Note Title 08-11-2016

Hydrogen atom

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r} \quad \ldots \text{(1)}$$

$$\hat{H} = \hat{T}_N + \hat{T}_e + V(r)$$

$$= -\frac{\hbar^2}{2m_N}\nabla_N^2 - \frac{\hbar^2}{2m_e}\nabla_e^2 + V(r) \quad \ldots \text{(2)}$$

Shifting to centre of mass

$$\hat{H} = \underbrace{-\frac{\hbar^2}{2M}\nabla^2}_{\text{translational motion}} \underbrace{- \frac{\hbar^2}{2\mu}\nabla^2 + V(r)}_{\text{Internal Motion (Relative)}} \quad \ldots \text{(3)}$$

$$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi) \quad \ldots \text{(4)}$$

$$\hat{H}\,\Psi(r,\theta,\phi) = \hat{H}\,R(r)\,Y(\theta,\phi) = E\,R(r)\,Y(\theta,\phi) \quad \ldots \text{(5)}$$

Radial Solutions

$$\frac{\partial^2 u}{\partial r^2} + \frac{2\mu}{\hbar^2}\left(E - V_{eff}\right)u = 0$$

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

$\underline{\underline{r \to \infty}}$

$$V_{eff} = 0$$

$$\frac{d^2 u}{dr^2} + \frac{2\mu E}{\hbar^2} u = 0$$

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

Bound states $\Rightarrow$ $E < 0$

$$R(r) \approx e^{-2\mu E/\hbar^2 \, r}$$

$\underline{r \to 0}$

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

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

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

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

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

$$u = A r^{l+1} + \frac{B}{r^l}$$

$u = rR$; as $r \to 0$ then $u \to 0$

$$B = 0$$

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

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

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

<u>General form of wave function</u>

$$R(r) = N_{nl}\, \rho^l\, L^{2l+1}_{n-l-1}(\rho) \exp(-\rho/2) \quad \ldots \text{(A)}$$

$$\rho = \frac{2Zr}{n a_0}$$

$L^{2l+1}_{n-l-1} \Rightarrow$ associated Laguerre polynomials