The Davisson-Germer Experiment

→ 3 years after deBroglie's work, Davisson & Germer measured the wavelength λ of electrons accidentaly

→ Davisson & Germer used 54 eV electrons (low energy) projected on a nickel target in a vacuum

→ nickel target accidentally oxidized ⟼ resulting in a treatment with heating in a flowing stream of hydrogen to remove the oxide coating

⇓

→ large crystal regions of the nickel target ⇒ 3D grating

⇒ maxima & minima @

specific angles (like the von Laue's pattern)

→ after careful diffraction measurements using e^- scattered on single-crystal targets

$p = \frac{h}{\lambda}$ was confirmed for electrons

→ Thomson: observed e^- diffraction patterns for e^- passing through very thin gold foils

→ other particles:

→ helium atoms
→ hydrogen atoms
→ neutrons

wave nature of particles established

Quiz: An electron & proton are moving with $v \ll c$ (non-relativistic speeds). Both have the same speed. Which quantity is the same for both particles?

(a) momentum : $p = mv$

(b) de Broglie wavelength $\lambda = \frac{h}{p}$

(c) kinetic energy $K = \frac{1}{2}mv^2$

(d) frequency $f = \frac{v}{\lambda}$

~~(e)~~ none of the above

The Quantum Particle Model

→ combine properties of a wave & a particle with a single mathematical description

→ superposition of two (2) waves

$$y_1 = A\cos(k_1 x - \omega_1 t) \qquad k = \frac{2\pi}{\lambda}$$

$$y_2 = A\cos(k_2 x - \omega_2 t)$$

→ assume $k_1 \neq k_2$

$\omega_1 \neq \omega_2$

but $\left.\begin{array}{l} k_1 \,\&\, k_2 \\ \omega_1 \,\&\, \omega_2 \end{array}\right\}$ not too different

→ superposition:

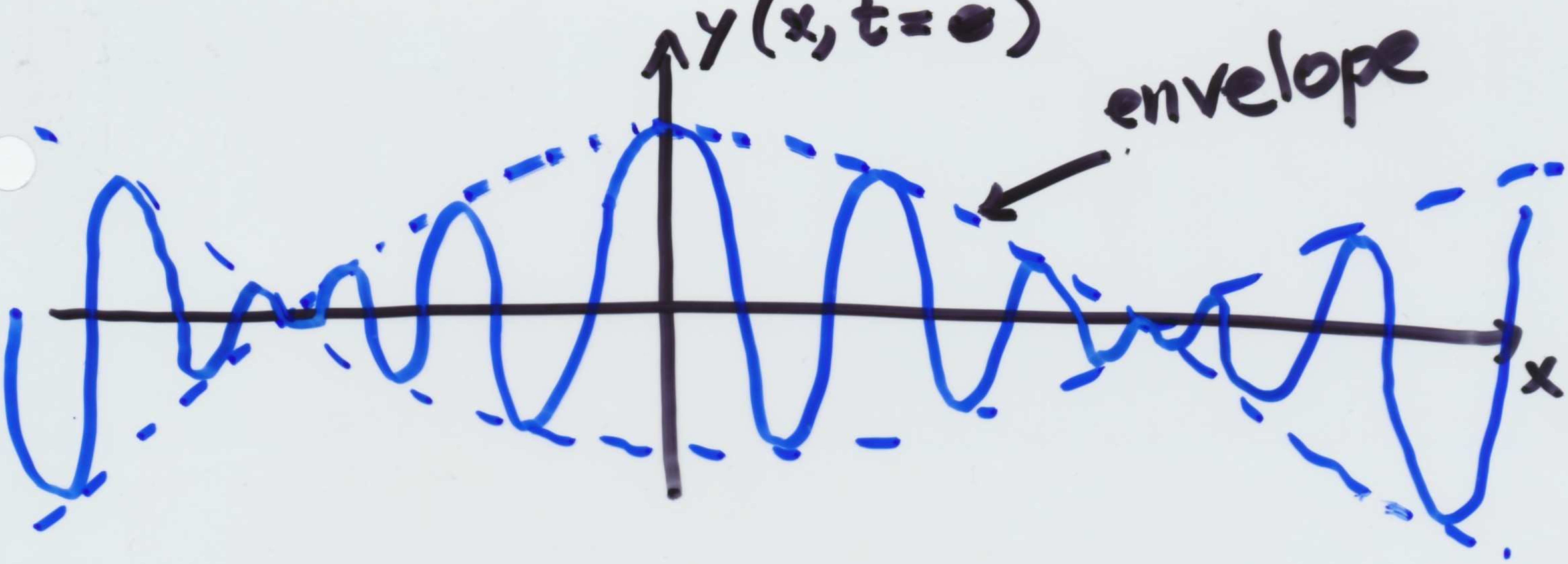
$$y = y_1 + y_2 =$$
$$= A\cos(k_1 x - \omega_1 t) + A\cos(k_2 x - \omega_2 t)$$
$$= 2A\cdot\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cdot$$
$$\cdot\cos(\bar{k}x - \bar{\omega}t)$$

