De Broglie wave.

$$E = \frac{1}{2}mv^2 = hf = \hbar\omega$$

$$p = mv = \frac{h}{\lambda} = \hbar k \Rightarrow k = \frac{2\pi}{\lambda}$$ wave number

$$\boxed{k^2 = \frac{2mE}{\hbar^2}}$$

Bohr model

$$E_H = -\frac{mq^4}{2(4\pi\epsilon\hbar n)^2} = -\frac{13.6}{n^2}\ eV$$

Schrodinger wave equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = j\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

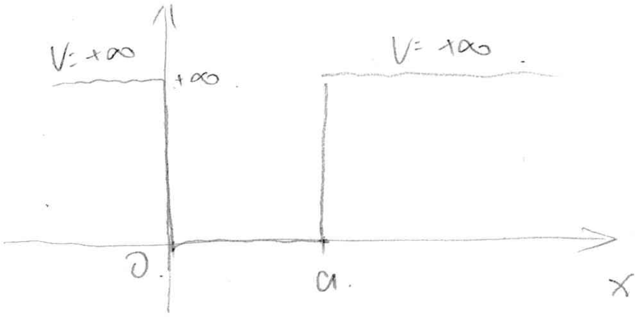
$$\xrightarrow{\text{time-independent}} \frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0.$$

Physical meaning of wave function.

$|\Psi(x,t)|^2 \rightarrow$ probability density function

$$\therefore \int_{-\infty}^{\infty} |\psi(x)|^2\,dx = 1$$

# Electrons in Infinite Quantum Well




$$V(x) = \begin{cases} 0, & 0 \le x \le a \\ +\infty, & x<0,\ x>a. \end{cases}$$

① when $x<0$ or $x>a$, no particle can be found.

$$\varphi(x) = 0.$$

② when $0 \le x \le a$.

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} + 0\cdot\varphi(x) = E\cdot\varphi(x).$$

$$\therefore \frac{d^2\varphi(x)}{dx^2} + \frac{2mE}{\hbar^2}\varphi(x) = 0 \xrightarrow{k^2=\frac{2mE}{\hbar^2}} \frac{d^2\varphi(x)}{dx^2} + k^2\cdot\varphi(x) = 0.$$

$$\Rightarrow \varphi(x) = A\cos kx + B\sin kx$$

$$\because \varphi(0)=0 \Rightarrow A=0 \Rightarrow \varphi(x) = B\sin kx.$$

$$\because \varphi(a)=0 \Rightarrow ka = n\pi \Rightarrow k=\frac{n\pi}{a}.$$

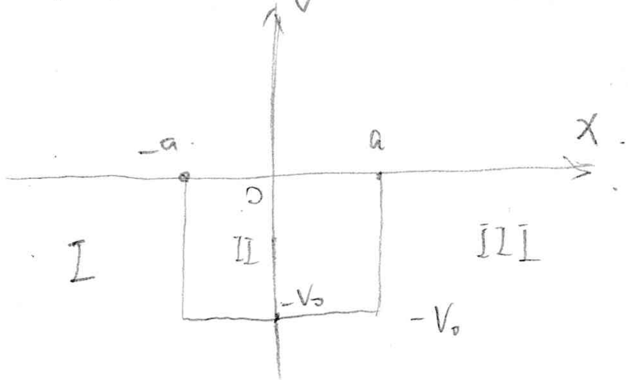
$$\because k^2 = \frac{2mE}{\hbar^2} \quad \therefore E = \frac{\hbar^2\pi^2}{2ma^2}\cdot n^2, \quad n=1,2,3\ldots$$

→ Energy is quanitized.

$$\because \int_0^a |\varphi(x)|^2 dx = 1 \Rightarrow \int_0^a B\sin\left(\frac{n\pi}{a}x\right)dx = 1 \Rightarrow B=\sqrt{\frac{2}{a}}$$

$$\therefore \varphi(x) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right), & 0 \le x \le L \\ 0, & \text{otherwise}. \end{cases}$$

Electrons in finite Quantum Well




$$V(x) = \begin{cases} -V_0, & -a \le x \le a \\ 0, & \text{otherwise} \end{cases}$$

$-V_0 < E < 0$.

In region I $(x < -a)$

$$\frac{d^2 \varphi_I(x)}{dx^2} - k_1^2 \varphi_I(x) = 0, \quad \text{where } k_1^2 = -\frac{2mE}{\hbar^2} > 0.$$

$\therefore \varphi_I(x) = A e^{k_1 x} + A' e^{-k_1 x}$

$\because$ When $x \to -\infty$, $\varphi_I(x) = 0 \Rightarrow A' = 0$

$\therefore \varphi_I(x) = A \cdot e^{k_1 x}$

In region III $(x > a)$

Similarly, we get $\varphi_{III}(x) = B \cdot e^{-k_1 x}$

In region II

$$\frac{d^2 \varphi_{II}(x)}{dx^2} + k_2^2 \varphi_{II}(x) = 0, \quad \text{where } k_2^2 = \frac{2m}{\hbar^2}(E + V_0) > 0.$$

$\therefore \varphi_{II}(x) = C_1 \cos k_2 x + C_2 \sin k_2 x$

$\because$ Potential energy is symmetric $\therefore$ wave function either even or odd

even

$$\varphi(x) = \begin{cases} A e^{k_1 x}, & x < -a \\ C_1 \cos k_2 x, & -a \le x \le a \\ A e^{-k_1 x}, & x > a \end{cases}$$

odd

$$\varphi(x) = \begin{cases} A e^{k_1 x}, & x < -a \\ C_2 \sin k_2 x, & -a \le x \le a \\ -A e^{-k_1 x}, & x > a \end{cases}$$

Considering of $\psi(x)$ and $\psi'(x)$ at $x=\pm a$.

Due to symmetry, we only consider $x=-a$

$$\therefore \begin{cases} \psi_{I}(-a) = \psi_{II}(-a) \\ \psi_{I}'(-a) = \psi_{II}'(-a) \end{cases}$$

$\therefore$

even

$$\begin{cases} A\cdot e^{-k_1 a} = C_1 \cos k_2 a \\ k_1\cdot A e^{-k_1 a} = C_1 k_2 \sin k_2 a \end{cases}$$

$$\Downarrow$$

$$k_1 = k_2 \tan k_2 a$$

odd

$$\begin{cases} A e^{-k_1 a} = -C_2 \sin k_2 a \\ k_1 A e^{-k_1 a} = C_2 k_2 \cos k_2 a \end{cases}$$

$$\Downarrow$$

$$k_1 = -k_2 \cot k_2 a$$

$\therefore$ $k_1 a = k_2 a\cdot \tan(k_2 a)$ ①   $k_1 a = -k_2 a \cot(k_2 a)$ ②

Recall that $\because k_1^2 = -\frac{2mE}{\hbar^2}$, $k_2^2 = \frac{2m}{\hbar^2}(E+V_0)$

$$\therefore (k_1 a)^2 + (k_2 a)^2 = \frac{2ma^2}{\hbar^2}\cdot V_0 \quad ③$$