- Free particle $\longrightarrow$ Classical

Particle in 1-D box

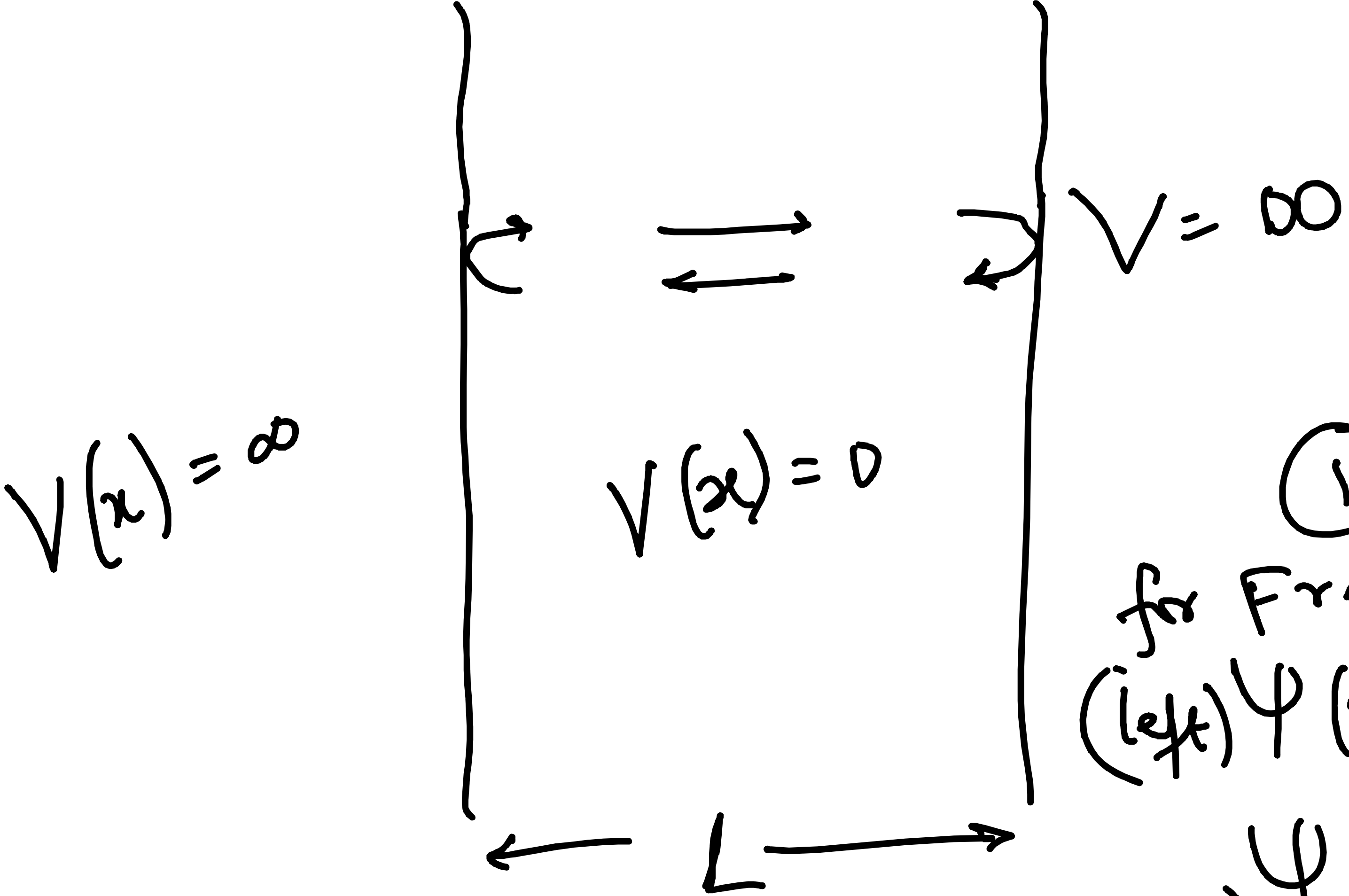
$$\hat{H}\Psi = E\Psi$$

restricts

$$\hat{H} = -\frac{1}{2m}\hbar^2 \frac{d^2}{dx^2} + \underbrace{V(x)}_{=0}$$

$= 0$ free particle

within a region in space



1 for Free particle

$$(\text{left})\ \psi(x) = Ae^{ikx}$$

$$(\text{right})\ \psi(x) = Be^{-ikx}$$

$$2\quad \boxed{\psi(x) = Ae^{ikx} + Be^{-ikx}}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \& \quad \psi = Ae^{ikx} + Be^{-ikx}$$

$$k = \sqrt{\frac{2Em}{\hbar^2}}$$

How to get A & B ?

