277(2): Application of 3D Orbit Theory to New Characterizations of the H Atom

From 3D orbit theory it is known that the Hamiltonian:

$$H = \frac{p^2}{2m} - \frac{k}{r} \quad -(1)$$

produces the beta ellipse:

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

where

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

and where the kinetic energy is:

$$T = \frac{p^2}{2m} = \frac{1}{2}mv^2 \quad -(4)$$

The velocity is:

$$v^2 = \dot{r}^2 + r^2\dot{\beta}^2 \quad -(5)$$

where

$$\dot{\beta}^2 = \dot{\theta}^2 + \sin^2\theta\,\dot{\phi}^2 \quad -(6)$$

On quantization the hamiltonian (1) becomes:

$$\hat{H}\psi = E\psi \quad -(7)$$

where:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{k}{r} \quad -(8)$$

2)

The energy levels are given as in note 268(1):

$$\langle E \rangle = \langle E_1 \rangle + \langle E_2 \rangle \quad -(9)$$

where:

$$\langle E_1 \rangle = -\frac{\hbar^2}{2m} \int \psi^* \nabla^2 \psi \, d\tau \quad -(10)$$

and

$$\langle E_2 \rangle = -\int \psi^* \frac{k}{r} \psi \, d\tau \quad -(11)$$

For the orbitals of the H atom:

$$\langle E_1 \rangle = \frac{\hbar^2}{2 m r_B^2 n^2} \quad -(12)$$

and

$$\langle E_2 \rangle = -\frac{e^2}{4\pi \epsilon_0 r_B} \quad -(13)$$

where the Bohr radius is:

$$r_B = \frac{4\pi \epsilon_0 \hbar^2}{m e^2} \quad -(14)$$

So:

$$\langle E \rangle = \frac{m e^4}{32 \pi^2 \epsilon_0^2 \hbar^2 n^2} - \frac{m e^4}{16 \pi^2 \epsilon_0^2 \hbar^2 n^2} \quad -(15)$$

where n is the principal quantum number.

3)

The theory of the H atom is transformed into the theory of quantized three dimensional orbits by:

$$\boxed{r_B = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \rightarrow \frac{\hbar^2}{m^2 MG}} \quad -(16)$$

So the theory of quantized three dimensional orbits is exactly the same as the theory of quantized atoms and molecules using the replacement rule (16).

This rule is equivalent to:

$$k = \frac{e^2}{4\pi\epsilon_0} \rightarrow mMG \quad -(17)$$

and

$$r_B = \frac{\hbar^2}{mk} \quad -(18)$$

The Bohr radius for planetary systems in three dimensions is many orders of magnitude smaller than the Bohr radius in quantum chemistry. However, three dimensional orbits in general are quantized in exactly the same way as the orbitals of the H atom.

4) The energy levels of the H atom are:

$$E = -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2n^2} \quad -(19)$$

$$= -\frac{k^2 m}{2\hbar^2 n^2}$$

where

$$k = \frac{e^2}{4\pi\epsilon_0} \quad -(20)$$

So the energy levels of the quantized three dimensional orbits are:

$$\boxed{E = -\frac{k^2 m}{2\hbar^2 n^2} = -\frac{m^3 M^2 G^2}{2\hbar^2 n^2}} \quad -(21)$$

Conversely, and of much greater practical importance, the H atom is characterized by the Beta ellipse:

$$r = \frac{\alpha}{1+\epsilon\cos\beta} \quad -(22)$$

where:

$$\alpha = \frac{L^2}{m^2 M G} \quad -(23)$$

and:

5)

$$\epsilon^2 = 1 + \frac{2EL^2}{m^2 M G} \quad -(24)$$

if

$$k = mMG \quad -(25)$$

So:

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

and

$$\epsilon^2 = 1 + \frac{2EL^2}{mk^2} \quad -(27)$$

Therefore for the H atom:

$$k = \frac{e^2}{4\pi\epsilon_0} \quad -(28)$$

and

$$\alpha = \frac{4\pi\epsilon_0 L^2}{me^2} \quad -(29)$$

and

$$\epsilon^2 = 1 + \frac{2EL^2}{m}\left(\frac{4\pi\epsilon_0}{e^2}\right)^2 \quad -(30)$$

where

$$L^2 = \ell(\ell+1)\hbar^2 \quad -(31)$$

So

$$\boxed{\alpha = \ell(\ell+1)\, r_B} \quad -(32)$$

where ℓ is the angular momentum quantum number.

and
$$\boxed{\epsilon = 1 - \frac{\ell(\ell+1)}{n^2}} \quad -(33)$$

where:
$$\ell = 0, 1, 2, \ldots, n-1. \quad -(34)$$

Therefore the H atom can be characterized by the expectation value of the beta conic section, in this case the beta ellipse.

$$\boxed{\langle r \rangle = \int \psi^* \frac{\alpha}{1+\epsilon\cos\beta} \psi \, d\tau} \quad -(35)$$

or
$$\boxed{\left\langle \frac{1}{r} \right\rangle = \int \psi^* \left(\frac{1+\epsilon\cos\beta}{\alpha} \right) \psi \, d\tau} \quad -(36)$$

and the method can be extended to the whole of quantum physics and chemistry.

From eq. (36):

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{\alpha} \left(\int \psi^* \psi \, d\tau + \epsilon \int \psi^* \cos\beta \, \psi \, d\tau \right) \quad -(37)$$

So:

7)

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{\alpha} + \frac{\epsilon}{\alpha} \int \phi^* \cos\beta \, \phi \, d\tau \quad -(38)$$

where

$$\frac{1}{\alpha} = \frac{1}{\ell(\ell+1) r_B} \quad -(39)$$

and

$$\frac{\epsilon}{\alpha} = \frac{1}{\ell(\ell+1) r_B} \left(1 - \frac{\ell(\ell+1)}{n^2} \right) \quad -(40)$$

Finally express $\cos\beta$ in terms of ϕ and θ using:

$$\tan\beta = \frac{L}{L_Z} \tan\phi \quad -(41).$$

where

$$L = (\ell(\ell+1))^{1/2} \hbar \quad -(42)$$

$$L_Z = m_\ell \hbar \quad -(43)$$

where

$$m_\ell = -\ell, \dots, \ell \quad -(44)$$

so

$$\cos\beta = \frac{\cos\phi}{\left(\cos^2\phi + \left(\frac{L}{L_Z} \right)^2 \sin^2\phi \right)^{1/2}} \quad -(45)$$

$$= \left(1 + \left(\frac{1}{1 - \left(\frac{L_Z}{L} \right)^2} \right) \cos^2\theta \right)^{1/2}$$