

$$Y_0^0 = \frac{1}{2} \sqrt{\frac{1}{\pi}}$$

$$Y_1^{-1}(\theta, \varphi) = \frac{1}{2} \sqrt{\frac{3}{2\pi}} \cdot e^{-i\varphi} \cdot \sin \theta$$

$$Y_1^0(\theta, \varphi) = \frac{1}{2} \sqrt{\frac{3}{\pi}} \cdot \cos \theta$$

$$Y_1^1(\theta, \varphi) = \frac{-1}{2} \sqrt{\frac{3}{2\pi}} \cdot e^{i\varphi} \cdot \sin \theta$$

$$Y_2^{-2}(\theta, \varphi) = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \cdot e^{-2i\varphi} \cdot \sin^2 \theta$$

$$Y_2^{-1}(\theta, \varphi) = \frac{1}{2} \sqrt{\frac{15}{2\pi}} \cdot e^{-i\varphi} \cdot \sin \theta \cdot \cos \theta$$

$$Y_2^0(\theta, \varphi) = \frac{1}{4} \sqrt{\frac{5}{\pi}} \cdot (3 \cos^2 \theta - 1)$$

$$Y_2^1(\theta, \varphi) = \frac{-1}{2} \sqrt{\frac{15}{2\pi}} \cdot e^{i\varphi} \cdot \sin \theta \cdot \cos \theta$$

$$Y_2^2(\theta, \varphi) = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \cdot e^{2i\varphi} \cdot \sin^2 \theta$$

Identify l and m in

$$\frac{3}{8} \sqrt{\frac{5}{2\pi}} \cdot e^{2i\varphi} \cdot \sin^2 \theta \cdot (7 \cos^2 \theta - 1)$$

$$\frac{-3}{32} \sqrt{\frac{1001}{\pi}} \cdot e^{5i\varphi} \cdot \sin^5 \theta \cdot \cos \theta$$

Given the θ part you can identify
 l & $|m|$

$$L^2 Y_{lm} = l(l+1) \hbar^2 Y_{lm}$$

$$L_z Y_{lm} = m \hbar Y_{lm} \quad s, p, d, \text{ etc } \quad \text{Orbitals}$$

H-atom

$$\hat{H} = \hat{T}_{nuc} + \hat{T}_{el} + V$$

$$= \hat{T}_M + \left[\hat{T}_\mu + V(r_e - r_n) \right] + Ze$$

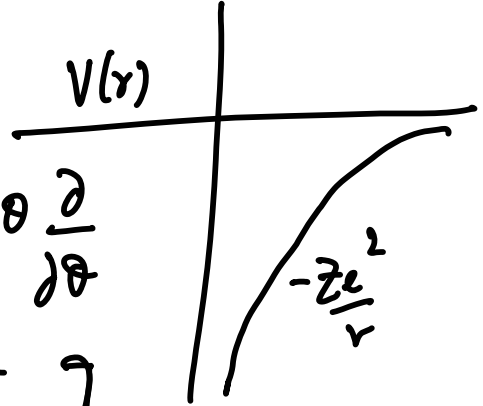
electrostatic attraction $\rightarrow e$

$$\frac{1}{\mu} = \frac{1}{m_N} + \frac{1}{m_e}$$

behaves like a free particle

$$\hat{H} = -\frac{\hbar^2}{2\mu} \nabla_{\mu}^2 - \frac{ze^2}{r} \quad \frac{1}{4\pi\epsilon_0} = 1$$

$$\nabla_{\mu}^2 = \frac{1}{r^2} \left[\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right] + \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2}$$



Schrödinger equation

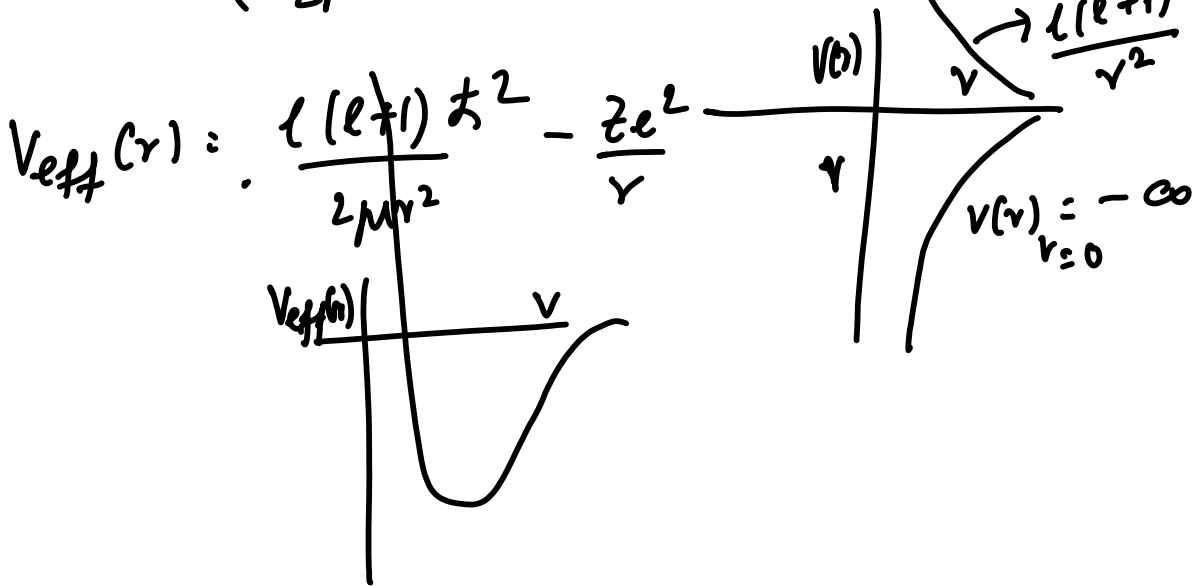
$$\hat{H}\psi = \left(-\frac{\hbar^2}{2M} \nabla_n^2 - \frac{Ze^2}{r} \right) \psi = E\psi$$

