71(7): New Radial Wavefunctions of Atoms and Molecules

From the Lagrangian:

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

it is found that:

$$r = \frac{\alpha}{1+\epsilon\cos\beta} \quad -(2)$$

and

$$\dot{\beta} = \frac{L}{mr^2} \quad -(3)$$

where L is a constant of motion. By definition:

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

and

$$U = \frac{-e^2}{4\pi\epsilon_0 r} \quad -(5)$$

for the H atom. The classical orbit of the electron around the proton is given by eq. (2). The classical velocity is

$$v^2 = \left(\frac{dr}{dt}\right)^2 + r^2\left(\frac{d\beta}{dt}\right)^2. \quad -(6)$$

Use

$$\frac{dr}{dt} = \frac{dr}{d\beta}\frac{d\beta}{dt} \; ; \; \frac{d\beta}{dt} = \frac{L}{mr^2} \quad -(7)$$

to find that:

$$v^2 = \frac{L^2}{\alpha}\left(\frac{2}{r} - \frac{1}{a}\right) \quad -(8)$$

where

$$a = \frac{\alpha}{1-\epsilon^2} \quad -(9)$$

2) is the semimajor axis of the ellipse (2).

Quantization occurs via:

$$-\hbar^2 \nabla^2 \psi = p^2 \psi \quad -(10)$$

where

$$\nabla^2 \psi = \frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r}\frac{\partial \psi}{\partial r} \quad -(11)$$

So:

$$\boxed{\frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r}\frac{\partial \psi}{\partial r} = -\frac{L^2}{\hbar^2 \alpha}\left(\frac{2}{r} - \frac{1}{a}\right)\psi} \quad -(12)$$

Solving this with Maxima gives new radial wavefunctions of the H atom, and also the radial wavefunctions of the Newtonian orbit.