SCHRODINGER EQUATION FOR HYDROGEN ATOM

The Shrödinger equation of H_2 atom containing one electron & one proton is given by (in spherical polar co-ordinate)

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{d\psi}{dr}\right]+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right]+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2\mu}{\hbar^2}[E-V]\psi=0 \quad \text{— (A)}$$

Where μ = reduced mass of electron & Proton, E is total energy and V = Potential energy.
The three variable r, θ & ϕ are orthogonal to each other.

Let $\psi(r,\theta,\psi)=R(r)Y(\theta)Z(\phi)$ ——— (B)

where R_r = function of r only, $Y(\theta)$ = function of θ only and $Z(\phi)$ = function of ϕ only

$$\frac{\partial\psi}{\partial r}=YZ\cdot\frac{\partial R}{\partial r},\ \frac{\partial\psi}{\partial\theta}=RZ\cdot\frac{\partial Y}{\partial\theta} \text{ and } \frac{\partial^2\psi}{\partial\phi^2}=RY\frac{\partial^2 Z}{\partial\phi^2}$$

Substituting these value in equation B.

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 YZ\cdot\frac{\partial R}{\partial r}\right]+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[RZ\frac{\partial Y}{\partial\theta}\right]+\frac{1}{r^2\sin^2\theta}RY\frac{\partial^2 Z}{\partial\phi^2}+\frac{2\mu}{\hbar^2}[E-V]RYZ=0$$

Multiplying by $r^2\sin^2\theta/RYZ$ We get

$$\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left[r^2\frac{\partial R}{\partial r}\right]+\frac{\sin\theta}{Y}\frac{\partial}{\partial\theta}\left[\sin\theta\cdot\frac{\partial Y}{\partial\theta}\right]+\frac{1}{Z}\cdot\frac{\partial^2 Z}{\partial\phi^2}+\frac{2\mu}{\hbar^2}[E-V]r^2\sin^2\theta=0$$

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$$\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left[r^2\frac{dR}{\partial r}\right]+\frac{\sin\theta}{Y}\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{\partial Y}{\partial\theta}\right)$$

$$+\frac{2\mu}{\hbar^2}[E-V]\,r^2\sin^2\theta=-\frac{1}{Z}\frac{\partial^2 Z}{\partial\phi^2} \quad \text{— (C)}$$

Let $-\frac{1}{Z}\frac{\partial^2 Z}{\partial\phi^2}=m^2$

or, $$\frac{d^2 Z}{\partial\phi^2}+m^2 Z=0 \quad \text{— (D)}$$

This is the independent equation for ϕ. Now equation (C) may be written as

$$\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left[r^2\frac{dR}{dr}\right]+\frac{\sin\theta}{Y}\frac{\partial}{\partial\theta}\left[\sin\theta\cdot\frac{\partial Y}{d\theta}\right]$$

$$+\frac{2\mu r^2\sin^2\theta}{\hbar^2}[E-V]=m^2$$

or, $$\frac{1}{R}\frac{\partial}{\partial r}\left[r^2\frac{dR}{dr}\right]+\frac{2\mu r^2}{\hbar^2}[E-V]$$

$$=\frac{m^2}{\sin^2\theta}-\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial Y}{\partial\theta}\right] \quad \text{— (E)}$$

The L.H.S is the function of r only and R.H.S is the function of θ only. They are equal to a constant $l(l-1)$ (let) where l is greater than m.

$$\frac{1}{R}\frac{d}{dr}\left[r^2\frac{dR}{dr}\right]+\frac{2\mu r^2}{\hbar^2}[E-V]=l(l+1)$$

or, $$\frac{d^2R}{dr^2}+\frac{2}{R}\frac{dR}{dr}+\frac{2\mu R}{\hbar^2}[E-V]=\frac{l(l+1)R}{r^2} \quad \text{— (F)}$$

And $\frac{m^2}{\sin^2\theta} - \frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{dY}{\partial\theta}\right] = l(l+1)$ (33)

or, $\frac{m^2}{\sin^2\theta} - \frac{1}{Y}\left[\frac{\partial^2 Y}{\partial\theta^2} + \cot\theta\frac{\partial Y}{\partial\theta}\right] = l(l+1)$ — (G)

The eqn D E & G are independent of ϕ, r & θ. The eqn (G) is K/a radial equation. It's soln is given by "associated Laguarre Polynomial function" (P_l^m). This equation may be solved when the energy of bound electron,

$$E_n = -\frac{Z^2 e^4 \mu}{2\hbar^2 n^2}$$

This is the energy eigen value for H-atom with Z = 1.

The solution of eqn (G) is given by.

$$Y(\theta) = \sqrt{\frac{(2l+1)}{2} \cdot \frac{(l-m)}{l+m}}\, P_l^m(\cos\theta)$$

where l = azimuthal quantum number. The soln of equation D is given by

$$Z(\phi) = \frac{1}{\sqrt{2\pi}} e^{2m\phi}$$

where m = magnetic quantum Number.

These $Y(\theta)$ & $Z(\phi)$ gives the spherical distribution of electron in H_2-atom. So they are called the spherical Eigen function.