+27(5): Hamiltonians of Relativistic Quantum in Theory

. In the notation of UFT 250, the Dirac theory produces the equation:

$$H = \left(mc^2 + e\phi + \frac{1}{2m}\underline{\sigma}\cdot(\underline{p}-e\underline{A})\left(1+\frac{e\phi}{2mc^2}\right)\underline{\sigma}\cdot(\underline{p}-e\underline{A})\right) \quad -(1)$$

where E is the total energy, e the charge on the proton, ϕ the scalar potential, $\underline{A}$ the vector potential and $\underline{p}$ the momentum. Eq. (1) can be expanded as:

$$H = mc^2 + e\phi + \frac{1}{2m}\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{p} + \frac{e^2}{2m}\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{A}$$
$$-\frac{e}{2m}\left(\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{p} + \underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{A}\right) \quad -(2)$$
$$+\underline{\sigma}\cdot(\underline{p}-e\underline{A})\frac{e\phi}{2mc^2}\underline{\sigma}\cdot(\underline{p}-e\underline{A}).$$

Therefore:

$$H = mc^2 + e\phi + H_1 + H_2 + H_3 + H_4 \quad -(3)$$

where:

$$H_1 = \frac{1}{2m}\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{p} = \frac{p^2}{2m} \quad -(4)$$

$$H_2 = -\frac{e}{2m}\left(\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{p} + \underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{A}\right) \quad -(5)$$

$$H_3 = \frac{e^2}{2m}\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{A} \quad -(6)$$

$$H_4 = \frac{1}{2m}\underline{\sigma}\cdot(\underline{p}-e\underline{A})\frac{e\phi}{2mc^2}\underline{\sigma}\cdot(\underline{p}-e\underline{A}) \quad -(7)$$

Eq. (4) is the free particle kinetic energy, eq. (5) is the Zeeman effect hamiltonian, eq. (6) is the second order effect due to $\underline{A}$ and eq. (7) is the fine structure hamiltonian

In R theory the hamiltonian is:

$$H = \frac{1}{m(r)^{1/2}} \frac{p^2}{2m}\left(1 - \frac{U}{2mc^2}\right)^{-1} + m(r)^{1/2}\left(mc^2 + U\right) \quad -(8)$$

In order to prepare for quantization this is written in the SU(2) basis as:

$$H = \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \left(\frac{1}{m(r)^{1/2}} \left(1 - \frac{U}{2mc^2}\right)^{-1} \right) \underline{\sigma} \cdot \underline{p} + m(r)^{1/2}\left(mc^2 + U\right)$$

$$\sim \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \left(\frac{1}{m(r)^{1/2}} \left(1 + \frac{U}{2mc^2}\right) \right) \underline{\sigma} \cdot \underline{p} + m(r)^{1/2}\left(mc^2 + U\right) \quad -(9)$$

The effect of an external magnetic field is described by the minimal prescription:

$$\underline{p} \rightarrow \underline{p} - e\underline{A}, \quad -(10)$$

and using

$$U = e\phi \quad -(11)$$

Eq. (9) becomes:

$$H \sim \frac{1}{2m} \underline{\sigma} \cdot \left(\underline{p} - e\underline{A}\right) \left(\frac{1}{m(r)^{1/2}} \left(1 + \frac{e\phi}{2mc^2}\right) \right) \underline{\sigma} \cdot \left(\underline{p} - e\underline{A}\right) + m(r)^{1/2}\left(mc^2 + U\right) \quad -(12)$$

$$= m(r)^{1/2}\left(mc^2 + U\right) + H_1 + H_2 + H_3 + H_4 \quad -(13)$$

where:

$$H_1 = \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \frac{1}{m(r)^{1/2}} \underline{\sigma} \cdot \underline{p} \quad -(14)$$

$$H_2 = -\frac{e}{2m} \left(\underline{\sigma} \cdot \underline{A} \frac{1}{m(r)^{1/2}} \underline{\sigma} \cdot \underline{p} + \underline{\sigma} \cdot \underline{p} \frac{1}{m(r)^{1/2}} \underline{\sigma} \cdot \underline{A} \right)$$

$$H_3 = \frac{e^2}{2m} \underline{\sigma} \cdot \underline{A} \frac{1}{m(r)^{1/2}} \underline{\sigma} \cdot \underline{A} \quad -(15)$$

$$H_4 = \frac{1}{2m}\,\underline{\sigma}\cdot\left(\underline{p}-e\underline{A}\right)\frac{e\phi}{2mc^2 n(r)^{1/2}}\,\underline{\sigma}\cdot\left(\underline{p}-e\underline{A}\right) \quad -(16)$$

It is seen that each one of the well known hamiltonians of Dirac theory, eqs. (4) to (7) is changed by $n(r)^{1/2}$. Therefore the spectral structure of atoms and molecules is changed by $n(r)^{1/2}$:

1) the main structure of the atom or molecule (H_1);
2) the structure of the Zeeman effect (H_2)
3) the second order structure (H_3)
4) the fine structure of atoms and molecules (H_4).

