the relativistic four momentum:

$$p^\mu = \left(\frac{E}{c}, \underline{p}\right), \quad -(6)$$

$$p_\mu = \left(\frac{E}{c}, -\underline{p}\right) \quad -(7)$$

2) then eq. (1) is

$$p^{\mu} p_{\mu} = m^2 c^2 \quad -(8)$$

The relativistic hamiltonian is:

$$H = E + U \quad -(9)$$

where U is the potential energy. The non relativistic hamiltonian is

$$H_0 = H - mc^2 \quad -(10)$$

From eqs. (1) and (9):

$$(H - U)^2 = p^2 c^2 + m^2 c^4 \quad -(11)$$

so

$$(H - U)^2 - m^2 c^4 = p^2 c^2 \quad -(12)$$

Factorizing:

$$(H - U)^2 - m^2 c^4 = (H - U - mc^2)(H - U + mc^2) \quad -(13)$$

From eqs. (12) and (13):

$$H - U - mc^2 = \frac{p^2 c^2}{H - U + mc^2} \quad -(14)$$

so

$$H_0 = H - mc^2 = \frac{p^2 c^2}{H - U + mc^2} + U \quad -(15)$$

which is another way of writing the Einstein energy equation.

3) Dirac or one of his contemporaries introduced a 'rough approximation' to eq. (15). The rigorously correct equation is:

$$H_0 = \frac{p^2 c^2}{E + mc^2} + U \quad -(16)$$

where we have used:

$$E = H - U \quad -(17)$$

From eqs. (2) and (16):

$$H_0 = \frac{p^2 c^2}{(1+\gamma) mc^2} + U$$

$$= \frac{p^2}{m(1+\gamma)} + U \quad -(18)$$

Eq. (18) reduces to the classical, non-relativistic result as follows:

$$H_0 \xrightarrow[\gamma \to 1]{} \frac{p_0^2}{2m} + U. \quad -(19)$$

Note carefully that $\underline{p}$ in eq. (18) is the relativistic momentum, while $\underline{p_0}$ in eq. (19) is the classical momentum:

$$\underline{p} = \gamma \underline{p_0} \xrightarrow[\gamma \to 1]{} \underline{p_0} \quad -(20)$$

Dirac approximated eq. (15) by assuming:

$$H \sim mc^2 \quad -(21)$$

to obtain:

$$H_0 \sim \frac{p^2 c^2}{2mc^2 - U} + U$$

$$= \frac{p^2}{2m\left(1 - \frac{U}{2mc^2}\right)} + U \quad -(22)$$

So Dirac assumed:

$$E = H - U \sim mc^2 - U = \gamma mc^2 \quad -(23)$$

i.e.

$$\gamma = 1 - \frac{U}{mc^2} \quad -(24)$$

The correct γ is:

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

$$\sim \left(1 + \frac{1}{2}\frac{p_0^2}{m^2 c^2}\right) \quad -(25)$$

if

$$v_0 << c \quad -(26)$$

Comparing eqs. (24) and (25):

$$\frac{p_0^2}{2m} \sim -U \quad -(27)$$

5) Eq. (27) means that:

$$H_0 = \frac{p_0^2}{2m} + U = 0. \quad -(28)$$

This does not seem to be a meaningful approximation, although it has been used for ninety years!

Accepting this approximation for the sake of argument, eq. (22) is traditionally developed by assuming:

$$U << 2mc^2 \quad -(29)$$

so

$$H_0 \sim \frac{p^2}{2m}\left(1 - \frac{U}{2mc^2}\right) + U \quad -(30)$$

$$= \frac{p^2}{2m} - \frac{U}{4m^2c^2}p^2 + U$$

Using the SU(2) basis:

$$H_0 = \frac{p^2}{2m} - \frac{1}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,U\,\underline{\sigma}\cdot\underline{p} + U \quad -(31)$$

where $\underline{p}$ is the relativistic momentum.

The first term in eq. (31) was developed in UFT331, and was shown to give rise to a new type of relativistic fine structure in the Zeeman effect. The second term is the traditional spin orbit

6) term. The ordering of the terms as $\underline{\sigma} \cdot \underline{p}\, U\, \underline{\sigma} \cdot \underline{p}$ is entirely arbitrary. The only justification for it is that it results in agreement with experiment. This could therefore be described as an empirical procedure.

