266(5): Hamiltonian for Precessing Orbits and Atomic and Molecular Orbitals

The Hamiltonian derived in Note 266(4) is:

$$H = \frac{1}{2}mv^2 - x^2\frac{mMG}{r} + (x^2-1)\frac{L^2}{2mr^2} \quad -(1)$$

where

$$v^2 = \left(\frac{dr}{dt}\right)^2 + r^2\left(\frac{d\theta}{dt}\right)^2, \quad -(2)$$

$$= \left(\frac{dr}{dt}\right)^2 + \frac{L^2}{m^2r^2}.$$

So:

$$H = \frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + \frac{L^2}{2mr^2} - x^2\frac{mMG}{r} + (x^2-1)\frac{L^2}{2mr^2}.$$

$$\boxed{\begin{aligned} H &= \frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + x^2\left(-\frac{mMG}{r} + \frac{L^2}{2mr^2}\right) \\ &= T + U \end{aligned}} \quad -(3)$$

The Lagrangian is:

$$\mathcal{L} = T - U \quad -(4)$$

For planetary precession:

$$x = 1 + \frac{3MG}{c^2 d} \quad -(5)$$

The kinetic energy is:

2)

$$T = \frac{1}{2} m \left(\frac{dr}{dt}\right)^2 \quad -(6)$$

and the potential energy is:

$$U = x^2 \left(-\frac{mMG}{r} + \frac{L^2}{2mr^2}\right) \quad -(7)$$

This x theory gives all orbital precession to state of the art experimental precision.

Atoms and Molecules

The same Hamiltonian and Lagrangian give the Bohr Sommerfeld and Bohr quantization with the replacements:

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

and

$$x \rightarrow n \quad -(9)$$

where n is the principal quantum number.

So:

$$\boxed{H = \frac{1}{2} m \left(\frac{dr}{dt}\right)^2 + n^2 \left(-\frac{e^2}{4\pi\epsilon_0 r} + \frac{L^2}{2mr^2}\right) \quad -(10)}$$

The angular momentum is:

$$L = \hbar l \quad -(11)$$

3) where l is the angular momentum quantum number defined by:

$$\Delta^2 Y = -l(l+1)\underline{Y} \quad -(12)$$

in three dimensions, where Δ^2 is the legendrian and Y are the spherical harmonics. This procedure introduces the quantum numbers l and m.

The hamiltonian (3) corresponds to:

$$r = \frac{\alpha}{1+\epsilon\cos(x\theta)} \quad -(13)$$

where

$$\alpha = \frac{L^2}{m^2 \underline{M} G} \quad -(14)$$

and

$$\epsilon = \left(1 - \frac{2EL^2}{m^3 \underline{M}^2 G^2}\right), \quad -(15)$$

$$x = 1 + \frac{3MG}{c^2 \alpha}. \quad -(16)$$

Using the replacement rules (8) and (9) the hamiltonian (10) is:

$$r = \frac{\alpha}{1+\epsilon\cos(n\theta)} \quad -(17)$$

with:

$$n = 1 + \frac{3\hbar}{mc}\left(\frac{\alpha_f}{\alpha}\right) \quad -(18)$$

 where the fine structure constant is:

$$\alpha_f = \frac{e^2}{4\pi\hbar c \epsilon_0} = 0.007297351 \quad -(19)$$

and where the de Broglie / Compton wavelength is:

$$\lambda_c = \frac{h}{mc} = 2.426309 \times 10^{-12}\,m \quad -(20)$$

The half right latitude is changed as follows:

$$\alpha = \frac{L^2}{m^2 M G} \rightarrow \frac{4\pi\epsilon_0 L^2}{e^2 m}$$

$$= \frac{L^2}{\hbar c \alpha_f m} \quad -(21).$$

and for an ellipse the eccentricity becomes:

$$\epsilon = \left(1 - \frac{2E}{mc^2}\left(\frac{L}{\hbar\alpha_f}\right)^2\right)^{1/2} \quad -(22)$$

For a hyperbola:

$$\epsilon = \left(1 + \frac{2E}{mc^2}\left(\frac{L}{\hbar\alpha_f}\right)^2\right)^{1/2} \quad -(23)$$

Quantization is defined by:

5)

$$\oint L \, d\theta = 2\pi L = h l \quad -(24)$$

and

$$m \oint \frac{dr}{dt} dr = L \oint \left(\frac{1}{r} \frac{dr}{d\theta} \right)^2 d\theta = n h \quad -(25)$$

Therefore in this theory:

$$L = \hbar l \quad -(26)$$

Note carefully that L is a function and not an operator, because wavefunctions do not appear in this theory.

The eccentricity is therefore, for an ellipse:

$$\epsilon = \left(1 - \frac{2E}{mc^2} \left(\frac{l}{\alpha_f} \right)^2 \right)^{1/2} \quad -(27)$$

and for a hyperbola:

$$\epsilon = \left(1 + \frac{2E}{mc^2} \left(\frac{l}{\alpha_f} \right)^2 \right)^{1/2} \quad -(28)$$

where

$$l = 0, 1, 2, 3, \ldots \quad -(29)$$

is the angular momentum quantum number.

The usual quantization of L^2 as an operator is:

6) Fm Eqs. (18) and (21)

$$n = 1 + 3\alpha_f^2 \left(\frac{\hbar^2}{L^2} \right) \quad -(30)$$

So:

$$\boxed{L^2 = \left(\frac{3\alpha_f^2}{n-1} \right) \hbar^2} \quad -(31)$$

Summary

The Hamiltonian (10) corresponds to:

$$r = \frac{\alpha}{1 + \epsilon \cos(n\theta)} \quad -(32)$$

where:

$$\alpha = \frac{L^2}{\hbar c m \alpha_f} = \frac{3\alpha_f \hbar}{(n-1) m c} \quad -(33)$$

$$\epsilon = \left(1 \mp \frac{2E}{mc^2} \left(\frac{\ell}{\alpha_f} \right)^2 \right)^{1/2} \quad -(34)$$

$$n = 1 + 3 \frac{\hbar}{mc} \left(\frac{\alpha_f}{\alpha} \right) \quad -(35)$$

where

$$n = 0, 1, 2, \ldots \quad -(36)$$

$$\ell = 0, 1, 2, \ldots$$