$$\cos a + \cos b = 2\cos\frac{a-b}{2}\cos\frac{a+b}{2}$$

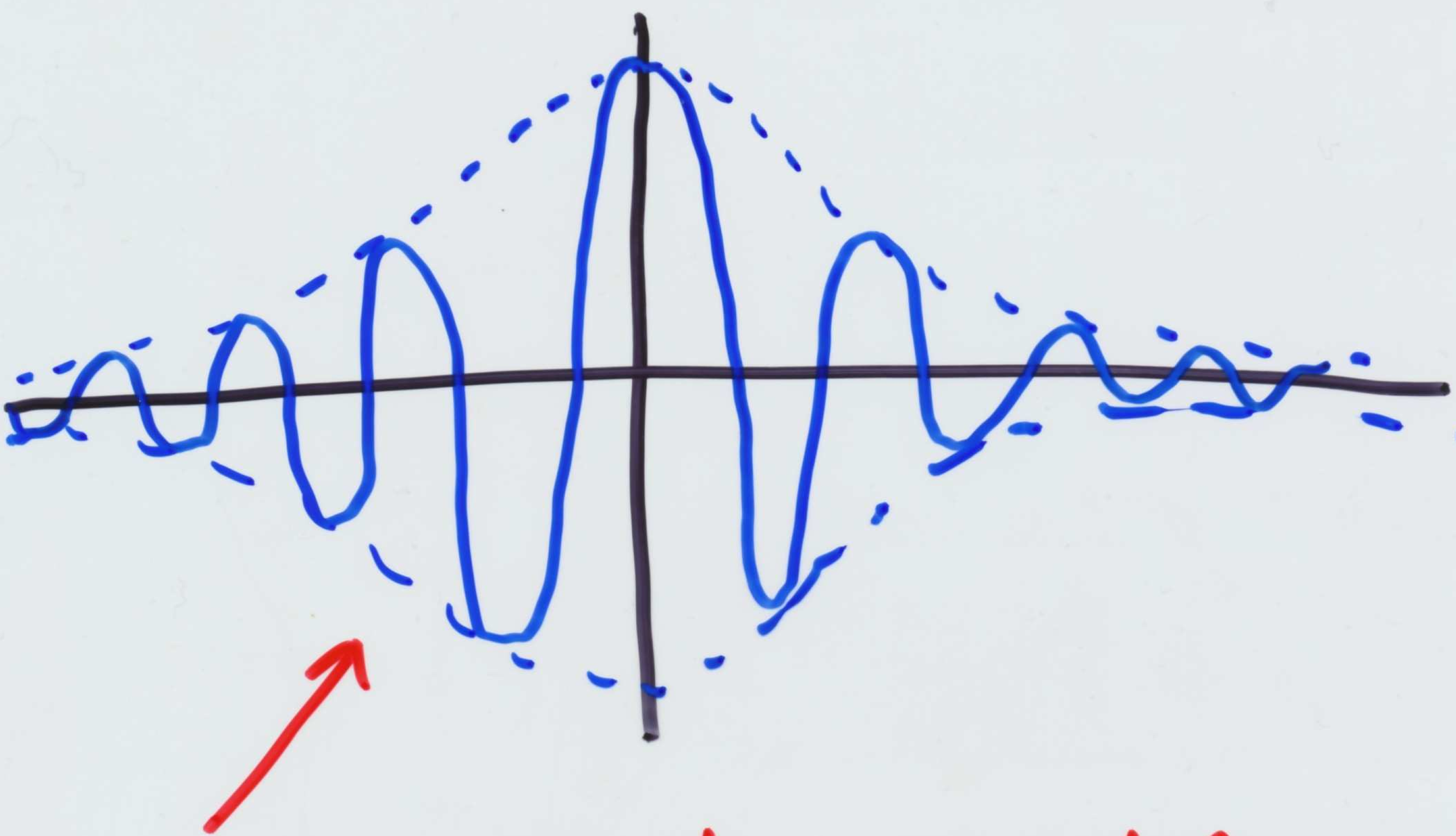
→ definitions

$$\Delta k = k_1 - k_2 \quad \& \quad \Delta\omega = \omega_1 - \omega_2$$
$$\bar{k} = \tfrac{1}{2}(k_1 + k_2) \quad \& \quad \bar{\omega} = \tfrac{1}{2}(\omega_1 + \omega_2)$$

$$y = \underbrace{2A\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)}_{\text{envelope (slow changing)}}\underbrace{\cos(\bar{k}x - \bar{\omega}t)}_{\text{fast changing}}$$



→ WAVE PACKET = a superposition of many wavelengths (many different k-waves)



a mathematical representation of a particle (quantum)

→ two types of speeds associated with a wave packet

phase speed v_p

group speed v_g

→ v_p ... the speed by which an individual crest moves

$$v_p = \frac{\omega}{k}$$

→ v_g ... the speed by which the envelope moves

$$v_g = \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk}$$

→ group velocity of a wave packet (quantum particle) is equal to the speed of the particle:

$$v_g \overset{\text{def.}}{=} \frac{d\omega}{dk} = \frac{d(\hbar\omega)}{d(\hbar k)} = \frac{dE}{dp}$$

