Quantum Mechanics

Physical state $\longleftrightarrow$ Wave function

$$\Psi = \Psi(\vec{r}, t)$$

$$\underbrace{\psi = \psi(\vec{r})}_{\text{complex valued functions}}$$

Physical quantity or observable x, p, E, L $\longleftrightarrow$ Operator: $\hat{O}$

$$\Phi = \hat{O}\Psi$$

Expectation value: average value of several measurements: $\langle O \rangle = \bar{O}$

$$\langle O \rangle = \int_{-\infty}^{+\infty} \Psi^* \hat{O} \Psi \, dx = \langle \Psi^*, \hat{O}\Psi \rangle$$

Schrödinger equation:

time dependent: $\hat{E}\Psi(x,t) = \hat{K}\Psi(x,t) + \hat{V}(x,t)\Psi(x,t)$

time independent: $\hat{K}\psi(x) + \hat{V}(x)\psi(x) = E\psi(x)$

$\hat{E}$: total energy operator

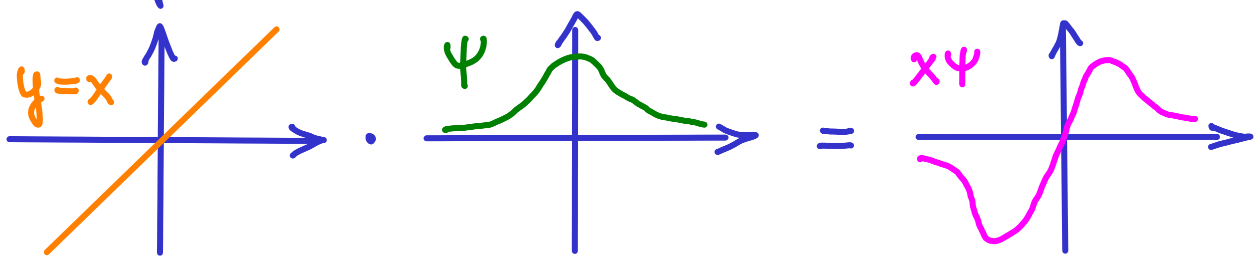
$\hat{K}$: kinetic energy operator

$\hat{V}(x,t)$, $\hat{v}(x)$: potential energy operator

$E \in \mathbb{R}$: total energy of the system

Operators in one dimension

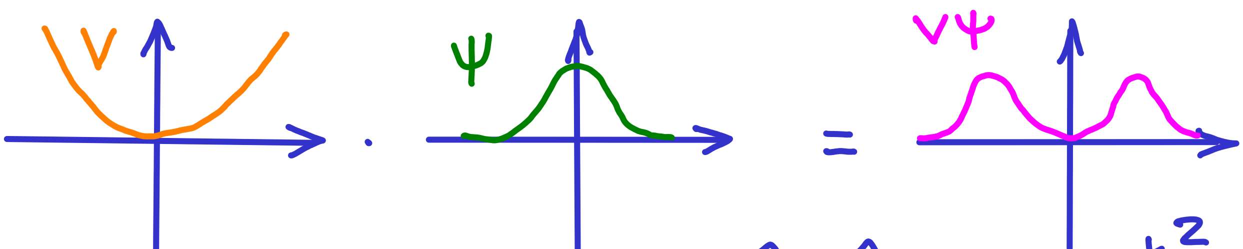
→ position : $\hat{x}$: $\hat{x}\Psi(x) = x\Psi(x)$



→ momentum : $\hat{p}_x$: $\hat{p}_x \Psi(x) = -i\hbar \frac{\partial}{\partial x}\Psi(x)$

first derivative w.r.t. x

→ potential energy : $\hat{V}$: $\hat{V}\Psi(x) = V(x)\Psi(x)$



→ kinetic energy : $\hat{K}$: $\hat{K}\Psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x)$

second derivative w.r.t. x : wavyness

($K = \frac{p^2}{2m}$ still holds)

In the case of a time dependent problem:

→ total energy : $\hat{E}$: $\hat{E}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$

first derivative w.r.t. time

Wave functions

- Ψ must be single valued
- Ψ must be finite everywhere
- $\lim\limits_{x \to \pm\infty} \Psi = 0 \iff \int_{-\infty}^{+\infty} \Psi^* \Psi \, dx$ must be finite
- Ψ and $\frac{d\Psi}{dx}$ must be continuous

  Exception: when $V(x)$ is infinite $\frac{d\Psi}{dx}$ will jump.

