Hydrogen Atom

$$V(r) = \frac{-e^2}{4\pi\epsilon_0} \cdot \frac{1}{r}$$

$$-\frac{\hbar^2}{2m} u''(r) + \left[\frac{-e^2}{4\pi\epsilon_0} \cdot \frac{1}{r} + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2}\right] u(r) = E\, u(r)$$

Long, pay attention

Let $k = \frac{\sqrt{-2mE}}{\hbar}$ $\quad E < 0$ so $k = \frac{\sqrt{2M|E|}}{\hbar}$

$$-\frac{\hbar^2 u''}{2mE} + \left[\frac{-e^2}{E\,4\pi\epsilon_0} \cdot \frac{1}{r} + \frac{\hbar^2}{2mE} \frac{\ell(\ell+1)}{r^2}\right] u(r) = u(r)$$

$$\frac{u''}{k^2} + \left[\frac{-e^2}{4\pi\epsilon_0 E} \cdot \frac{1}{r} - \frac{\ell(\ell+1)}{(kr)^2}\right] u(r) = u(r)$$

$$\frac{u''}{k^2} = u(r)\left[1 + \frac{e^2}{4\pi\epsilon_0 E r} + \frac{\ell(\ell+1)}{(kr)^2}\right] \rightarrow E = -\frac{\hbar^2 k^2}{2M}$$

$$\frac{u''}{k^2} = u(r)\left[1 - \frac{2Me^2}{2\pi\epsilon_0 \hbar^2 k} \cdot \frac{1}{(kr)} + \frac{\ell(\ell+1)}{(kr)^2}\right] \qquad \boxed{u(r) = r\,R(r)}$$

$$\boxed{\text{Let } \rho = kr} \qquad \boxed{\rho_0 = \frac{Me^2}{2\pi\epsilon_0 \hbar^2 k}}$$

$$\frac{u''}{k} = u(r)\left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right]$$

Now $u(r) \to u(\rho)$ -

$$\frac{du}{dr} = \frac{du}{d\rho}\frac{d\rho}{dr} = k\frac{du}{d\rho} \qquad \frac{d^2u}{dr^2} = \frac{d}{dr}\left[k\frac{du}{d\rho}\right] = k\frac{d}{dr}\left[\frac{du}{d\rho}\right]$$

$$= k\frac{d}{d\rho}\frac{d\rho}{dr}\frac{du}{d\rho} = k^2\frac{d^2u}{d\rho^2}$$

So $$\frac{d^2u}{d\rho^2} = u(\rho)\left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right] \qquad \boxed{\rho = kr \quad u = rR(r)}$$

Still HARD!!

$$\boxed{\rho_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2 k}}$$

Look at asymptotes! $\rho \to \infty$

$$\frac{d^2u}{d\rho^2} = u(\rho) \qquad u'' - u = 0 \qquad (D^2-1)u = 0 \qquad (D+1)(D-1)u = 0$$

$$\to \underset{\rho\to\infty}{u} = Ae^{-\rho} + Be^{\rho} \qquad \text{But } e^{\rho} \to \infty \text{ as } \rho\to\infty$$

$$\boxed{\text{So } \underset{\rho\to\infty}{u(\rho)} = Ae^{-\rho}}$$

$$\rho \to 0 \to \frac{d^2u}{d\rho^2} = \frac{\ell(\ell+1)}{\rho^2}\, u$$

Let $\rho = \rho^a$ $\quad \frac{du}{d\rho} = a\rho^{a-1} \quad \frac{d^2u}{d\rho^2} = a(a-1)\rho^{a-2} = \frac{a(a-1)}{\rho^2}$

or $a(a-1) = \ell(\ell+1) \to a^2 - a = \ell^2 + \ell$

if $a = -\ell$ ✓ if $a = \ell+1$ ✓

$$\underset{\rho \to 0}{u(\rho)} = C\rho^{\ell+1} + D\rho^{-1} \quad \text{but } \rho^{-1} \to \infty \text{ for } \rho \to 0$$

$$\boxed{\text{So } \underset{\rho \to 0}{u(\rho)} = C\rho^{\ell+1}}$$

Now $u(\rho) = \rho^{\ell+1} e^{-\rho} V(\rho)$

↑ not known

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right] u(\rho)$$

$$\frac{du}{d\rho} = \frac{d}{d\rho}\left[\underset{A}{\rho^{l+1}}\,\underset{B}{e^{-\rho}}\,\underset{C}{v(\rho)}\right] = (l+1)\rho^{l}BC + A(-e^{-\rho})C + ABv'(\rho)$$

$$= (l+1)\rho^{l}e^{-\rho}v(\rho) - \rho^{l+1}e^{-\rho}v(\rho) + \rho^{l+1}e^{-\rho}v'(\rho)$$

$$= \rho^{l}e^{-\rho}\left[(l+1)v(\rho) - \rho v(\rho) + \rho v'(\rho)\right]$$

$$= \rho^{l}e^{-\rho}\left[(l+1-\rho)v(\rho) + \rho\frac{dv(\rho)}{d\rho}\right]$$

