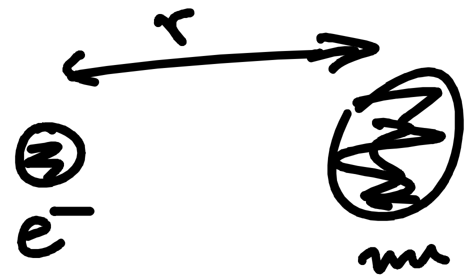
H-atom Problem.

1e⁻ 1nu

1p i.e. e⁺



$$\hat{H} = \widehat{(KE)}_{nu} + \widehat{(KE)}_{e} + V$$ potential energy

$$\boxed{H\Psi = E\Psi}$$

$$V = -\frac{e^2}{4\pi\varepsilon_0 r}$$ radial

$$\Psi(r,\theta,\phi) = R(r)\cdot Y(\theta,\phi)$$

$m_{nu} + m_e \sim m_{nu}$

CM + Internal coordinates

Reduced mass

② m_e

m_2

③

m_{nu}

m_1

$m_1 \gg m_2$

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$\mu = \frac{m_e \cdot m_{nu}}{m_{nu} + m_e} \simeq m_e$$

$$\hat{H}_{relative} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$\frac{\hbar^2}{2\mu}\nabla^2\psi(r,\theta,\phi) - \frac{e^2}{4\pi\epsilon_0 r}\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

$$\nabla^2 = \underline{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)} + \underbrace{\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}}_{\hat{L}^2}$$

$$\psi(r,\theta,\phi) = N \cdot R(r)\, Y_{l,m_l}(\theta,\phi)$$

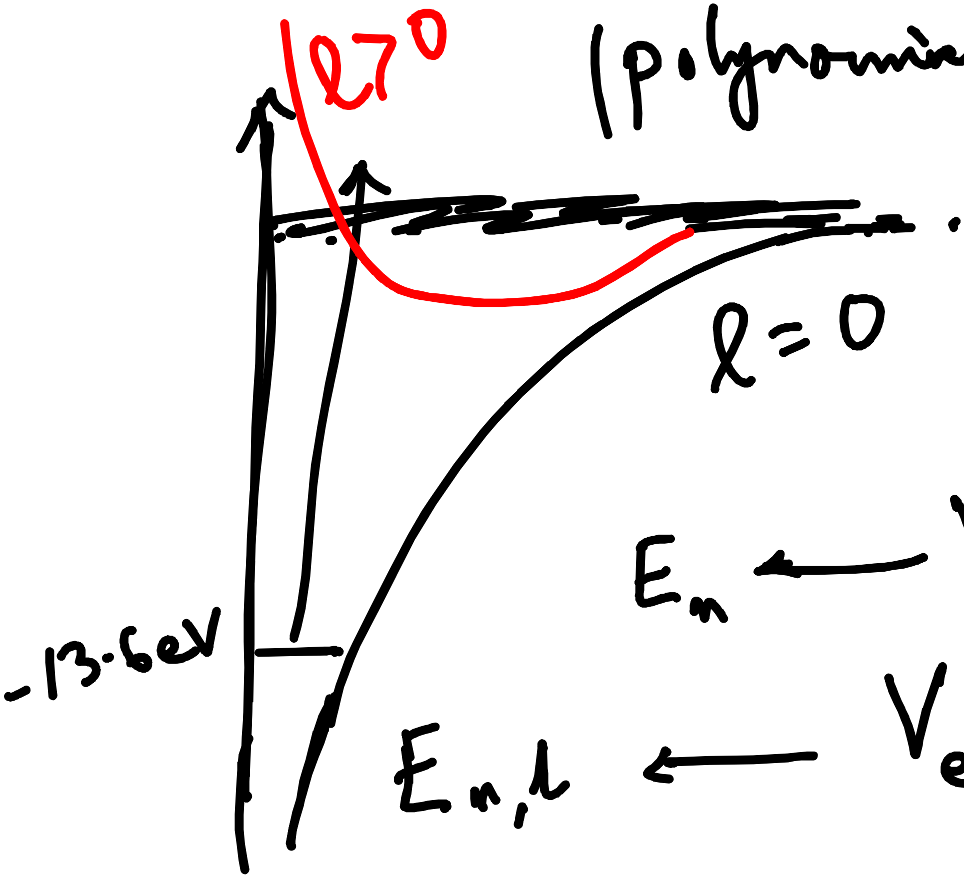
Normalization Const

$R(r)$: Quantum Number (n)

$(\text{polynomial in } r) \cdot \exp(\quad)_r$

integer

$l \to 0$



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

$$E_n \longleftarrow V = -\frac{e^2}{4\pi\varepsilon_0 r}$$

$$E_{n,l} \longleftarrow V_{\text{eff.}} = -\frac{e^2}{4\pi\varepsilon_0 r} + \frac{\hbar^2}{2\mu r^2} l(l+1)$$

H-atom case $\quad l = 0$

m_e

$$E_n = \frac{-\mu e^4}{\underbrace{32\pi\varepsilon_0^2\hbar^2}} \cdot \frac{1}{n^2} \quad , \quad n = 1, 2, \ldots$$

Rydberg const $= 109679 \text{ cm}^{-1}$

R_H $\quad hc$

$$E_n = -\frac{R_H}{n^2}$$

$$\langle r \rangle \longrightarrow \quad a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = 0.53\ \text{Å}$$

$$R_{n\ell}(r) = N_{n\ell m_\ell} \left(\frac{2r}{n a_0}\right)^{\ell} L_{n\ell}\left(e^{-r/na_0}\right)$$

$$\langle r \rangle_n \sim n^2 a_0$$

Bohr Radius

$$\left(\frac{-\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r}\right)\underbrace{\psi(r,\theta,\phi)} = E\underbrace{\psi(r,\theta,\phi)}$$

Orbital

$$\longrightarrow \underline{\psi_{n\ell m_\ell}} \longrightarrow E_n$$

Degeneracy

Orbital $\longrightarrow$ 1e$^-$ wave f^n. $\longleftarrow$ visualize

$$\int_0^R dr \int_0^\pi d\theta \int_0^{2\pi} d\phi \left(r^2 \sin\theta\right) = \frac{4}{3}\pi R^3$$

$|\psi|^2$

$$\psi_{100} \propto \exp\left(-\frac{r}{a_0}\right)$$

n, l, m_l

$l=0$

$$\psi_{200} \propto \left(2 - \frac{r}{a_0}\right)\exp\left(-\frac{r}{a_0}\right)$$

$n = 1$, $l = 0$ $\longrightarrow$ $1s-$ orbital

$n = 2$, $l = 0$ $\longrightarrow$ $2s-$ orbital

$$l = 1 \begin{cases} m_l = -1 \\ m_l = 0 \\ m_l = +1 \end{cases} \Bigg\} \ p\text{- orbital}$$

p_0 p_{-1} p_{+1}

$$E_n = -\frac{13.6}{n^2} \text{ eV}$$

$l = 0, 1, 2, \ldots (n-1)$

$m_l = 0, \pm 1, \pm 2, \cdots \pm l$

$$\sum_{l=0}^{n-1} (2l+1) = \underline{n^2}$$