Quantization of the spin orbit Hamiltonian:

$$H_{so} = -\frac{1}{4m^2c^2}\, \underline{\sigma} \cdot \underline{p}\, U\, \underline{\sigma} \cdot \underline{p} \quad -(32)$$

proceeds by assuming that the first $\underline{p}$ is an operator and that the second is a function. Again this is an arbitrary procedure. It is also assumed that the relativistic quantization:

$$-i\hbar \underline{\nabla} \phi = \underline{p}\, \phi \quad -(33)$$

is the same as the non relativistic Schroedinger quantization and reduces to the latter in the limit

$$\gamma \rightarrow 1 \quad -(34)$$

This is again an arbitrary assumption, its only justification is that it appears to work.

Therefore eq. (32) quantizes to:

$$H_{so}\phi = \frac{i\hbar}{4m^2c^2}\, \underline{\sigma} \cdot \underline{\nabla} U\, \underline{\sigma} \cdot \underline{p}\, \phi \quad -(35)$$

7) It is now assumed that:

$$H_{so}\phi = \frac{i\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\left(U\,\underline{\sigma}\cdot\underline{p}\,\phi\right) \quad -(36)$$

Using the Leibnitz theorem:

$$\underline{\nabla}\left(U\,\underline{\sigma}\cdot\underline{p}\,\phi\right) = \underline{\nabla}U\left(\underline{\sigma}\cdot\underline{p}\,\phi\right) + U\,\underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\,\phi\right) \quad -(37)$$

Spectral fine structure energies from the first term on the right hand side of eq. (37), so:

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

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

The Coulomb potential between electron and proton in the H atom is:

$$U = -\frac{e^2}{4\pi\epsilon_0 r} \quad -(39)$$

so

$$\underline{\nabla}U = -\frac{e^2}{4\pi\epsilon_0 r^3}\,\underline{r} \quad -(40)$$

It follows that:

8)

$$H_{so}\phi = \frac{-i\hbar e^2}{16\pi\epsilon_0 m^2 c^2 r^3}\, \underline{\sigma}\cdot\underline{r}\,\underline{\sigma}\cdot\underline{p}\,\phi \quad -(41)$$

$+ \ldots\ldots$

Using Pauli algebra:

$$\underline{\sigma}\cdot\underline{r}\,\underline{\sigma}\cdot\underline{p} = \underline{r}\cdot\underline{p} + i\,\underline{\sigma}\cdot\underline{L} \quad -(42)$$

where

$$\underline{L} = \underline{r}\times\underline{p} \quad -(43)$$

is the relativistic angular momentum:

$$\underline{L} = \gamma\,\underline{L}_0 \quad -(44)$$

where the classical angular momentum is:

$$\underline{L}_0 = \underline{r}\times\underline{p}_0 \quad -(45)$$

Therefore the real and physical part of H_{so} is:

$$\boxed{\mathrm{Re}\,H_{so}\phi = \frac{\hbar e^2}{16\pi\epsilon_0 m^2 c^2 r^3}\,\underline{\sigma}\cdot\underline{L}\,\phi \quad -(46)}$$

This is the spin orbit hamiltonian.

Note carefully that it is:

$$\mathrm{Re}\,H_{so}\phi = \frac{\hbar e^2\gamma}{16\pi\epsilon_0 m^2 c^2 r^3}\,\underline{\sigma}\cdot\underline{L}_0\,\phi \quad -(47)$$

where:

$$\gamma = \left(1 - \frac{p_0^2}{m^2c^2}\right)^{-1/2} \quad -(48)$$

The factor γ in eq. (47) appears to have been omitted in the development of the past ninety years. Using

$$\gamma \sim 1 + \frac{1}{2}\frac{p_0^2}{m^2c^2} \quad -(49)$$

Eq. (47) becomes:

$$\boxed{\mathrm{Re}\, H_{SO}\,\phi = \frac{\hbar e^2}{16\pi\epsilon_0 m^2c^2r^3}\left(1 + \frac{1}{mc^2}\frac{p_0^2}{2m}\right)\underline{\sigma}\cdot\underline{L}_0\,\phi} \quad -(50)$$

which is the relativistically corrected spin orbit hamiltonian. The spin quantum operator $\hat{S}$ is defined as:

$$\hat{\underline{S}} = \frac{\hbar}{2}\hat{\underline{\sigma}} \quad -(51)$$

where the Pauli matrix is regarded as an operator. So

$$\mathrm{Re}\, H_{SO}\,\phi = \frac{e^2}{8\pi\epsilon_0 m^2c^2r^3\hbar^2}\left(1 + \frac{1}{mc^2}\frac{p_0^2}{2m}\right)\underline{S}\cdot\underline{L}_0\,\phi \quad -(52)$$

