277(1): Analogy between 3D Orbit Theory and Orbital Theory.

The classical hamiltonian of the orbit theory is:

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

where:

$$U(r) = -\frac{k}{r} \quad -(2)$$

and

$$k = mMG. \quad -(3)$$

Here:

$$\dot{\beta}^2 = \dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta \quad -(4)$$

and the spherical polar coordinate system is defined by:

$$X = r \sin\theta \cos\phi \quad -(5)$$

$$Y = r \sin\theta \sin\phi \quad -(6)$$

$$Z = r \cos\theta. \quad -(7)$$

The starting point of the quantum theory of orbitals is eqn. (1) with:

$$k = \frac{e^2}{4\pi\epsilon_0} \quad -(8)$$

The kinetic energy in eq. (1) is the same for both orbit and the classical limit of the orbital theory:

$$T = \frac{p^2}{2m} = \frac{1}{2} m v^2 \quad -(9)$$

) where:

$$v^2 = \dot{r}^2 + r^2 \dot{\beta}^2 \quad -(10)$$

Quantization takes place through:

$$\underline{p}\, \phi = -i\hbar \underline{\nabla} \phi \quad -(11)$$

in three dimensions. Therefore:

$$-\frac{\hbar^2}{2m} \nabla^2 \phi = \frac{p^2}{2m} \phi = \frac{1}{2} m \left(\dot{r}^2 + r^2 \dot{\beta}^2 \right) \phi \quad -(12)$$

The laplacian in spherical polar coordinates is:

$$\nabla^2 \phi = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \phi}{\partial r} \right) + \frac{\Lambda^2 \phi}{r^2} \quad -(13)$$

where the Legendrian is:

$$\Lambda^2 = \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \phi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial \phi^2} . \quad -(14)$$

Here:

$$\Lambda^2 Y = -\ell(\ell+1) Y \quad -(15)$$

where Y are the spherical harmonics and where ℓ is an integer.

For a particle constrained on a sphere:

$$\dot{r} = 0 \quad -(16)$$

3) and the moment of inertia is:

$$I = mr^2 \quad -(17)$$

It follows that:

$$E\phi = -\frac{\hbar^2}{2I}\Lambda^2\phi$$
$$= \frac{\hbar^2}{2I}\ell(\ell+1)\phi \quad -(18)$$

if

$$\phi = Y \quad -(19)$$

Therefore the eigenvalues of the rotational kinetic energy are:

$$E = \frac{\hbar^2}{2I}\ell(\ell+1) \quad -(20)$$

The Schroedinger equation is:

$$\Lambda^2\phi = -\left(\frac{2IE}{\hbar^2}\right)\phi = -\ell(\ell+1)\phi \quad -(21)$$

Therefore

$$\boxed{\dot{\beta}^2 = \ell(\ell+1)\frac{\hbar^2}{I^2}} \quad -(22)$$

The particle constrained on a sphere is

4) also a spherical orbital, which is quantized in the same way.

The expectation value of the energy is:

$$\langle E \rangle = \int \psi^* E \psi \, d\tau = \frac{1}{2} m r^2 \dot{\beta}^2 \quad -(23)$$

where

$$E = \frac{\hbar^2}{2I} l(l+1) \quad -(24)$$

The expectation value of $\dot{\beta}^2$ is:

$$\langle \dot{\beta}^2 \rangle = \frac{2E}{I} = \int \psi^* \dot{\beta}^2 \psi \, d\tau \quad -(25)$$

where

$$\dot{\beta}^2 = \frac{\hbar^2}{I^2} l(l+1) \quad -(26)$$

Classically: $$\langle \dot{\beta} \rangle = \frac{L}{mr^2} = \frac{L}{I} \quad -(27)$$

so $$\langle L \rangle = I \langle \dot{\beta} \rangle = I\omega \quad -(27)$$

and $$L = \hbar \left(l(l+1) \right)^{1/2} \quad -(28)$$

$$\dot{\beta} = \frac{\hbar}{I} \left(l(l+1) \right)^{1/2} \quad -(29)$$

5)

Therefore for a particle on a sphere or a spherical orbit the quantized β is:

$$\boxed{\beta = \frac{\hbar}{I}\left(l(l+1)\right)^{1/2} t} \quad -(30)$$

and its classical value is:

$$\boxed{\langle\beta\rangle = \frac{L}{I} t} \quad -(31)$$

Now the classical $\langle\beta\rangle$ can be related to ϕ and θ as in previous work.

This analysis must now be repeated for the Schroedinger equation.