330(4): Systematic Development of Schemes of Quantization

The classical spin orbit hamiltonian in the SU(2) basis is:

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

where $\underline{p}$ is the relativistic momentum. The quantization scheme in the Dirac equation is:

$$p^\mu = i\hbar \partial^\mu \quad -(2)$$

and quantization takes place through the relativistic four momentum

$$p^\mu = \left(\frac{E}{c}, \underline{p} \right) \quad -(3)$$

This fact almost never appears in the textbooks. Here:

$$E = \gamma mc^2, \quad \underline{p} = \gamma m \underline{v} = \gamma \underline{p}_0 \quad -(4)$$

where $\underline{p}_0$ is the classical momentum:

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

The Schroedinger equation is not relativistic, so quantization takes place through the classical momentum. The wave functions of the Dirac equation are denoted ϕ_r, and those of the Schroedinger equation are denoted ϕ. It follows that:

$$-i\hbar \underline{\nabla} \phi_r = \underline{p} \phi_r \quad -(6)$$

and

$$-i\hbar \underline{\nabla} \phi = \underline{p}_0 \phi \quad -(7)$$

) In eq. (6):

$$\underline{p}\,\psi_r = \gamma\,\underline{p_0}\,\psi_r = -i\hbar\,\underline{\nabla}\,\psi_r \quad -(8)$$

Therefore:

$$H_{so} = \frac{1}{4m^2c^2}\,\underline{\sigma}\cdot\gamma\,\underline{p_0}\;U\;\underline{\sigma}\cdot\gamma\,\underline{p_0} \quad -(9)$$

$$= \frac{1}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\;U\;\underline{\sigma}\cdot\gamma\,\underline{p_0}$$

So:

$$H_{so}\psi_r = -\frac{\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\;U\;\underline{\sigma}\cdot\gamma\,\underline{p_0}\,\psi_r \quad -(10)$$

$$= -\frac{\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\left(U\,\underline{\sigma}\cdot\gamma\,\underline{p_0}\,\psi_r\right)$$

as in previous notes for UFT330.

If the relativistic wavefunction ψ_r is approximated by the Schroedinger wavefunction ψ then to a first approximation:

$$\psi_r \sim \psi \quad -(11)$$

and

$$\underline{p}\,\psi = \gamma\,\underline{p_0}\,\psi \quad -(12)$$

so eq. (10) is approximated by:

3)

$$H_{SO}\phi = -\frac{\hbar\gamma}{4m^2c^2}\underline{\sigma}\cdot\underline{\nabla}\left(U\underline{\sigma}\cdot\gamma_{p_0}\phi\right) \quad -(13)$$

The advantage of using the approximation (13) is that the hydrogenic ϕ are known analytically.

In these scheme:

$$\gamma = 1 + \frac{H_0 - U}{mc^2} \quad -(14)$$

where

$$U = -\frac{e^2}{4\pi\epsilon_0 r}. \quad -(15)$$

Therefore:

$$\gamma = 1 + \frac{H_0}{mc^2} + \frac{e^2}{4\pi\epsilon_0 mc^2 r}. \quad -(16)$$

In the H atom:

$$H_0 = \langle H_0\rangle = -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2n^2} \quad -(17)$$

where n is the principal quantum number.

So:

$$\gamma = 1 - \frac{e^4}{32\pi^2\epsilon_0^2\hbar^2c^2n^2} + \frac{e^2}{4\pi\epsilon_0 mc^2 r} \quad -(18)$$

Using the Bohr radius:

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} \quad -(19)$$

it follows that

$$H_0 = \langle H_0 \rangle = -\frac{e^2}{8\pi\epsilon_0 mc^2 a_0} \quad -(20)$$

so

$$\boxed{\gamma = 1 - \frac{e^2}{4\pi\epsilon_0 mc^2}\left(\frac{1}{2a_0} - \frac{1}{r}\right)} \quad -(21)$$

A lot of new information appears by careful consideration of γ in various quantization schemes. Consider the definition of the fine structure constant:

$$\alpha = \frac{e^2}{4\pi\hbar c\epsilon_0}, \quad -(22)$$

then:

$$\gamma = 1 - \alpha\left(\frac{\hbar}{mc}\right)\left(\frac{1}{2a_0} - \frac{1}{r}\right) \quad -(23)$$

i.e.

$$\boxed{\gamma = 1 - \alpha\lambda_c\left(\frac{1}{2a_0} - \frac{1}{r}\right)} \quad -(24)$$

where

$$\lambda_c = \frac{\hbar}{mc} \quad -(25)$$

is the Compton wavelength.

