269(1): Synthesis of Three Dimensional Dynamics with a Combination of Two Ellipses.

The force equation in three dimensions is:

$$F = -\frac{k}{r^2} = F_1 + F_2 \quad -(1)$$

where

$$F_1 = m\ddot{r} - \frac{L_1^2}{mr^3} \quad -(2)$$

and

$$F_2 = -\frac{L_2^2}{mr^3 \sin^2\theta} \quad -(3)$$

The force F_1 is generated from the Binet equation:

$$F_1 = -\frac{L_1^2}{mr^2}\left(\frac{d^2}{d\theta^2}\left(\frac{1}{r_1}\right) + \frac{1}{r_1}\right) \quad -(4)$$

and the force F_2 is generated from the Binet equation:

$$F_2 = -\frac{L_2^2}{\sin^2\theta}\left(\frac{d^2}{d\theta^2}\left(\frac{1}{r_2}\right) + \frac{1}{r_2}\right) \quad -(5)$$

Here:

$$\frac{1}{r_1} = \frac{1}{\alpha_1}\left(1 + \epsilon_1 \cos\theta\right) \quad -(6)$$

$$\frac{1}{r_2} = \frac{1}{\alpha_2}\left(1 + \epsilon_2 \cos\phi\right) \quad -(7)$$

From eq. (4) and (6):

$$F_1 = m\ddot{r} - \frac{L_1^2}{mr^3} = -\frac{L_1^2}{mr^2}\left(\frac{d^2}{d\theta^2}\left(\frac{1}{r_1}\right) + \frac{1}{r_1}\right) \quad -(8)$$

2) Now use:

$$\frac{d^2}{d\theta^2}\left(\frac{\epsilon_1}{\alpha_1}\cos\theta\right) = \frac{1}{\alpha_1} - \frac{1}{r} \quad -(9)$$

so

$$F_1 = -\frac{L_1^2}{\alpha_1 m r^2} = m\ddot{r} - \frac{L_1^2}{mr^3} \quad -(10)$$

and we obtain the Leibniz equation:

$$m\ddot{r} = -\frac{L_1^2}{\alpha_1 m r^2} + \frac{L_1^2}{mr^3} \quad -(11)$$

where we have used:

$$\frac{1}{r} = \frac{1}{\alpha_1}\left(1+\epsilon_1\cos\theta\right) = \frac{1}{\alpha_2}\left(1+\epsilon_2\cos\phi\right). \quad -(12)$$

$$= \frac{1}{r_1} = \frac{1}{r_2}$$

The second ellipse (7) gives

$$F_2 = -\frac{L_2^2}{mr^3\sin^2\theta} \quad -(13)$$

using

$$\frac{d}{d\theta}\cos\phi = 0 \quad -(14)$$

Therefore it has seen shown that any three dimensional force can be analyzed as two Binet equations for any type of planar orbit.

3) The analysis can be developed in terms of the conserved Binet equation:

$$F = -\frac{L^2}{mr^2}\left(\frac{d^2}{d\theta^2}\left(\frac{1}{r}\right) + \frac{1}{r}\right) \quad -(15)$$

where:

$$L^2 = L_1^2 + \frac{L_2^2}{\sin^2\theta} \quad -(16)$$

and

$$\frac{1}{r} = \frac{1}{\alpha_1}\left(1+\epsilon_1\cos\theta\right) = \frac{1}{\alpha_2}\left(1+\epsilon_2\cos\phi\right) \quad -(17)$$

This gives:

$$m\ddot{r} = -\frac{L^2}{mr^2}\frac{d^2}{d\theta^2}\left(\frac{1}{r}\right) \quad -(18)$$

$$= \frac{L^2}{mr^2}\left(\frac{1}{r} - \frac{1}{\alpha_1}\right)$$

<u>Expectation Values</u>

1)

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{\alpha_1}\left(1+\epsilon_1\langle\cos\theta\rangle\right) \quad -(19)$$

$$= \frac{1}{\alpha_2}\left(1+\epsilon_2\langle\cos\phi\rangle\right)$$

For the hydrogenic orbitals:

$$\langle\cos\theta\rangle = \langle\cos\phi\rangle = 0 \quad -(20)$$

so:

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{\alpha_1} = \frac{1}{\alpha_2} \quad -(21)$$

