$\boxed{\text{SCHRÖDINGER EQUATION}}$

$$H\Psi = E\Psi$$

$$(KE + V)\Psi = E\Psi$$

$$KE \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

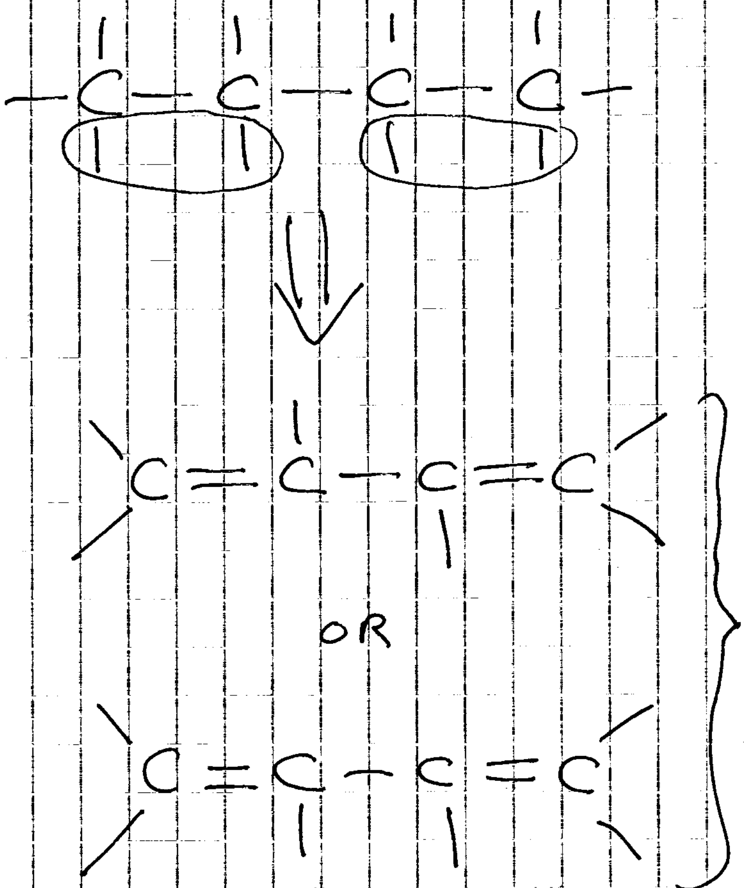
$$V \equiv \text{Potential Energy}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V(x)\Psi = E\Psi$$

$E \Rightarrow$ QUANTIZED ENERGY.

APPLIED TO THE HYDROGE ATOM, SCHRODINGER OBTAINED THE SAME ENERGY LEVELS AS IN THE BOHR ATOM.