The $\underline{J}$ angular momentum is defined by:

$$\underline{J} = \underline{L}_0 + \underline{S} \quad -(53)$$

10) This was inferred by Sommerfeld and named the inner quantum number. Upon quantization:

$$J^2 \psi = J(J+1)\hbar^2 \psi \quad -(54)$$
$$L_0^2 \psi = L(L+1)\hbar^2 \psi \quad -(55)$$
$$S^2 \psi = S(S+1)\hbar^2 \psi \quad -(56)$$

The inner quantum number J is defined by the Clebsch Gordan series:

$$J = L+S,\ L+S-1,\ \ldots\ |L-S| \quad -(57)$$

Now note:
$$J^2 = L^2 + S^2 + 2\,\underline{L_0}\cdot\underline{S} \quad -(58)$$

It follows that:
$$\underline{L_0}\cdot\underline{S}\,\psi = \frac{1}{2}\hbar^2\left(J(J+1) - L(L+1) - S(S+1)\right)\psi \quad -(59)$$
$$-(60)$$

From eqs. (53) and (59):

$$\boxed{\mathrm{Re}\,H_{so}\,\psi = \frac{e^2}{16\pi\epsilon_0 m^2c^2r^3}\left(1 + \frac{1}{mc^2}\frac{p_0^2}{2m}\right)\left(J(J+1) - L(L+1) - S(S+1)\right)\psi}$$

For an electron:
$$S = \pm\frac{1}{2} \quad -(61)$$

so
$$J = L + \frac{1}{2} \text{ and } L - \frac{1}{2} \quad -(62)$$

11) In the usual theory the energy levels or fine structure of spin orbit interaction are given by the expectation value: — (63)

$$\langle \mathrm{Re} H_{SO} \rangle = \frac{e^2}{16\pi \epsilon_0 m^2 c^2} \left(J(J+1) - L(L+1) - S(S+1) \right) \int \phi^* \frac{1}{r^3} \phi \, d\tau$$

where:

$$\left\langle \frac{1}{r^3} \right\rangle = \int \phi^* \frac{1}{r^3} \phi \, d\tau = \frac{1}{a_0^3 L \left(L + \frac{1}{2}\right)(L+1) n^3} \quad -(64)$$

where n is the principal quantum number. Here:

$$a_0 = \frac{4\pi \epsilon_0 \hbar^2}{m e^4} \quad -(65)$$

is the Bohr radius.

So in the traditional theory: — (66)

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

where:

$$L = 0, \ldots, n-1 \quad -(67)$$

and

$$J = L + 1/2, \; L - 1/2 \quad -(68)$$

So the fine structure in atomic H depends on four quantum numbers, n, J, L and S.

12) In the relativistically corrected theory:

$$\langle ReH_{so} \rangle = \frac{e^2}{16\pi\epsilon_0 m^2 c^2}\left(\frac{J(J+1)-L(L+1)-S(S+1)}{a_0^3 n^3 L(L+\frac{1}{2})(L+1)}\right)\left(1+\frac{1}{mc^2}\left\langle \frac{p_0^2}{2m} \right\rangle\right) \quad -(69)$$

From note 331(5):

$$\frac{1}{mc^2}\left\langle \frac{p_0^2}{2m} \right\rangle = \frac{1}{2}\left(\frac{\lambda_c}{a_0}\right)\frac{\alpha}{n^2} \quad -(70)$$

$$= \frac{2.662567 \times 10^{-5}}{n^2}$$

So:

$$\langle ReH_{so} \rangle = \frac{e^2}{16\pi\epsilon_0 m^2 c^2}\left(\frac{J(J+1)-L(L+1)-S(S+1)}{a_0^3 n^3 L(L+1/2)(L+1)}\right)\left(1+\frac{2.662567 \times 10^{-5}}{n^2}\right) \quad -(71)$$

For the 2p level of atomic hydrogen the fine structure splitting is 0.365 cm^{-1}, where:

$$1 \text{ cm}^{-1} = 2.997925 \times 10^{10} \text{ Hz} \quad -(72)$$

$$\sim 30 \text{ GHz}$$

so the hyperfine spin orbit splitting in the Dirac approximation is in the MHz range approximately, within reach of double resonance spectroscopy. A computer program could be written to show the spectra from eq. (71)