269(3): Summary of the Three Dimensional Theory

The basic Hamiltonian is:

$$H = \frac{1}{2} m v^2 - \frac{k}{r} \quad -(1)$$

$$= \frac{p^2}{2m} - \frac{k}{r}$$

In spherical polar coordinates:

$$H = \frac{1}{2} m \left(\dot{r}^2 + r^2 \left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta \right) \right) - \frac{k}{r}$$

$$= \frac{1}{2} m \left(\frac{dr}{dt} \right)^2 + \frac{L^2}{2mr^2} - \frac{k}{r} \quad -(2)$$

where

$$L^2 = L_x^2 + L_y^2 + L_z^2 \quad -(3)$$

$$= m^2 r^4 \left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta \right)$$

The individual components of angular momentum are:

$$L_x = -mr^2 \left(\dot{\theta} \sin \phi + \dot{\phi} \sin \theta \cos \theta \cos \phi \right) \quad -(4)$$

$$L_y = mr^2 \left(\dot{\theta} \cos \phi - \dot{\phi} \sin \theta \cos \theta \sin \phi \right) \quad -(5)$$

$$L_z = mr^2 \dot{\phi} \sin^2 \theta \quad -(6)$$

The conserved quantities are L^2, L_x, L_y and L_z.

It would be interesting to work out the expectation values of these quantities:

2)

$$\langle L^2 \rangle = m^2 \int \phi^* r^4 \left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta\right) \phi \, d\tau \quad -(7)$$

$$\langle L_x \rangle = -m \int \phi^* r^2 \left(\dot{\theta} \sin\phi + \dot{\phi} \sin\theta \cos\theta \cos\phi\right) \phi \, d\tau \quad -(8)$$

$$\langle L_y \rangle = m \int \phi^* r^2 \left(\dot{\theta} \cos\phi - \dot{\phi} \sin\theta \cos\theta \sin\phi\right) \phi \, d\tau \quad -(9)$$

$$\langle L_z \rangle = m \int \phi^* r^2 \dot{\phi} \sin^2\theta \, \phi \, d\tau \quad -(10)$$

Now define the angle β by:

$$\dot{\beta}^2 = \dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta \quad -(11)$$

Then:

$$H = \frac{1}{2} m \left(\dot{r}^2 + r^2 \dot{\beta}^2\right) - \frac{k}{r} \quad -(12)$$

It follows that this three dimensional hamiltonian has the same format as the two dimensional hamiltonian:

$$H = \frac{1}{2} m \left(\dot{r}^2 + r^2 \dot{\phi}^2\right) - \frac{k}{r} \quad -(13)$$

therefore many characteristics of eq. (12) can be deduced, notably its orbit is:

$$r = \frac{\alpha}{1 + \epsilon \cos\beta} \quad -(14)$$

3) where:

$$\alpha = \frac{L^2}{mk}, \quad \epsilon^2 = 1 + \frac{2EL^2}{mk^2} \quad -(15)$$

The Binet equation governing the system is:

$$F = -\frac{L^2}{mr^2}\left(\frac{d^2}{d\beta^2}\left(\frac{1}{r}\right) + \frac{1}{r}\right) \quad -(16)$$

$$= m\ddot{r} - \frac{L^2}{mr^3}$$

$$= -\frac{k}{r^2}$$

For the ellipse (14):

$$F = -\frac{L^2}{m\alpha r^2} = -\frac{k}{r^2}. \quad -(17)$$

and

$$V = -\frac{k}{r}. \quad -(18)$$

For the precessing ellipse:

$$r = \frac{\alpha}{1 + \epsilon\cos(x\beta)} \quad -(19)$$

$$F = -x^2\frac{k}{r^2} + (x^2 - 1)\frac{L^2}{mr^3} \quad -(19)$$

and $$V = -x^2 \frac{k}{r} + (x^2-1)\frac{L^2}{2mr^2} \quad -(20)$$

The Hamiltonian is changed from:

$$H = \frac{p^2}{2m} - \frac{k}{r} \quad -(21)$$

to $$H = \frac{p^2}{2m} - x^2\frac{k}{r} + \frac{(x^2-1)L^2}{2mr^2} \quad -(22)$$