$$k = \frac{2\pi}{\lambda}$$
$$\hbar = \frac{h}{2\pi}$$
$$\omega = 2\pi f$$

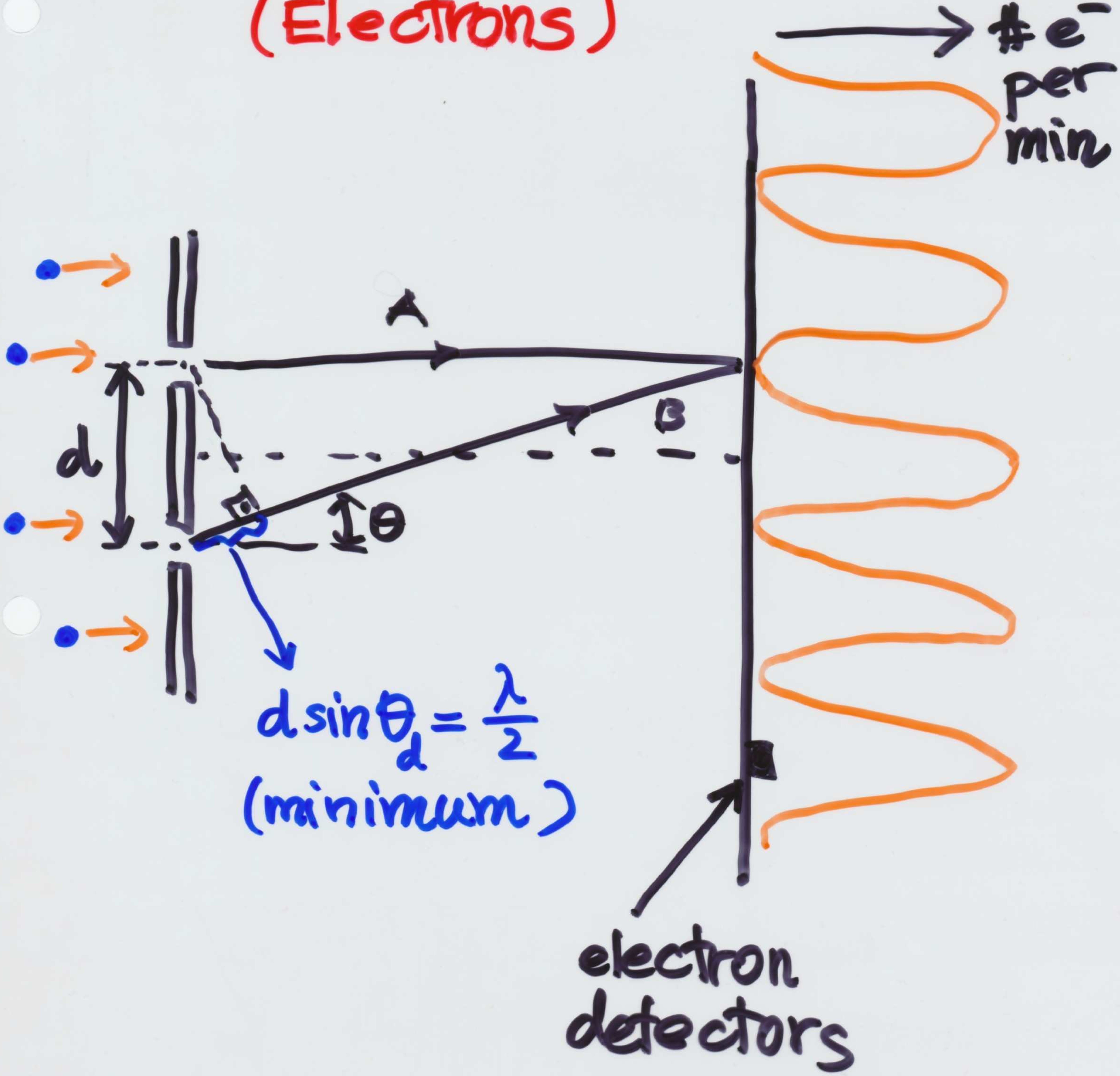
$$E = \hbar\omega$$
$$p = \hbar k$$

classical (non-relativistic) particle:

$$\underbrace{p = mv \quad \& \quad E = \frac{1}{2}mv^2}$$

$$E = \frac{p^2}{2m} \Rightarrow \frac{dE}{dp} = \frac{p}{m} = v$$

The Double-Slit Experiment
(Electrons)



→ interference pattern emerges even at very low intensity of incoming e^-

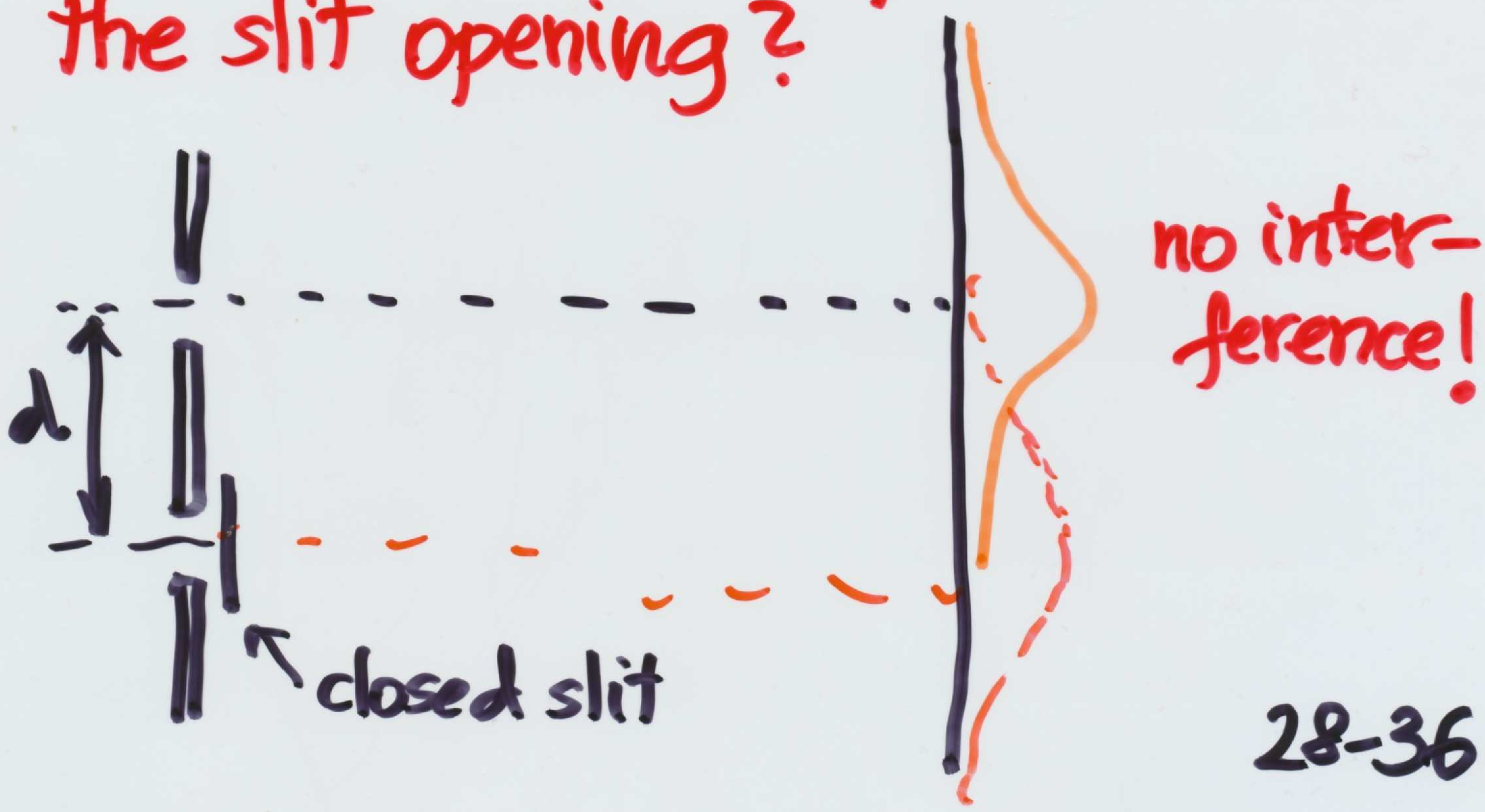
→ λ of electrons can be expressed by the momentum p_x:

$$\lambda = \frac{h}{p_x}$$

→ the angle θ at which the 1st minimum occurs:

$$\sin\theta \approx \theta \approx \frac{h}{2p_x d}$$

Does each electron pass one of the slit opening?



The only way to observe the interference is to have e^- pass through <u>two</u> open slits <u>simultaneously</u>!

The Uncertainty Principle

It is fundamentally impossible to make simultaneous measurements of a particle's position and momentum with infinite accuracy:

$$\Delta x \cdot \Delta p_x \geq \frac{\hbar}{2}$$

→ consequence of the quantum structure of matter

Example: a particle with exact wavelength λ:

$$p_x = \frac{h}{\lambda} \Rightarrow \Delta p_x = 0$$

$\rightarrow$ Heisenberg uncertainty principle

$\Delta x \rightarrow \infty$ such that

$$\Delta x \cdot \Delta p_x \gtrsim \frac{\hbar}{2}$$

$\Downarrow$

the particle can be anywhere along x

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

plane wave $\mapsto$ wave function

$\uparrow$

the only particle with exact λ or p_x

Two forms of the Heisenberg uncertainty principle:

(1) $\Delta x \cdot \Delta p_x \gtrsim \frac{\hbar}{2}$

OR $\Delta y \, \Delta p_y \gtrsim \frac{\hbar}{2}$

$\Delta z \, \Delta p_z \gtrsim \frac{\hbar}{2}$

<u>but</u> not $\cancel{\Delta x \, \Delta p_y \gtrsim \frac{\hbar}{2}}$

(2) $\Delta E \cdot \Delta t \gtrsim \frac{\hbar}{2}$

$E = hf$

<u>Example:</u> e^- $v = 5 \times 10^3 \, m/s \pm 0.003\%$

$\Delta x = ?$

$p_x = m_e v = 4.56 \times 10^{-27} \, kg\,m/s$

$\Delta p_x = 0.00003 \cdot p_x = 1.37 \times 10^{-31} \, kg\,m/s$

$\Delta x \gtrsim \hbar / 2\Delta p_x \approx \underline{0.384 \, nm}$

An Interpretation of QM

→ description of the quantum particle (wave or particle):

probability amplitude OR wave function $\Psi(\vec{r},t)$
(complex function)

$$\Psi(\vec{r},t) = \psi(\vec{r})\, e^{-i\omega t}$$

$i = \sqrt{-1}$

separation of $\vec{r}$ & t part when describing STATIONARY conditions of a quantum particle

→ remember:

$$e^{i\theta} = \cos\theta + i\sin\theta$$

→ consider only stationary solutions ⇒ only $\psi(\vec{r})$

→ simplify to one dimension

$\psi(x)$ ... complex function

$$\underbrace{\psi^*(x)\,\psi(x)}_{= |\psi(x)|^2} \text{ ... real function}$$

→ $\underbrace{(a+ib)}_{\psi}\,\underbrace{(a-ib)}_{\psi^*} = a^2+b^2$

$(i^2=-1)$

→ probability density

$P(x)$

$$P(x) \stackrel{\text{def.}}{=} |\Psi(x)|^2$$

→ wave function $\Psi(x)$ is normalized:

$$\int_{-\infty}^{\infty} P(x)\,dx = 1$$

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

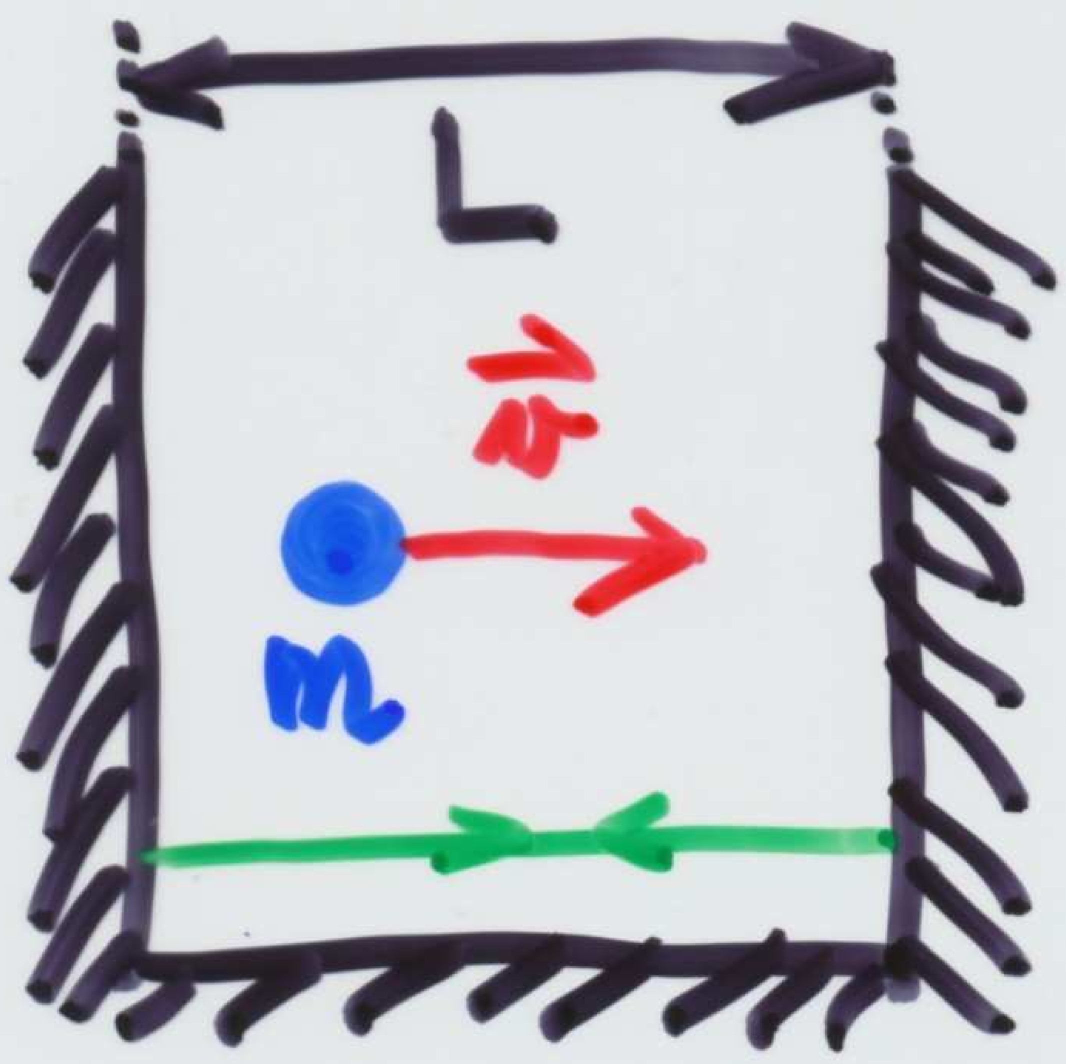
→ $P_{ab} = \int_a^b |\Psi|^2\,dx$ prob. to find a QP at $a \leq x \leq b$

→ $\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* x \Psi\,dx$ expectation value of x

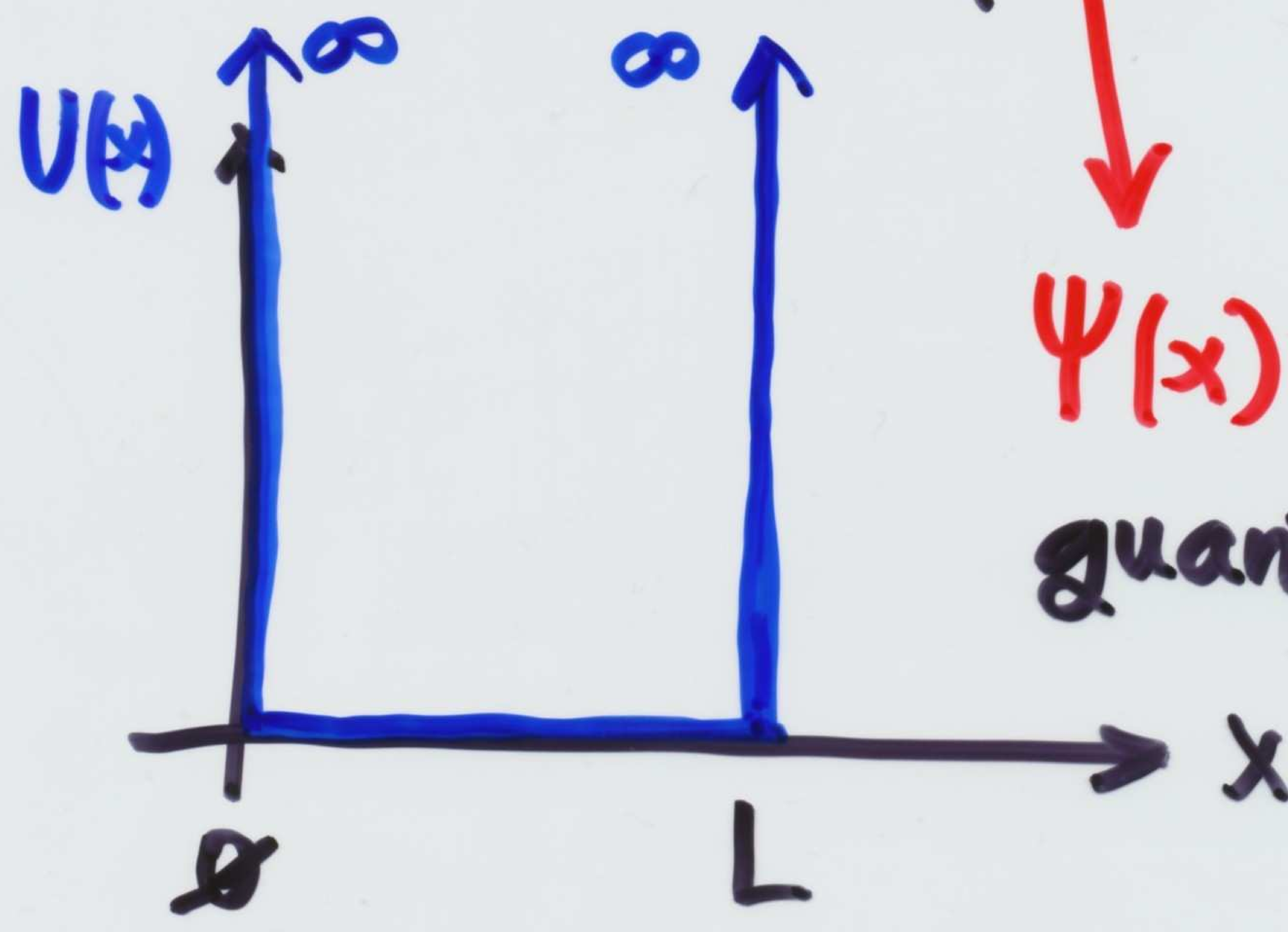
→ $\langle f(x) \rangle = \int_{-\infty}^{\infty} \Psi^* f(x) \Psi\,dx$ general

A Particle in a Box

How does the classical physics describe a particle in a box?