In S.I. units:

5)

$$\alpha = 0.007297351 \quad -(26)$$

$$a_0 = 5.29177 \times 10^{-11}\,\text{m} \quad -(27)$$

$$\lambda_c = 3.861591 \times 10^{-13}\,\text{m} \quad -(28)$$

Therefore

$$H_0 = \langle H_0 \rangle = -\frac{\alpha \lambda_c}{2 a_0} \quad -(29)$$

and

$$U = -\frac{\alpha \lambda_c}{r} \quad -(30)$$

The fundamental approximation used is:

$$\gamma = \left(1 - \frac{p_0^2}{m^2 c^2}\right)^{-1/2} \quad -(31)$$

where

$$H_0 = \frac{p_0^2}{2m} + U \quad -(32)$$

so

$$p_0^2 = 2m\left(H_0 - U\right) \quad -(33)$$

The Hamiltonian of the Schroedinger H atom is given by eq. (29) and is negative valued. The reason for this is that H_0 defines binding states between electron and proton, and is defined by:

$$H_0 = \langle H_0 \rangle = -\frac{\hbar^2}{2m}\int \psi^* \nabla^2 \psi \, d\tau - \frac{e^2}{4\pi\epsilon_0}\int \psi^* \frac{1}{r} \psi \, d\tau$$

$$-(34)$$

) The expectation value of p_0^2 is:

$$p_0^2 = \langle p_0^2 \rangle = -\hbar^2 \int \psi^* \nabla^2 \psi \, d\tau \quad -(35)$$

and is negative valued. This indicates that p_0 is complex valued in the H atom, and this is the result of the Schroedinger equation.

The richness of structure follows from the Leibnitz equation applied to Eq. (10):

$$\underline{\nabla}\left(U \underline{\sigma} \cdot \underline{p} \, \psi_r\right) = \underline{\nabla}\left(\underline{\sigma} \cdot \underline{p}\right)\left(U\psi_r\right) + \underline{\sigma} \cdot \underline{p} \, \underline{\nabla}\left(U\psi_r\right)$$

$$= \underline{\nabla}\left(\underline{\sigma} \cdot \gamma \underline{p}_0\right)\left(U\psi_r\right) + \underbrace{\gamma \underline{\sigma} \cdot \underline{p}_0 \, \underline{\nabla}\left(U\psi_r\right)}_{\text{Note 330(2)}} \quad -(36)$$

The first term in Eq. (36) can be developed using the Leibnitz theorem:

$$\underline{\nabla}\left(\gamma \underline{\sigma} \cdot \underline{p}_0\right) = \left(\underline{\nabla}\gamma\right) \underline{\sigma} \cdot \underline{p}_0 + \gamma \underline{\nabla}\left(\underline{\sigma} \cdot \underline{p}_0\right) \quad -(37)$$

So there is a new term:

$$\hat{H}_{SO}\psi = -\frac{i\hbar}{4m^2c^2}\left(\underline{\sigma} \cdot \underline{\nabla}\gamma \, \underline{\sigma} \cdot \underline{p}_0\right) U\psi_r \quad -(38)$$

$$+ \ldots$$

1) where:

$$\underline{\nabla}\gamma = -\frac{1}{mc^2}\underline{\nabla}U = \frac{e^2}{4\pi mc^2\epsilon_0}\frac{\underline{r}}{r^3} \quad -(39)$$

giving:

$$\hat{H}_{SO}\phi_r = -\frac{i\hbar}{4m^2c^2}\left(\frac{e^2}{4\pi mc^2\epsilon_0 r^3}\right)\left(\frac{-e^2}{4\pi\epsilon_0 r}\right) \times \underline{\sigma}\cdot\underline{r}\;\underline{\sigma}\cdot\underline{p}_0\,\phi_r \quad -(40)$$

giving:

$$\mathrm{Re}\,\hat{H}_{SO}\phi_r = \frac{-e^4\hbar}{128m^3c^4\epsilon_0^2}\frac{\underline{\sigma}\cdot\underline{L}}{r^4} \quad -(41)$$