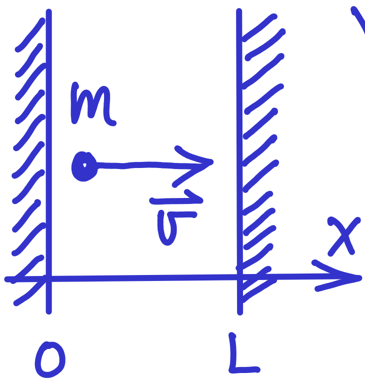
Normalization:

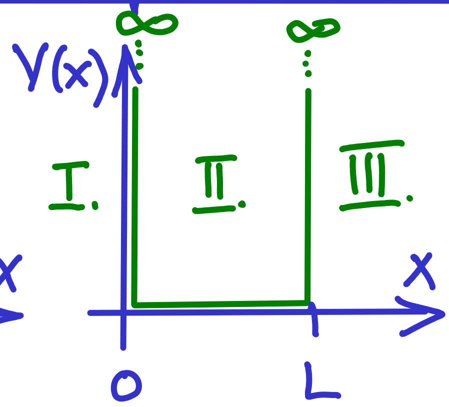
$$\int_{-\infty}^{+\infty} \Psi^* \Psi \, dx = 1$$

$\rho = \Psi^* \Psi$: probability density

- Hilbert space

Infinite square potential well in 1D





$$V(x) = \begin{cases} \infty & \text{if } x \leq 0 \\ 0 & \text{if } 0 < x < L \\ \infty & \text{if } L \leq x \end{cases}$$

Schrödinger equation:

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

<u>Region I and III</u>: $\psi(x) = 0$: an impenetrable wall is impenetrable even in quantum mechanics.

Region II:

$$-\frac{\hbar^2}{2m} \cdot \frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2} \cdot \psi$$

$$\frac{d^2\psi}{dx^2} = -k^2 \cdot \psi$$

$$k = \frac{\sqrt{2mE}}{\hbar} = \frac{p}{\hbar} = \frac{p}{\frac{h}{2\pi}} = \frac{2\pi}{\lambda}$$

$k = \frac{2\pi}{\lambda}$: wave number

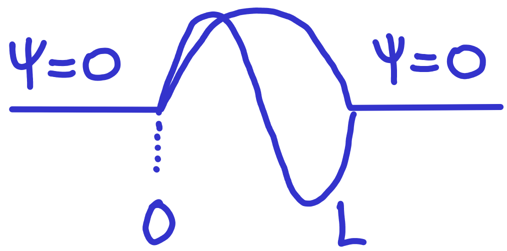
Note: $E = KE$ b/c $V(x) = 0$

Infinite square well in 1D, part 2.

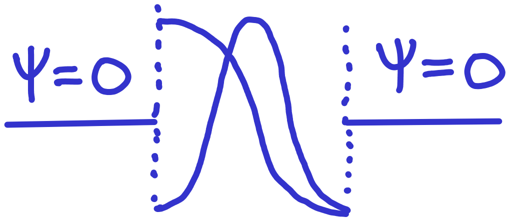
$$\frac{d^2\psi(x)}{dx^2} = -k^2 \cdot \psi(x)$$

General solution:

$$\psi(x) = A \cdot \sin(kx) + B \cdot \cos(kx)$$



sine functions : OK



cosine functions: NOT OK, because the wave function ψ is not continuous at $x=0$ and $x=L$.

The derivative of the wave function: $\frac{d\psi}{dx}$ is not continuous at $x=0$ and $x=L$ for the first group of functions, but that is because $V(x)=\infty$ at those locations.