In the H atom the energy levels are changed to:

$$E = \langle H \rangle = \left\langle \frac{p^2}{2m} \right\rangle - x^2 \left\langle \frac{k}{r} \right\rangle + \frac{(x^2-1)}{2m}\left\langle \frac{L^2}{r^2} \right\rangle \quad -(23)$$

where

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2 n^2} \quad -(24)$$

$$\left\langle \frac{k}{r} \right\rangle = -\frac{me^4}{16\pi^2\epsilon_0^2\hbar^2 n^2} \quad -(25)$$

$$\langle L^2 \rangle = \ell(\ell+1)\hbar^2 \quad -(26)$$

so the new energy levels are:

$$E = \frac{(1-2x^2)me^4}{32\pi^2\epsilon_0^2\hbar^2 n^2} + \frac{(x^2-1)\hbar^2\ell(\ell+1)}{2m}\left\langle \frac{1}{r^2} \right\rangle \quad -(27)$$

5) where:

$$\left\langle \frac{1}{r^2} \right\rangle = \int \phi^* \frac{1}{r^2} \phi \, d\tau \quad -(28)$$

The fine structure of the H atom can be reproduced by comparing Eq. (27) with the result for spin orbit theory:

$$(E - mc^2)\phi = \left(\frac{p^2}{2m} - \frac{k}{r} - \frac{e^2}{16\pi\epsilon_0 m^2 c^2} \underline{\sigma} \cdot \underline{p} \frac{1}{r} \underline{\sigma} \cdot \underline{p} \right) \phi$$

$$-(29)$$

so:

$$-x^2 \left\langle \frac{k}{r} \right\rangle + (x^2 - 1) \ell(\ell+1) \frac{\hbar^2}{2m} \left\langle \frac{1}{r^2} \right\rangle$$

$$= - \left\langle \frac{k}{r} \right\rangle - \frac{e^2}{16\pi\epsilon_0 m^2 c^2} \left\langle \underline{\sigma} \cdot \underline{p} \frac{1}{r} \underline{\sigma} \cdot \underline{p} \right\rangle$$

$$= - \left\langle \frac{k}{r} \right\rangle + \frac{e^2 \hbar^2}{16\pi\epsilon_0 m^2 c^2 r_{B0}^3} \left(\frac{j(j+1) - \ell(\ell+1) - s(s+1)}{n^3 \ell(\ell+1/2)(\ell+1)} \right)$$

$$-(30)$$

where:

$$r_{B0} = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \quad -(31)$$

so x can be expressed in terms of n, j, ℓ and s using:

6)

$$\left(1-x^2\right)\left\langle\frac{k}{r}\right\rangle = \left(x^2-1\right)\frac{me^4}{16\pi^2\epsilon_0^2\hbar^2n^2} \quad -(32)$$

So:

$$\left(x^2-1\right)\left[\frac{me^4}{16\pi^2\epsilon_0^2\hbar^2n^2} + l(l+1)\frac{\hbar^2}{2m}\left\langle\frac{1}{r^2}\right\rangle\right]$$

$$= \frac{e^2\hbar^2}{16\pi\epsilon_0 m^2c^2r_{B0}^3}\left(\frac{j(j+1)-l(l+1)-s(s+1)}{n^3 l(l+1/2)(l+1)}\right) \quad -(33)$$

Eckardt Quantization

In this case x is postulated to be integral so a different approach is needed, starting with the ellipse:

$$r = \frac{\alpha}{1+\epsilon\cos(n\beta)}, \quad -(34)$$

which is the Eckardt ellipse, with β replaced by $n\beta$, and $\dot{\beta}$ by $n\dot{\beta}$, so the angular momentum is changed from L to nL. This is Bohr quantization:

$$L = n\hbar \quad -(35)$$

if n is the principal quantum number.