

### 329(1): Numerical Corrections to Sommerfeld and Dirac Quantization.

Consider the Hamiltonian of special relativity:

$$H = \gamma mc^2 + U = (p^2 c^2 + m^2 c^4)^{1/2} + U. \quad (1)$$

For the Sommerfeld and Dirac atoms (Hydrogen):

$$U = -\frac{ee_1}{4\pi\epsilon_0 r} \quad (2)$$

where  $e$  is the charge of the proton and  $e_1$  the charge on the electron. The distance between the proton and electron is  $r$  and  $\epsilon_0$  is the vacuum permittivity. In eq. (1)  $\underline{p}$  is the relativistic momentum:

$$\underline{p} = \gamma m \underline{v}_0 \quad (3)$$

and  $\gamma$  is the Lorentz factor:

$$\gamma = \frac{dt}{d\tau} = \left(1 - \frac{v_0^2}{c^2}\right)^{-1/2} \quad (4)$$

The proper time  $\tau$  is defined by the infinitesimal line element of special relativity:

$$c^2 d\tau^2 = (c^2 - v_0^2) dt^2 \quad (5)$$

Eq. (1) can be written as:

$$2) (H-U)^2 = p^2 c^2 + m^2 c^4 = E^2 - (6)$$

$$\text{i.e.: } (H-U)^2 - m^2 c^4 = p^2 c^2 - (7)$$

Factorizing the left hand side:

$$(H-U-mc^2)(H-U+mc^2) = p^2 c^2 - (8)$$

$$\text{so } H-U-mc^2 = \frac{p^2 c^2}{H-U+mc^2} - (9)$$

$$= \frac{p^2 c^2}{E+mc^2}$$

Eq. (9) can be written as:

$$H_0 = H-mc^2 = \frac{p^2 c^2}{E+mc^2} + U - (10)$$

$$\text{In the limit: } E \rightarrow mc^2 - (11)$$

eq. (10) becomes the classical:

$$H_0 = \frac{p^2}{2m} + U - (12)$$

In the well known Dirac approximation, it is assumed that:

$$H \rightarrow E \rightarrow mc^2 - (13)$$

i.e.

$$U \ll E \quad (14)$$

so eq. (9) becomes:

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

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

$$H_0 \sim \frac{p^2}{2m} \left( 1 + \frac{U}{2mc^2} \right) + U \quad (16)$$

The Dirac approximation is very rough, and is accepted because it gives a variety of results such as the Thomas factor, spin-orbit coupling and so on.

Therefore the relativistic Hamiltonian (1) has been approximated by Eq. (16). This approximation can be used both for Schrödinger and Dirac quantization. In Schrödinger quantization:

$$(H_0 - U)\psi = -\frac{\hbar^2 \nabla^2}{2m} \left( \left( 1 + \frac{U}{2mc^2} \right) \right) \psi \quad (17)$$

i.e.:

$$4) H_0 \psi = -\frac{\hbar^2 \nabla^2}{2m} \left( \left( 1 + \frac{U}{2mc^2} \right) \psi \right) + U \psi \quad (18)$$

In the limit:  $U \ll 2mc^2 \quad (19)$

this reduces to the Schrodinger equation:

$$H_0 \psi = -\frac{\hbar^2 \nabla^2}{2m} \psi + U \psi \quad (20)$$

Eq. (18) is the Schrodinger quantization of the Sommerfeld

atom.  
In Dirac quantization:

$$H_0 = \frac{\underline{\sigma} \cdot \underline{p}}{2m} \left( 1 + \frac{U}{2mc^2} \right) \underline{\sigma} \cdot \underline{p} + U \quad (21)$$

in the  $su(2)$  basis. Here:

$$\underline{\sigma} \cdot \underline{p} \psi = -i \hbar \underline{\sigma} \cdot \underline{\nabla} \psi, \quad (22)$$

so:

$$H_0 \psi = -\frac{\hbar^2}{2m} \underline{\sigma} \cdot \underline{\nabla} \left( \left( 1 + \frac{U}{2mc^2} \right) \underline{\sigma} \cdot \underline{\nabla} \right) \psi + U \psi \quad (23)$$

As in previous UFT papers eq. (23) give several Hamiltonians because  $\underline{\nabla}$  is on the left hand side of the brackets as well as on all to the right of it.

> A more accurate calculation requires the equation:

$$H_0 = H - mc^2 = \frac{p^2 c^2}{(p^2 c^2 + m^2 c^4)^{1/2} + mc^2} + U. \quad (24)$$

Consider for example the quantization scheme:

$$H_0 \psi = \left( \frac{-c^2 \hbar^2}{(p^2 c^2 + m^2 c^4)^{1/2} + mc^2} \right) \nabla^2 \psi + U \psi \quad (25)$$

In the numerator:

$$p^2 \psi = -\hbar^2 \nabla^2 \psi \quad (26)$$

In the denominator the classical but relativistic  $p^2$  must be calculated.

In two dimensions:

$$p = m \int \dot{r} dt \quad (27)$$

and from the Lagrangian:

$$L = -\frac{mc^2}{\gamma} + U \quad (28)$$

it can be shown in Notes for papers UFT324 and UFT325 that:

$$\ddot{r} = \frac{(-\gamma^2 \dot{v}^2 + \gamma^2 \dot{r}^2 - c^2) \underline{m} \underline{G} + r (\gamma^3 \dot{v}^4 + \gamma c^2 \dot{v}^2) + r \dot{r} (-\gamma^3 \dot{v}^2 - \gamma c^2)}{r^3 (\gamma^3 \dot{v}^2 + \gamma c^2)} \quad - (29)$$

For application to atoms:

$$\underline{m} \underline{G} \rightarrow \frac{1}{4\pi \epsilon_0} \quad - (30)$$

Therefore in two dimensions,  $p$  can be computed and used in eq. (25).

The accurate Dirac atom is given by:

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

which quantizes to:

$$H_0 \phi = - \underline{\sigma} \cdot \underline{\nabla} \left( \left( \frac{c^2 \hbar^2}{(\underline{p}^2 c^2 + m^2 c^4)^{1/2} + m c^2} \right) \underline{\sigma} \cdot \underline{\nabla} \right) \phi + U \phi \quad - (32)$$

## Computer Algebra

Use the two dimensional particle on a ring wave functions:

$$7) \psi(\theta) = \left(\frac{1}{2\pi}\right)^{1/2} \exp(i m_e \theta) - (33)$$

and calculate expectation values of  $H_0$  from eqs. (18) and (25) and compare. Use eq. (29) to compute  $P$  in the denominator of eq. (25).

Repeat for the Dirac atom by comparing the usual Dirac atom, eq. (23), with the corrected Dirac atom, eq. (32). There should be significant differences in energy levels between eqs. (23) and (32).

The next stage is to repeat these calculations in three dimensions and apply the results to the H atom.

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