A

$$\frac{d^2u}{d\rho^2} = \text{Lot's of Math} = \rho^{l}e^{-\rho}\left\{\left[-2l-2+\rho+\frac{l(l+1)}{\rho}\right]v + 2(l+1-\rho)v'(\rho) + \rho v''(\rho)\right\}$$

Equate to $\left[1-\frac{\rho_0}{\rho}+\frac{l(l+1)}{\rho^2}\right]u(\rho)$

$$\downarrow$$

$$\rho v''(\rho) + 2(l+1-\rho)v'(\rho) + [\rho_0 - 2(l+1)]v(\rho) = 0$$

Let $v(\rho) = \sum_{j=0}^{\infty} c_j\rho^j = c_0\rho^0 + c_1\rho^1 + c_2\rho^2 + c_3\rho^3 + \dots$

$$V(\rho) = c_0\rho^0 + c_1\rho^1 + c_2\rho^2 + c_3\rho^3 + c_4\rho^4 + \cdots = \sum_{j=0} c_j \rho^j$$

$$V'(\rho) = c_1\rho^0 + 2c_2\rho^1 + 3c_3\rho^2 + 4c_4\rho^3 + \cdots = \sum_{j=0} (j+1)\, c_{j+1}\, \rho^j$$

$$V''(\rho) = 1\cdot 2\cdot c_2\rho^0 + 2\cdot 3\cdot c_3\rho^1 + 3\cdot 4\,\rho^2 + \cdots = \sum_{j=0} j(j+1)\, c_{j+1}\, \rho^{j-1}$$

$$\rho V''(\rho) = 1\cdot 2\cdot c_2\rho^1 + 2\cdot 3\cdot c_3\rho^2 + 3\cdot 4\,\rho^3 + \cdots = \sum_{j=0} j(j+1)\, c_{j+1}\, \rho^j$$

$$\rho V'(\rho) = c_1\rho^1 + 2c_2\rho^2 + 3\cdot c_3\rho^3 + \cdots = \sum_{j=0} j\, c_j\, \rho^j$$

So $\rho v'' + \left[2(\ell+1) - 2\rho\right] v' + \left[\rho_0 - 2(\ell+1)\right] v = 0$

$$\rightarrow \sum j(j+1)\, c_{j+1}\rho^j + 2(\ell+1)\sum (j+1)\, c_{j+1}\rho^j - 2\sum j\, c_j \rho^j$$

$$+ \left[\rho_0 - 2(\ell+1)\right] \sum c_j \rho^j = 0$$

or $$\sum \Big[\big(j(j+1) + 2(\ell+1)(j+1)\big)\, c_{j+1} + \left[\rho_0 - 2(\ell+1) - 2j\right] c_j\Big] \rho^j = 0$$

or $$\big(j(j+1) + 2(\ell+1)(j+1)\big)\, c_{j+1} = \big(2\left[j+\ell+1\right] - \rho_0\big)\, c_j$$

or $$\frac{\left[2(j+\ell+1) - \rho_0\right] c_j}{(j+1)(j+2\ell+2)} = c_{j+1}$$

For j large $\frac{2jc_j}{j(j+1)} = c_{j+1} = \frac{2c_j}{j+1}$

$c_0,\ c_1 = \frac{4c_0}{2},\ c_2 = \frac{8c_0}{2\cdot 3},\ c_3 = \frac{16c_0}{2\cdot 3\cdot 4} \ldots$

$$c_j \sim \frac{2^j c_0}{j!} \rightarrow v(\rho) = c_0 \sum \frac{2^j}{j!} \rho^j = c_0 e^{2\rho}$$

$u(\rho) = c_0 \rho^{l+1} e^{-\rho} e^{2\rho} = c_0 \rho^{l+1} e^{\rho} \rightarrow$ Not Normalizable !!

Series must terminate at j_{max} where $c_{j_{max}+1} = 0$

So $2(j_{max} + l + 1) - \rho_0 = 0$

$\uparrow n = j_{max} + l + 1$

$$\boxed{\rho_0 = 2n}$$

or $\frac{\rho_0}{2} = n \rightarrow \frac{me^2}{4\pi\epsilon_0 \hbar^2 k} = n \qquad k = \frac{\sqrt{-2mE}}{\hbar}$

$$n^2 = \left(\frac{me^2}{4\pi\epsilon_0 \hbar}\right)^2 \cdot \frac{1}{(-2mE)} \rightarrow E = \frac{-me^4}{32\pi^2\epsilon_0^2\hbar^2} \cdot \frac{1}{n^2} = \frac{E_1}{n^2}$$

$$= \frac{-13.6\,eV}{n^2} !!!$$

and $\rho_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2 k} = 2n \rightarrow k = \frac{me^2}{4\pi\epsilon_0\hbar^2 n} = \frac{1}{an}$

$a =$ bohr radius $= \frac{4\pi\epsilon_0\hbar^2}{me^2} = .529 \cdot 10^{-10}\,m$

$\rho = kr = \frac{r}{an}$!!

$\Psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\,Y_\ell^m(\theta,\phi)$

$\frac{u(\rho)}{r} = R_{n\ell}(r) = \frac{1}{r}\rho^{\ell+1}e^{-\rho}v(\rho)$

With $c_{j+1} = \frac{2(j+\ell+1-n)}{(j+1)(j+2\ell+2)}$