329(2): The Sommerfeld and Dirac Equations in 3 - D

As in note 329(1) the basic equation is:

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

It is assumed that this quantizes using:

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

in the numerator. In the denominator it is assumed that p^2 remains classical. The expectation values of H_0 are:

$$\langle H_0 \rangle = \int \phi^* \frac{p^2c^2}{(p^2c^2+m^2c^4)^{1/2}+mc^2}\phi \, d\tau + \int \phi^* U \phi \, d\tau \quad -(3)$$

In the H atom these expectation values of total energy, which can be observed spectroscopically. From eq. (3):

$$\langle H_0 \rangle = -\hbar^2c^2 \int \frac{\phi^* \nabla^2 \phi \, d\tau}{(p^2c^2+m^2c^4)^{1/2}+mc^2} + \int \phi^* U \phi \, d\tau \quad -(4)$$

where

$$U = -\frac{e^2}{4\pi\epsilon_0 r} \quad -(5)$$

2)

In the non-relativistic limit the expectation values are:

$$\langle H_0 \rangle = -\frac{\hbar^2}{2m}\int \phi^* \nabla^2 \phi \, d\tau + \int \phi^* U \phi \, d\tau \qquad -(6)$$

It is clear that the relativistic (3) produces a shift in the energy levels (6).

In spherical polar coordinates:

$$p_x = m(\dot{r}\sin\theta\cos\phi + r\cos\theta\cos\phi\,\dot{\theta} - r\sin\theta\sin\phi\,\dot{\phi})$$
$$p_y = m(\dot{r}\sin\theta\sin\phi + r\cos\theta\sin\phi\,\dot{\theta} + r\sin\theta\cos\phi\,\dot{\phi})$$
$$p_z = m(\dot{r}\cos\theta - r\sin\theta\,\dot{\theta}) \qquad -(7)$$
$$L_x = -mr^2(\dot{\theta}\sin\phi + \dot{\phi}\sin\theta\cos\theta\cos\phi)$$
$$L_y = mr^2(\dot{\theta}\cos\phi - \dot{\phi}\sin\theta\cos\theta\sin\phi)$$
$$L_z = mr^2\sin^2\theta\,\dot{\phi}$$

Therefore in order to find p^2 it is necessary to find $\dot{r}$, $\dot{\theta}$ and $\dot{\phi}$.

On the non relativistic level as in 4FT270 and 4FT271

$$\dot{\phi} = \frac{L_z}{mr^2\sin^2\theta}, \qquad -(8)$$

$$\dot{\theta} = \frac{1}{mr^2}\left(L^2 - \frac{L_z^2}{\sin^2\theta}\right)^{1/2} \qquad -(9)$$

3) and $\dot{r}$ can be evaluated from:

$$m\ddot{r} = m\left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta\right) - \frac{mMG}{r^2} \quad -(10)$$

using

$$\dot{r} = \int \ddot{r}\, dt \quad -(11)$$

In the first approximation, the expectation values can be calculated from eqs. (4), and (8) to (10).

In a fully relativistic treatment the relativistic hamiltonian and lagrangian must be used:

$$H = \gamma m c^2 + U \quad -(12)$$

$$\mathcal{L} = -\frac{mc^2}{\gamma} - U \quad -(13)$$

where

$$\gamma = \left(1 - \frac{v^2}{c^2}\right)^{-1/2} \quad -(14)$$

with

$$v^2 = \dot{r}^2 + r^2\left(\dot{\theta}^2 + \sin^2\theta\, \dot{\phi}^2\right)$$
$$= \dot{r}^2 + \dot{\beta}^2 r^2 \quad -(15)$$

The relativistic equivalents of eqs. (8), (9) and (10) must be found because p^2 is the relativistic momentum.

In order to pursue this calculation use:

$$\frac{\partial \mathcal{L}}{\partial r} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{r}} \quad -(16)$$

$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\theta}} \quad -(17)$$

$$\frac{\partial \mathcal{L}}{\partial \phi} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\phi}} \quad -(18)$$

and

$$\frac{\partial \mathcal{L}}{\partial \beta} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\beta}} \quad -(19)$$

with the lagrangian:

$$\mathcal{L} = -mc^2\left(1 - \frac{1}{c^2}\left(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\,\dot{\phi}^2\right)\right)^{1/2} - U$$

$$= -mc^2\left(1 - \frac{1}{c^2}\left(\dot{r}^2 + \dot{\beta}^2 r^2\right)\right)^{1/2} - U \quad -(20)$$

in order to find the relativistic equivalents of eqs. (8) to (10). This means that $\dot{\theta}$, $\dot{\phi}$ and $\dot{r}$ can be expressed in terms of L^2 and L_Z^2. Finally $\dot{r}$ can be found from the relativistic equivalent of eq. (10) and the expectation value of eq. (4) computed using the hydrogenic ψ as a first approximation.