Boundary Cond^n

$x = 0$

$x = L$

$0 < x < L \rightarrow$ free particle

$$\int |\psi|^2 dx = 1$$

$$\boxed{|\psi^2(x)|_{\substack{x \leq 0 \\ x \geq L}} = 0}$$

$\Rightarrow \psi(0) = \psi(L) = 0$

① $A + B = 0$

② $Ae^{ikL} + Be^{-ikL} = 0$

(1) $B = -A$ & (2) $A\left(e^{ikL} - e^{-ikL}\right) = 0$

$$\exp(\pm ikL) = \cos(kL) \pm i\sin(kL)$$

$$2i\cancel{A}\sin(kL) = \sin(n\pi)$$

integers

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad kL = n\pi$$

$$E_n = \frac{\pi^2\hbar^2}{2mL}n^2$$

only allowed

To get: $\psi_n(x) \longrightarrow \hat{H}\psi_n = E_n \psi_n$

$$\psi_n(x) = 2i\underline{\underline{A}} \sin\left(\frac{n\pi x}{L}\right)$$

for $n = 1, 2, 3, \ldots$

Not $n = 0$; $\because$ will give $\psi_n = 0$ (no particle!)

<u>Quantized Energy</u> with <u>Quantum No. "n"</u>

$$\int_0^L \psi_n^*(x) \cdot \psi_n(x)\, dx = \int_0^L |\psi_n(x)|^2 dx = 1$$

ψ^* is complex conjugate of ψ

e.g. $\psi = a + ib$ then $\psi^* = a - ib$

$$|\psi|^2 = \psi \psi^* = a^2 + b^2$$

$$\psi_n(x) = \underbrace{2iA}\sin\left(\frac{n\pi x}{L}\right) = C\sin\left(\frac{n\pi x}{L}\right)$$

$$\int_0^L \left|\psi_n(x)\right|^2 dx = C^2\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$C^2\left(\frac{L}{2} - 0\right) = 1 \quad 4 \quad C = \pm\sqrt{\frac{2}{L}}$$

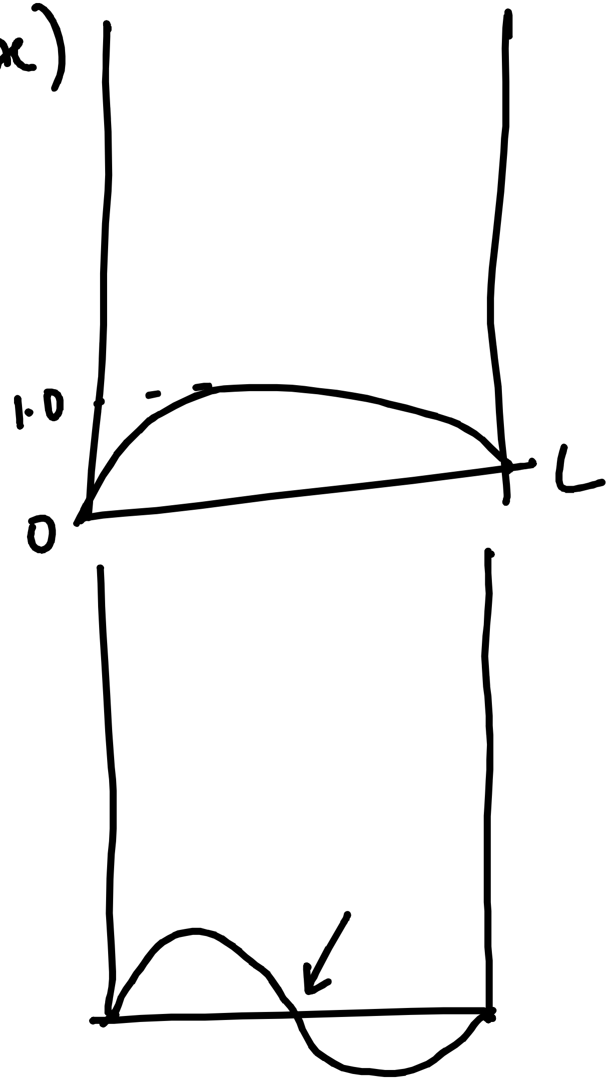
$$\rightarrow \quad \psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3 \cdots$$