Quantization now proceeds using:

$$\underline{p}\,\psi = -i\hbar\,\underline{\nabla}\,\psi \quad -(17)$$

In the Dirac theory, the energy levels of the H atom are given by:

$$H\psi = E\psi \quad -(18)$$

where

$$H = H_1 + e\phi$$

$$= \frac{1}{2m}\,\underline{\sigma}\cdot\underline{p}\;\underline{\sigma}\cdot\underline{p} - \frac{e^2}{4\pi\epsilon_0 r} \quad -(19)$$

$$= \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r}$$

so

$$H\psi = -\frac{\hbar^2\nabla^2}{2m}\psi - \frac{e^2}{4\pi\epsilon_0 r}\psi \quad -(20)$$

The energy levels of the H atom are given by:

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

$$= -\frac{\mu e^4}{32\pi^2\epsilon_0^2\hbar^2 n^2} \quad -(21)$$

where n is the principal quantum number:

$$n = 1, 2, 3, 4 \ldots \quad -(22)$$

and

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad -(23)$$

, the reduced mass of the electron and proton of the H atom. Here ϕ are the well known hydrogen wave functions.

In m theory the energy levels of the H atom are given by:

$$H\phi = E\phi \quad -(24)$$

where:

$$H = H_1 + m(r)^{1/2} e\phi \quad -(25)$$

$$= \frac{1}{2m}\underline{\sigma}\cdot\underline{p}\,\frac{1}{m(r)^{1/2}}\,\underline{\sigma}\cdot\underline{p} - m(r)^{1/2}\frac{e^2}{4\pi\epsilon_0 r}$$

$$= \frac{1}{2m}\underline{p}\cdot\left(\frac{1}{m(r)^{1/2}}\underline{p}\right) - \frac{e^2}{4\pi\epsilon_0}\frac{m(r)^{1/2}}{r}$$

So

$$H\phi = -\frac{i\hbar}{2m}\underline{\nabla}\cdot\left(\frac{1}{m(r)^{1/2}}\underline{p}\,\phi\right) - \frac{e^2}{4\pi\epsilon_0}\frac{m(r)^{1/2}}{r}\phi$$

$$= -\frac{\hbar^2}{2m}\underline{\nabla}\cdot\left(\frac{1}{m(r)^{1/2}}\underline{\nabla}\phi\right) - \frac{e^2}{4\pi\epsilon_0}\frac{m(r)^{1/2}}{r}\phi$$

$$-(26)$$

5) So:

$$H\psi = -\frac{\hbar^2}{2m\,m(r)^{1/2}}\nabla^2\psi - \frac{\hbar^2}{2m}\underline{\nabla}\left(\frac{1}{m(r)^{1/2}}\right)\cdot\underline{\nabla}\psi$$

$$-\frac{e^2}{4\pi\epsilon_0}\frac{m(r)^{1/2}}{r}\psi \quad -(27)$$

$$\xrightarrow[m(r)\to 1]{} -\frac{\hbar^2}{2m}\nabla^2\psi - \frac{e^2}{4\pi\epsilon_0 r}\psi$$

The theory reduces correctly to the Dirac theory when:

$$m(r) = 1 \quad -(28)$$

Q.E.D.

The energy levels are:

$$E = -\frac{\hbar^2}{2m}\int\psi^*\frac{1}{m(r)^{1/2}}\nabla^2\psi\,d\tau$$

$$-\frac{\hbar^2}{2m}\int\psi^*\underline{\nabla}\left(\frac{1}{m(r)^{1/2}}\right)\cdot\underline{\nabla}\psi\,d\tau \quad -(29)$$

$$-\frac{e^2}{4\pi\epsilon_0}\int\psi^*\frac{m(r)^{1/2}}{r}\psi\,d\tau$$

So the energy levels of the H atom are all changed to a different extent by m theory.