

275(6): Summary of the General Theory of 3D Orbitals

Consider the Hamiltonian:

$$H = \frac{1}{2}mv^2 + U(r) \quad - (1)$$

and the Lagrangian:

$$L = \frac{1}{2}mv^2 - U(r) \quad - (2)$$

where U is any function of r . The solution of eq. (1) is:

$$\frac{1}{r} = f(\beta) \quad - (3)$$

where f is any function of β .

The force law equivalent to Eq. (1) is:

$$F(r) = -\frac{L^2}{mr^3} \left(\frac{d^2}{d\beta^2} \left(\frac{1}{r} \right) + \frac{1}{r} \right) \quad - (4)$$

where:

$$m\ddot{r} = -\frac{L^2}{mr^3} \frac{d^2}{d\beta^2} \left(\frac{1}{r} \right) \quad - (5)$$

The transition from 2D to 3D orbital theory takes place through a transition in kinetic energy:

$$T = \frac{1}{2}mv^2, \quad - (6)$$

The potential energy $U(r)$ is the same in 2D and 3D.

In 2D:

$$v^2 = \dot{r}^2 + \dot{\phi}^2 r^2 \quad - (7)$$

and in 3D:

$$2) \quad v^2 = \dot{r}^2 + \dot{\beta}^2 r^2 - (8)$$

where:

$$\dot{\beta}^2 = \dot{\theta}^2 + \sin^2 \theta \dot{\phi}^2 - (9)$$

Eqs. (7) to (9) lead to:

$$\tan \phi = \frac{L_z}{L} \tan \beta - (10)$$

and

$$\cos \theta = \left(1 - \left(\frac{L_z}{L} \right)^2 \right)^{1/2} \sin \beta - (11)$$

i.e.:

$$\cos \beta = \frac{\cos \phi}{\left(\cos^2 \phi + \left(\frac{L}{L_z} \right)^2 \sin^2 \phi \right)^{1/2}} - (12)$$

$$\cos \beta = \left(1 - \left(\frac{1}{1 - \left(\frac{L_z}{L} \right)^2} \cos^2 \theta \right)^{1/2} \right) - (13)$$

Conclusion

In general, a three dimensional orbit is given by Eq. (3) with β defined by eq. (12). Therefore r may be expressed in terms of ϕ , in terms of θ , or a combination of ϕ and θ by adding eqs. (12) and (13):

3)

$$\cos \beta = \frac{1}{2} \left[\frac{\cos \phi}{\left(\cos^2 \phi + \left(\frac{L}{L_z} \right)^2 \sin^2 \phi \right)^{1/2}} + \left(1 - \left(\frac{1}{1 - \left(\frac{L_z}{L} \right)^2} \right) \cos^2 \theta \right)^{1/2} \right]$$

Eq. (14) gives an orbit $r(\theta, \phi)$ for any β and any force law or potential $u(r)$.

Example

$$u(r) = -\frac{L^2}{2m} (1+d^2) \frac{1}{r^2} \quad (15)$$

This gives:

$$F(r) = -\frac{L^2}{mr^3} (1+d^2) \quad (16)$$

and the logarithmic spiral orbit:

$$r = r_0 \exp(d\beta) \quad (17)$$

using eq. (4)
Using

$$\frac{d\beta}{dt} = \frac{L}{mr^2} \quad (18)$$

4) it is found that:

$$\beta(t) = \frac{1}{2d} \log_e \left(\frac{2dLt}{mr_0^2} \right) - (19)$$

and
$$r(t) = \left(\frac{2dLt}{m} \right)^{1/2} - (20)$$

Therefore from eqs. (10) and (11):

$$\phi(t) = \tan^{-1} \left(\frac{L_z}{L} \tan \beta(t) \right) - (21)$$

and
$$\theta(t) = \cos^{-1} \left(\left(1 - \left(\frac{L_z}{L} \right)^2 \right)^{1/2} \sin \beta(t) \right) - (22).$$