family } Normalized wave functions

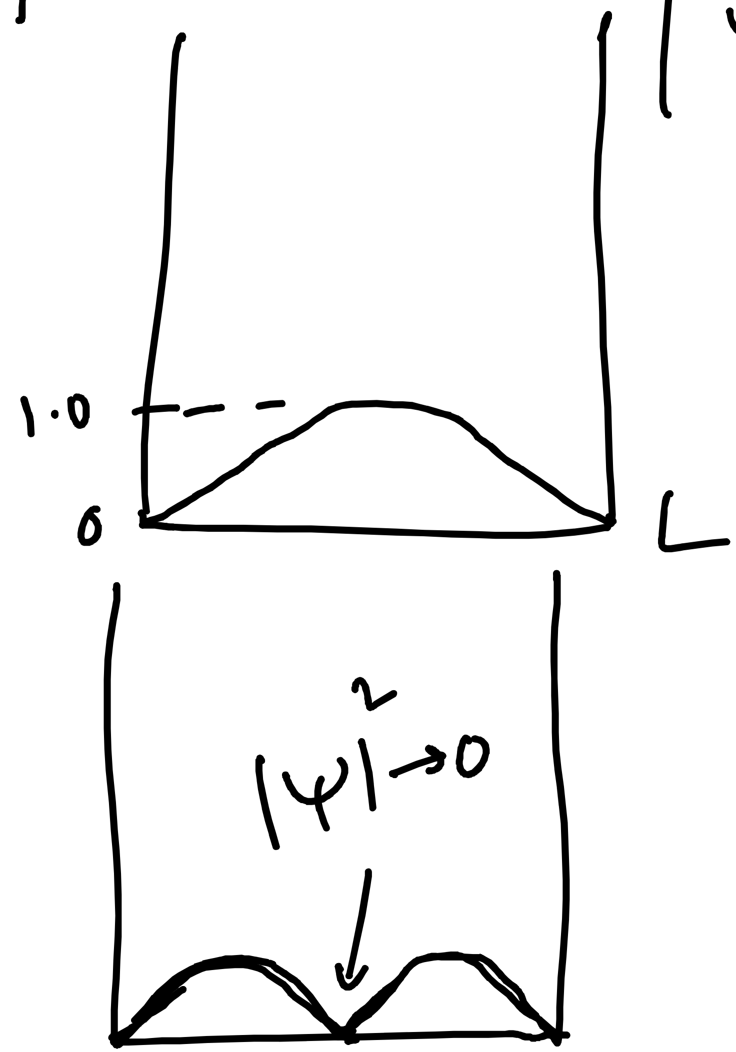
$\psi_n(x)$

n = 1

n = 2



$|\psi_n(x)|^2$



Points in space other than the edges of the 1-D box, probability can approach "zero", these are defined as <u>Nodes</u>

quantum # $\leftarrow$ $(n-1)$ nodes for <u>1-D particle in a box</u>

# of nodes +1

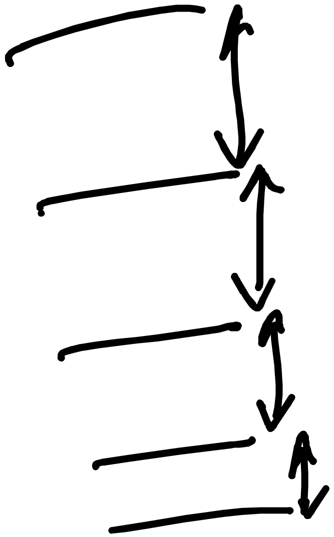
$E \propto$ No. of nodes

Lowest energy $= E_1 = \dfrac{\pi^2 \hbar^2}{2mL^2}$

Energy Spacing

$$E_{n+1} - E_n = \left(\frac{\pi^2 \hbar^2}{2mL^2}\right)(2n+1)$$

with increasing "n", gap increases.



$$\frac{E_{n+1} - E_n}{E_n}$$