4)
$$F = \frac{L^2}{mr^2}\left(\frac{1}{r} - \frac{1}{d_1} - \frac{1}{r}\right) \quad -(22)$$

from Eqs. (15) and (18), so:

$$F = -\frac{L^2}{mr^2 d_1} = -\frac{k}{r^2} \quad -(23)$$

where

$$k = \frac{e^2}{4\pi\epsilon_0} \quad -(24)$$

So

$$\frac{L^2}{md_1} = k \quad -(25)$$

and

$$d_1 = \frac{L^2}{mk} \quad -(26)$$

$$= \frac{1}{mk}\left(L_1^2 + \frac{L_2^2}{\sin^2\theta}\right)$$

The relevant force law is therefore:

$$m\ddot{r} = -\frac{k}{r^2} + \frac{L^2}{mr^3} \quad -(27)$$

corresponding to the effective potential energy:

$$V_{eff}(r) = -\frac{k}{r} + \frac{L^2}{2mr^2} \quad -(28)$$

In the hydrogen atom:

5)

$$L^2 \phi = \ell(\ell+1)\hbar^2 \phi \quad -(29)$$

so

$$V_{eff}(r) = -\frac{k}{r} + \frac{\ell(\ell+1)\hbar^2}{2mr^2} \quad -(30)$$

Defining the hydrogenic wave function as:

$$\phi = R_{n\ell}(r)\, Y_{\ell m}(\theta, \phi) \quad -(31)$$

and defining:

$$P = rR \quad -(32)$$

then:

$$-\frac{\hbar^2}{2m} \nabla^2 P + V_{eff} P = E P \quad -(33)$$

The complete Schroedinger equation is:

$$-\frac{\hbar^2}{2m} \nabla^2 \phi - \frac{k}{r}\phi = E\phi \quad -(34)$$

and the spherical harmonics are defined by:

$$\Lambda^2 Y = -\ell(\ell+1) Y \quad -(35)$$

where

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) \quad -(36)$$

The complete Laplacian is:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Lambda^2 \quad -(37)$$

6)

The effective potential (30) is made up of the Coulomb potential and the energy:

$$E_r = \frac{l(l+1)\hbar^2}{2mr^2} \quad -(38)$$

and in classical dynamics this is the <u>centrifugal energy</u>:

$$E_r\,(\text{classical}) = \frac{L^2}{2mr^2} \quad -(39)$$

so

$$L^2 \phi = l(l+1)\hbar^2 \phi \quad -(40)$$

$$\langle L^2 \rangle = l(l+1)\hbar^2 \quad -(41)$$

It follows from eqs. (16) and (41) that:

$$\langle L^2 \rangle = \langle L_1^2 \rangle + \left\langle \frac{L_2^2}{\sin^2\theta} \right\rangle = l(l+1)\hbar^2 \quad -(42)$$

The $\hat{L}^2$ operator is defined by:

$$\hat{L}^2 = -\hbar^2 \Lambda^2 \quad -(43)$$

$$= -\hbar^2 \left(\underbrace{\frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right)} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \right)$$

$$= \hat{L}_1^2 + \frac{\hat{L}_2^2}{\sin^2\theta}$$

7) So:

$$\hat{L}_1^2 = -\frac{\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) \quad -(44)$$

$$\hat{L}_2^2 = -\hbar^2\frac{\partial^2}{\partial\phi^2} \quad -(45)$$

It follows that:

$$\langle L_1^2\rangle = \int \psi^* \hat{L}_1^2 \psi \, d\tau \quad -(46)$$

$$= -\hbar^2 \int \psi^* \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) d\tau$$

and

$$\langle L_2^2\rangle = \int \psi^* \hat{L}_2^2 \psi \, d\tau \quad -(47)$$

$$= -\hbar^2 \int \psi^* \frac{\partial^2\psi}{\partial\phi^2} \, d\tau$$

and

$$\langle L^2\rangle = \langle L_1^2\rangle + \langle L_2^2\rangle \quad -(48)$$

$$= l(l+1)\hbar^2$$

This can be checked by computer algebra for the H wave functions

) Conclusions

Three dimensional classical dynamics can be represented by the force law (15), where the total angular momentum is defined by eq. (16). In general:

$$\boxed{\frac{1}{r} = \frac{1}{d_1}\left(1+\epsilon_1\cos\theta\right) = \frac{1}{d_2}\left(1+\epsilon_2\cos\phi\right)} \quad -(49)$$

where

$$d_1 = \frac{L^2}{mk} \quad -(50)$$

and

$$L^2 = L_1^2 + \frac{L_2^2}{\sin^2\theta} \quad -(51)$$

The elliptical equation (49) leads to the Leibniz equation:

$$m\ddot{r} = -\frac{k}{r^2} + \frac{L^2}{mr^3} \quad -(52)$$

and effective potential:

$$V_{eff}(r) = -\frac{k}{r} + \frac{L^2}{2mr^2} \quad -(53)$$

This quantizes with:

$$L^2\phi = \ell(\ell+1)\hbar^2\phi \quad -(54)$$

with $\langle L_1^2\rangle$ and $\langle L_2^2\rangle$ defined by eqs. (46) and (47)