Quantum Mechanics

Schrödinger equation

$$H\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

$$H = \underbrace{-\frac{\hbar^2}{2m}\nabla^2}_{\text{kinetic energy}} + \underbrace{V(\vec{r},t)}_{\text{Potential energy}}$$

$\psi(\vec{r},t)$: wave function of a particle

$|\psi^2(\vec{r},t)| = \psi(\vec{r},t)\,\psi^*(\vec{r},t)$

= Probability of finding the particle at $\vec{r}$

To see the physical meaning, consider a plane wave:

$$\psi(x,t) = e^{ikx-i\omega t}$$

k : wave vector

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,t) = \frac{\hbar^2k^2}{2m}\psi = \frac{p^2}{2m}\psi$$

Momentum $p = \hbar k$

or $\vec{P} = \hbar\vec{k} = -i\hbar\nabla$

RHS $i\hbar \frac{\partial}{\partial t} \psi(x.t) = -(i)^2 \hbar\omega \cdot \psi(x,t) = \hbar\omega\, \psi(x,t)$

$\Rightarrow$ Total energy $= \hbar\omega$

Wave function is normalized so

$$\int \psi^*(\vec{r}.t) \cdot \psi\, (\vec{r}.t) = 1$$

Measured physical quantity is the average value.

Position $\langle x \rangle = \int \psi^* x \cdot \psi\, d\vec{r}$

$$\langle \vec{r} \rangle = \int \psi^* \cdot \vec{r} \cdot \psi\, d\vec{r}$$

Momentum operator

$$\vec{p} = -i\hbar\nabla$$

$$\langle \vec{p} \rangle = \int \psi^* (-i\hbar) \nabla \psi \cdot d\vec{r}$$

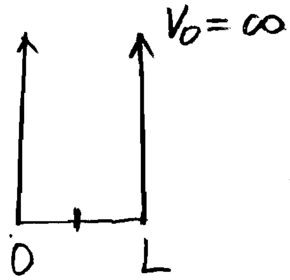
If $V(\vec{r},t)$ is Indepent of t

$\Rightarrow$ $\psi(\vec{r},t) = \psi(\vec{r}) \cdot e^{-i\omega t} = \psi(\vec{r}) \cdot e^{-i\frac{E}{\hbar}t}$

$\Rightarrow$ $-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E \cdot \psi(\vec{r})$

$\hookrightarrow$ Solve E, $\rightarrow \psi(\vec{r})$

Infinite Potential Well:



$$V(z) = 0 \quad \text{for } 0 < z < L$$
$$\infty \quad \text{outside}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\phi(z) = E\phi(z)$$

$$\frac{d^2}{dz^2}\phi(z) + \frac{2mE}{\hbar^2}\phi(z) = 0$$

General solution

$$\sin kz. \quad \cos kz$$

B.C. $\phi(0) = \phi(L) = 0 \Rightarrow \begin{cases} \sin kz \\ kL = n\pi \end{cases}$

$$\Rightarrow \phi_n(z) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} z\right)$$

$$\Rightarrow E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 \quad \propto n^2$$

Solution in 3-D

$$\psi(x.y,z) = \underbrace{\phi'(x.y)}_{\text{unconstrained}} \cdot \phi(z)$$

$$\Rightarrow \phi' = e^{ik_x x + ik_y y} \quad \frac{1}{\sqrt{A}}$$

$\uparrow$ Normalization const

$$\psi_n(x.y.z) = \frac{1}{\sqrt{A}}\sqrt{\frac{2}{L}} \cdot e^{ik_x x + ik_y y} \cdot \sin\left(\frac{n\pi}{L} z\right)$$

$$E_n = \frac{\hbar^2}{2m}\left[k_x^2 + k_y^2 + \left(\frac{n\pi}{L}\right)^2\right]$$ Quantized only in k_z

For electrons in 10-nm wide quantum well

$$E_1 = \frac{\hbar^2}{2m_0}\left(\frac{\pi}{L}\right)^2 = \frac{(6.5822\times10^{-16}\ \mathrm{eV\cdot s})^2}{2\times 9.11\times10^{-31}\ \mathrm{kg}} \cdot \frac{\pi^2}{(10^{-8})^2\cdot \mathrm{m}^2}$$

$$= 2.34\times10^{16}\ \frac{\mathrm{eV}^2}{\mathrm{J}}$$

$$= 3.75\ \mathrm{meV}$$

$$E_2 = 4E_1$$

$$E_3 = 9E_1$$

In semiconductor, $m_0 \to m^*$

GaAs. $m_e^* = 0.067\ m_0$

$$\Rightarrow E_1 = \frac{3.75}{0.067} = 56\ \mathrm{meV}$$