$$L^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm}$$

$$\psi = R(r) Y_{lm}(\theta, \varphi)$$

$$\hat{H}\psi = \left(-\frac{\hbar^2}{2Mr^2} \left\{ \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right\} + \frac{L^2}{2Mr^2} - \frac{Ze^2}{r} \right) \psi = E\psi$$

$\rightarrow \frac{l(l+1)\hbar^2}{r^2}$



As $r \rightarrow 0$, $V_{\text{eff}}(r) \rightarrow +\infty$

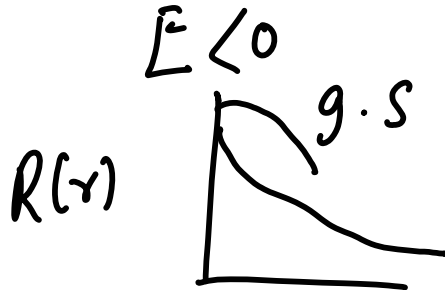
$R(r) \rightarrow 0$ as $r \rightarrow 0$

For $l=0$ (spherically symmetric state)
 $V = -\infty$ as $r \rightarrow 0$ so $R(r)$ is finite
at $r=0$

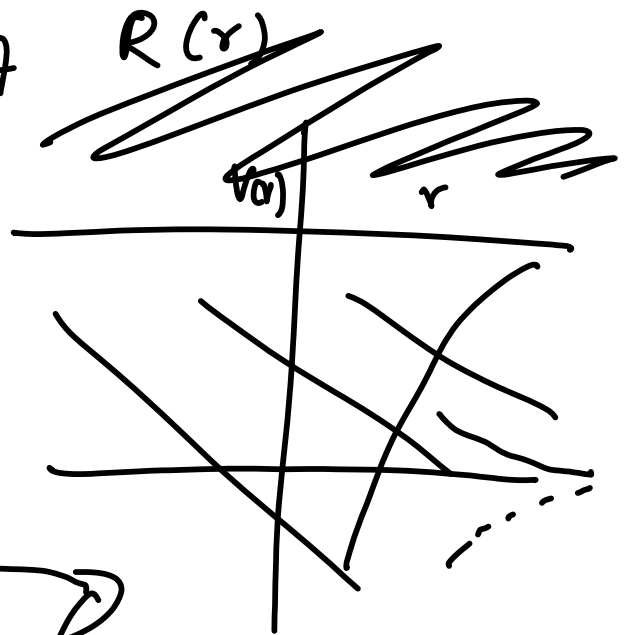
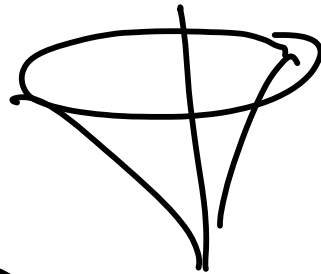
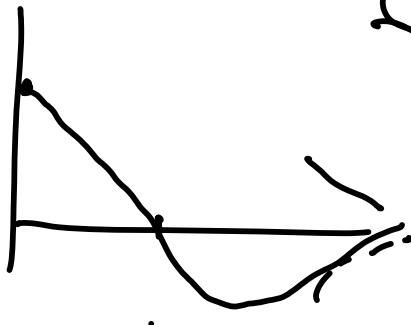
$V_{\text{eff}}^{\text{mir}}$ is a function of l

Qualitative form of $R(r)$

$$l=0$$



1st excited state



$$R(r) = \frac{g(r)}{r}$$

$$\left\{ -\frac{\hbar^2}{2\mu r^2} \left[\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right] - \frac{Ze^2}{r} \right\} R(r) = ER(r)$$

Look for the solution at large r

$$R(r) = \frac{g(r)}{r}$$

$$-\frac{\hbar^2}{2\mu} \frac{d^2 g}{dr^2} - \frac{Ze^2}{r} g(r) = E g(r)$$

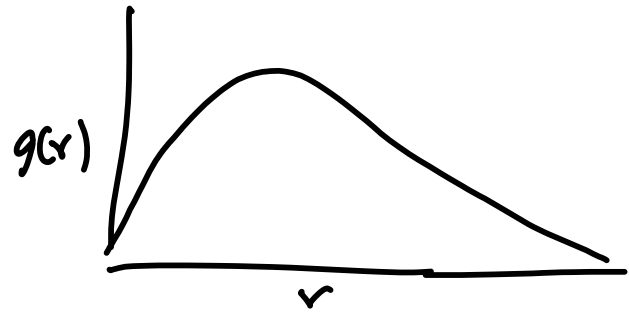
$$b^2 = -\frac{2\mu E}{\hbar^2}; \quad b = \frac{\sqrt{-2\mu E}}{\hbar}$$

$$g(r) \sim A e^{-br} + B e^{br}$$

$$g(r) = A r e^{-br} \quad E_1 = \frac{\mu Z^2 e^4}{2\hbar^2}$$

$$(ar - br^2) e^{-br}$$

$$g_1(r)$$



$$g_2(r)$$