How about a quantum particle in a box?



$\psi(x) = ?$

quantum description

$\psi(x)$ ... probability amplitude (wave function)

→ particle cannot exist outside the box ($U(x=0) = U(x=L) = \infty$):

$$\psi(x \leq 0) = 0 \ \& \ \psi(x \geq L) = 0$$

boundary conditions

→ inside the box :

$$U(x) = 0 \quad 0 < x < L$$

$$U(x \to 0) \to \infty \ \& \ U(x \to L) \to \infty$$

→ select a function that satisfies boundary conditions :

$$\psi(x) = A \sin kx$$

$$kL = n\pi \Rightarrow k_n = n\frac{\pi}{L}$$

OR $\quad \lambda_n = \frac{2\pi}{k_n} = \frac{1}{n} \cdot 2L$

$$\boxed{\psi_n(x) = A \cdot \sin\left(\frac{n\pi x}{L}\right)} \quad n = 1, 2, 3 \ldots$$

→ normalize the wave function

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

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

$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = A^2 \frac{L}{n\pi} \underbrace{\int_0^{n\pi} \sin^2 y \, dy}_{\frac{1}{2}n\pi}$$

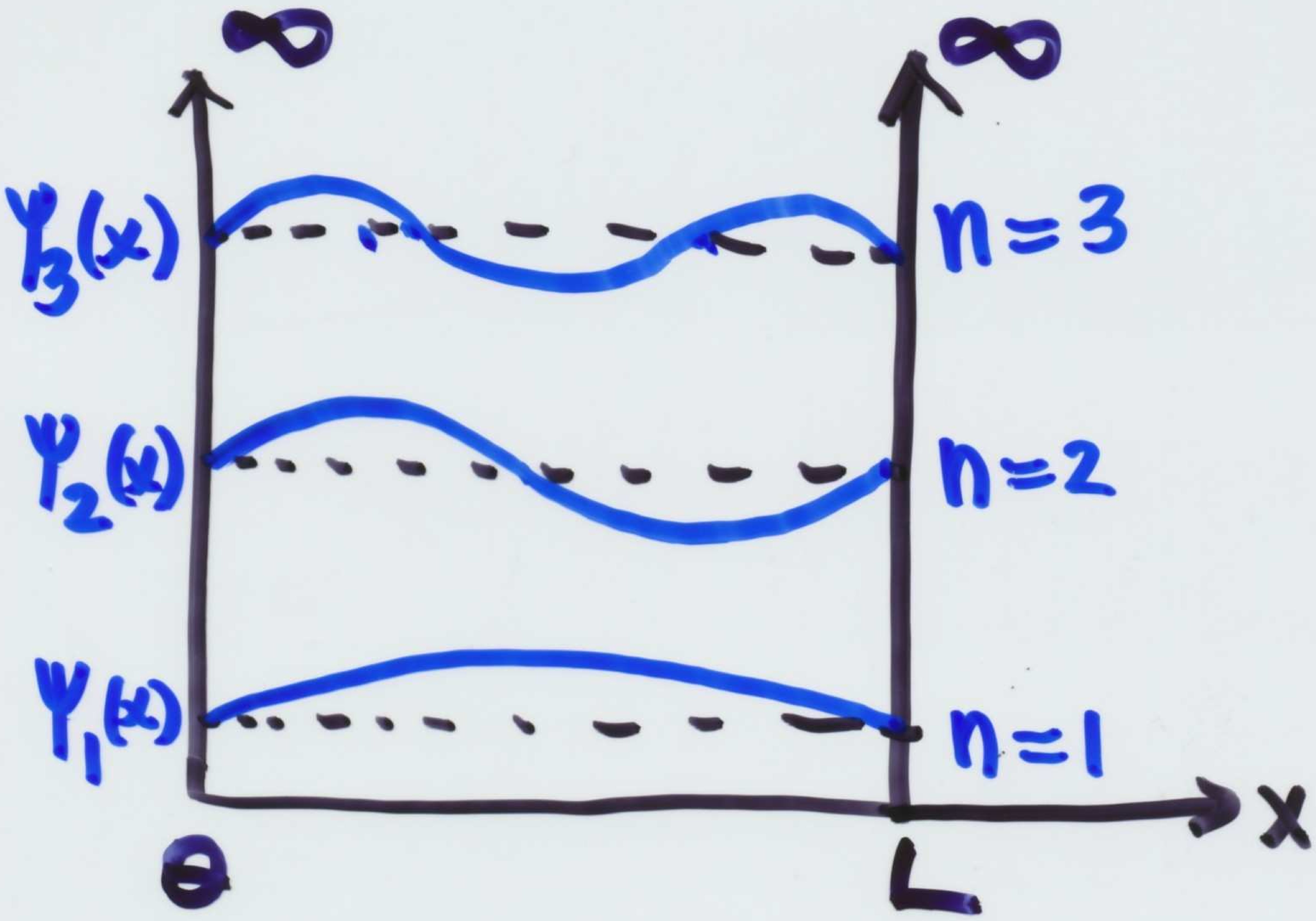
$$y = \frac{n\pi x}{L}$$

$$dy = \frac{n\pi}{L} dx \Rightarrow dx = \frac{L}{n\pi} dy$$

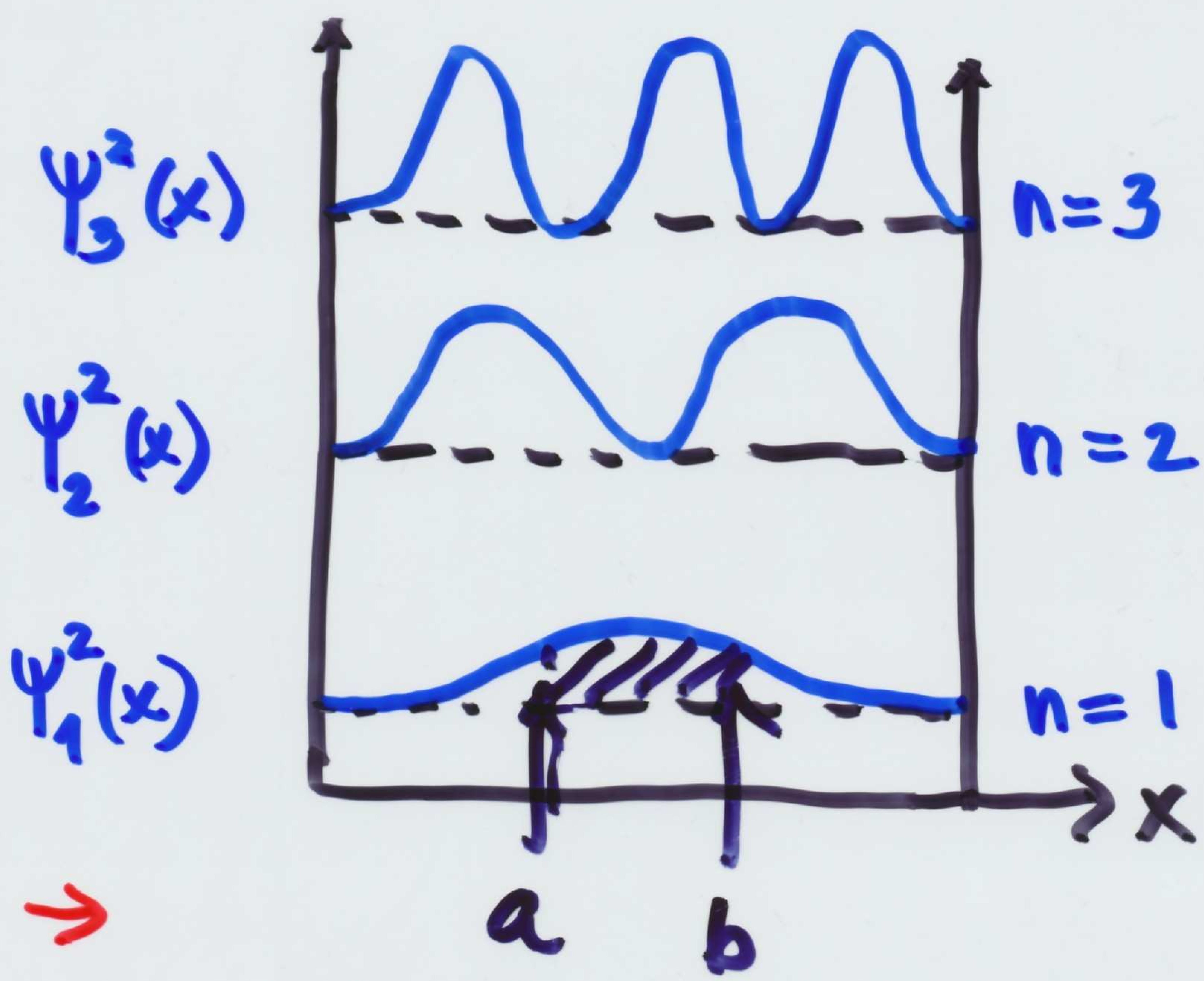
$$A^2 \frac{L}{\cancel{n\pi}} \cdot \frac{1}{2} \cancel{n\pi} = 1 \Rightarrow \underline{A = \sqrt{\frac{2}{L}}}$$

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

→ wave functions for $n = 1, 2, 3$



→ probability densities:



→

→ energy levels:

(What is the kinetic energy of a Q-particle in a box?)

