Note Title 09-11-2016

Hydrogen atom

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla^2 \underbrace{-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)}_{\text{internal motion}}$$

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$\psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi)$$

$$\hat{H}\psi(r,\theta,\phi) = \hat{H}R(r)\,Y(\theta,\phi)$$

$$\hat{H}R(r)\,Y(\theta,\phi) = E\,R(r)\,Y(\theta,\phi) \leftarrow \text{use this eqn.}$$

$\nabla^2 \equiv$ Laplacian in $\hat{H}$ takes the full form

Radial Wavefunction

$$\frac{\partial^2 u}{\partial r^2} + \frac{2\mu}{\hbar^2}(E - V_{eff})u = 0 \quad \cdots \text{(1)}$$

$$V_{eff} = \frac{\hbar^2}{2\mu r^2}l(l+1) + V_{coulombic}(r)$$

$$V_{eff} = \frac{\hbar^2}{2\mu r^2}l(l+1) - \frac{Ze^2}{4\pi\varepsilon_0 r} \quad \cdots \text{(2)}$$

$r \to \infty \qquad V_{eff} \to 0$

$$\frac{\partial^2 u}{\partial r^2} + \frac{2\mu}{\hbar^2} E u = 0$$

$$\frac{\partial^2 u}{\partial r^2} = -\frac{2\mu}{\hbar^2} E u \quad \cdots \quad (3)$$

Energies of states being considered are referred to as <u>bound states</u>!

$$E < 0, \qquad -\frac{2\mu E}{\hbar^2} > 0$$

$$R \simeq \exp\left(-\frac{2\mu E}{\hbar^2} r\right)$$

<u>$r \to 0$</u>

$$\frac{\partial^2 u}{\partial r^2} - \frac{2\mu}{\hbar^2} V_{eff}\, u = 0$$

$$V_{eff} = \frac{\hbar^2}{2\mu r^2} l(l+1)$$

$$\frac{\partial^2 u}{\partial r^2} - \frac{2\mu}{\hbar^2} \cdot \frac{\hbar^2}{2\mu r^2} l(l+1)\, u = 0$$

$$\frac{\partial^2 u}{\partial r^2} - \frac{1}{r^2} l(l+1) u = 0$$

$$\frac{\partial^2 u}{\partial r^2} = \frac{l(l+1)}{r^2} u \quad \ldots \quad (4)$$

$$u = A r^{l+1} + \frac{B}{r^l} \quad \text{(general soln.)}$$

$\underline{\underline{r \to 0}}$ $\quad u = rR$, $\therefore$ if $r \to 0$, $u \to 0$

$$\Downarrow$$

$$B = 0$$

$$u = A r^{l+1}$$

$$rR = A r^{l+1}$$

$$\underline{R = A r^l}$$

$$R_{nl}(r) = N_{n,l}\, \rho^l\, L^{2l+1}_{n-l-1}(\rho) \exp(-\rho/2)$$

$\uparrow$

General form of the radial soln. of H-atom

$$\rho = \frac{2Zr}{n a_0} \qquad a_0 \Rightarrow \text{Bohr's radius}$$

$N_{nl} \Rightarrow$ normalisation constant

$L^{2l+1}_{n-l-1}(\rho)$ = associated Laguerre polynomials