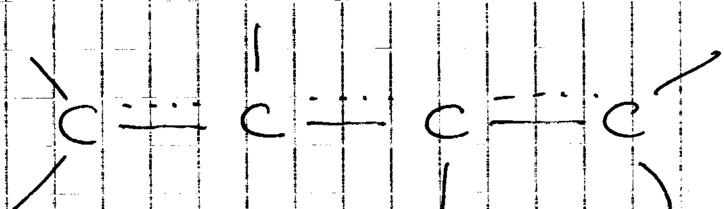
BACKGROUND



OR

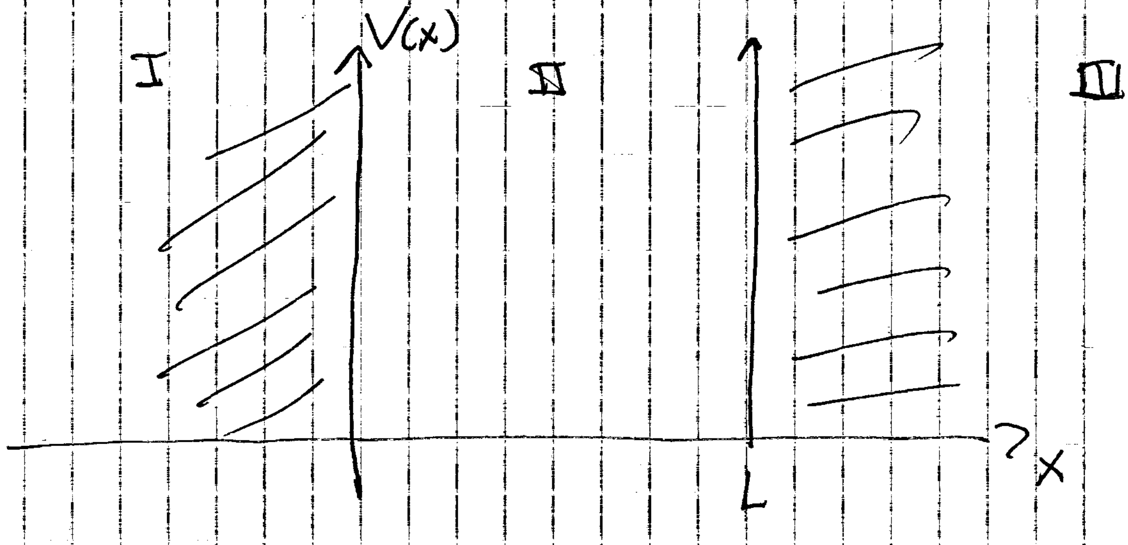
DISTANCE BETWEEN CARBONS

4 → π electrons ARE DELOCALIZED



4-πe^- TRAPPED IN A BOX

Particle in a Box



$$V(x) = \begin{cases} \infty & -\infty < x \le 0 \\ 0 & 0 < x < L \\ \infty & L \le x < \infty \end{cases}$$

Schrodinge Eq.

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V(x)\Psi = E\Psi$$

$$\Psi(x) = \begin{cases} \Psi_I(x) = 0 & -\infty < x \le 0 \\ \Psi_{II}(x) & 0 < x < L \\ \Psi_{III}(x) = 0 & L \le x < \infty \end{cases}$$

$$\Psi_{II}(x) = A\sin\left(\frac{2\pi}{L}x\right)$$

$$\Psi_{I}(0) = 0 = \Psi_{II}(0)$$

$$\Psi_{III}(0) = 0 = \Psi_{II}(L)$$

$$P(x)\,dx = |\Psi_{II}(x)|^2 dx$$

$$= |A|^2\left(\sin\left(\frac{2\pi}{L}x\right)\right)^2 dx$$

$$\boxed{\int_{-\infty}^{\infty} P(x)\,dx = 1 \Rightarrow A = \sqrt{\frac{2}{L}}}$$

ENERGY LEVELS

$$\Psi_{I}(0) = 0$$

FROM BOUNDARY CONDITIONS (BC)

a) $$\Psi_{II}(0) = \Psi_{I}(0) = 0$$

$$\sin(k0) = 0$$

b) $$\Psi_{III}(L) = \Psi_{II}(L) = 0$$

$$\sin(kL) = 0$$

$$\Rightarrow \quad kL = n\pi \qquad n = 1, 2, 3, \ldots$$

$$k = \frac{n\pi}{L}$$

$$k^2 = \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$$

$$\boxed{E_n = \frac{h^2}{8mL^2}\, n^2} \qquad n = 1, 2, 3, \ldots$$

$$\Delta E = E_{n+1} - E_n = \frac{h^2}{8mL^2}\left[(n+1)^2 - n^2\right]$$

$$\boxed{\Delta E = \frac{h^2}{8mL^2}(2n+1) = h\nu_{obs}}$$

FOR THE 3-D CASE

$$\boxed{E_n = \frac{h^2}{8m}\left[\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right]}$$

$$\boxed{\Psi_{n_x n_y n_z}(x) = A_{n_x n_y n_z} \sin\left(\frac{n_x \pi}{L_x}x\right)\sin\left(\frac{n_y}{L_y}\pi y\right)\sin\left(\frac{n_z \pi z}{L_z}\right)}$$