$$p = \frac{h}{\lambda} \quad \text{(de Broglie relat.)}$$

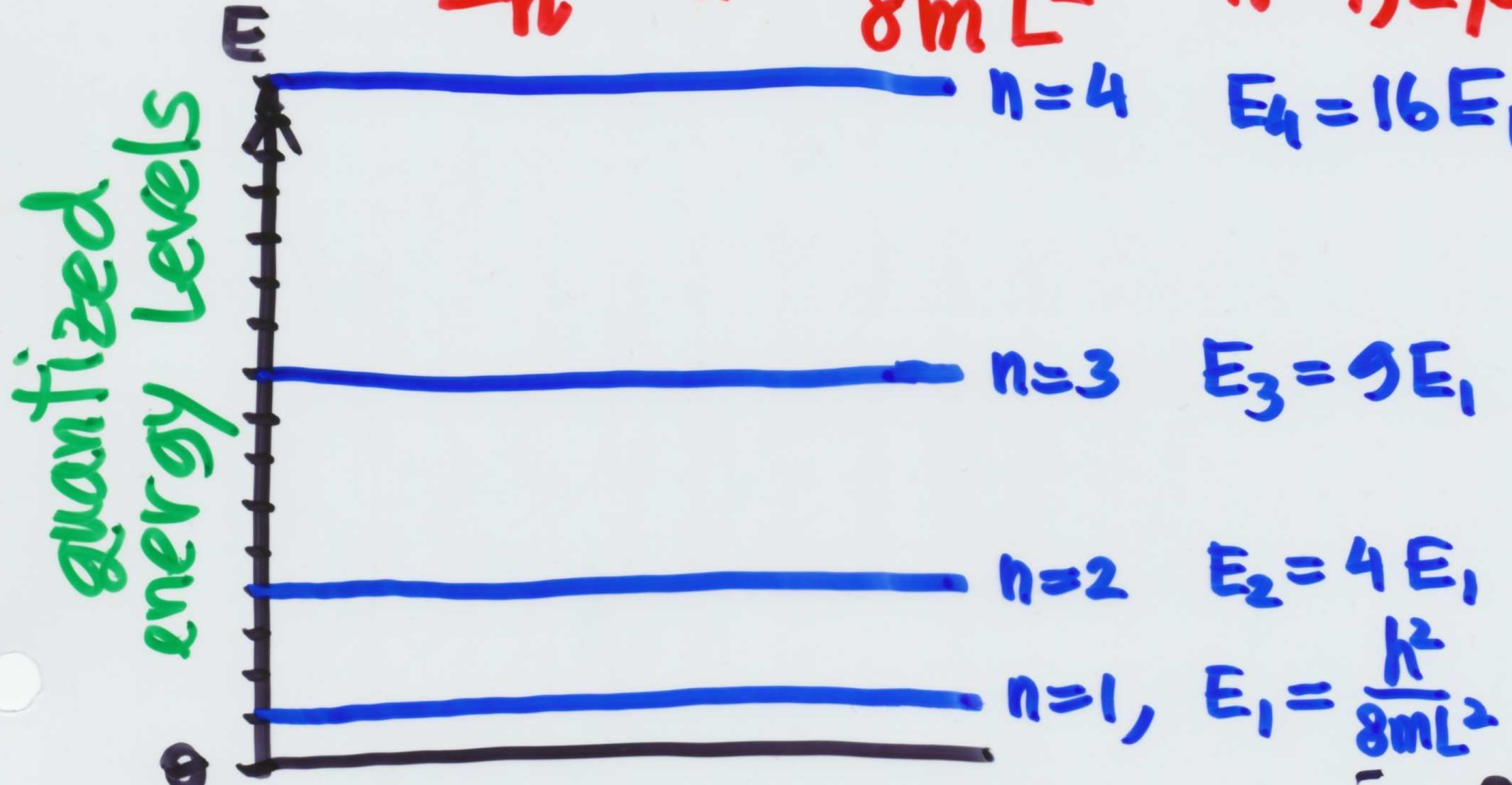
$$\lambda_n = \frac{2L}{n} \Rightarrow p_n = n\frac{h}{2L}$$

$$E_n = K_n + \underbrace{\cancel{U_n}}_{=0} = K_n = \frac{p_n^2}{2m}$$

$E_n = n^2 E_1$

$\boxed{\text{Q particle CANNOT be at rest in a box}}$

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



Example: A bound electron in a box of length $L = 2a_0 \approx 10^{-10}\,m$

the Bohr radius

→ calculate the lowest energy level

$$E_1 = \frac{h^2}{8 m_e L^2} = \frac{(hc)^2}{8 \underline{m_e c^2} L^2} =$$

$$= \frac{1240^2\, eV^{\cancel{2}}\, \cancel{nm^2}\; 10^{-4}}{8 \cdot 0.511 \times \cancel{10^6}\, \cancel{eV} \cdot \cancel{10^{-2}}\, \cancel{nm^2}} =$$

$$\approx \underline{\underline{37.6\, eV}}$$

→ the lowest kinetic energy of an e^- in a "box" of $2a_0$ (diameter of a H-atom)

$(-13.6\, eV)$

Macroscopic objects?

→ tennis ball of $m = 70\,g$

→ in a fence enclosure $L = 1m$

(A) $E_1 = ?$ $v_1 = ?$

$$E_1 = \frac{h^2}{8mL^2} = \frac{(6.63)^2 \times 10^{-68}\, J^{\cancel{2}}\, \cancel{s^2}\, \cancel{kg}\, \cancel{m^2}}{8 \cdot 0.07 \cdot \cancel{kg}\, \cancel{m^2} \cdot \cancel{s^2}}$$

$$\doteq 7.8 \times \underline{10^{-67}}\, J = \underline{4.9 \times 10^{-48}\, eV}$$

very small

$$K_1 = E_1 = \frac{1}{2} m v_1^2 \Rightarrow v_1 = \sqrt{2E_1/m} =$$

$$\doteq \underline{1.2 \times 10^{-23}\, m/s}$$

unmeasurably small

(B) If the speed of a tennis ball is $v = 2\,cm/s = 0.02\,m/s$, $n = ?$

$$\boxed{K = n^2 E_1}$$

$$K = \frac{1}{2} m v^2 = 1.4 \times 10^{-6}\, J$$

$$n = \sqrt{\frac{K}{E_1}} \doteq 1.3 \times 10^{30}$$

Quantum Particle & Boundary Conditions

Analogy:

→ mechanical waves on a string fixed at both ends

→ quantum particle in a box

→ probability amplitude at the boundaries is zero

⇓

quantized wavelengths, frequencies, energies

If an interaction between a Q-particle & environment restricts the QP to a finite region of space ⇒ quantization of energy of a QP

What equation do we use to mathematically describe the motion of the QP?

→ in classical physics

$$\vec{F} = \frac{d\vec{p}}{dt}$$ Newton's 2nd Law

→ in wave mechanics

$$\frac{\partial^2 B}{\partial x^2} = \varepsilon_0 \mu_0 \frac{\partial^2 B}{\partial t^2}$$ EM waves

wave equation

→ in quantum mechanics

the Schrödinger equation

The Schrödinger Equation

→ applies to a particle of mass m moving along x-direction in 1D, potential $U(x)$

→ stationary equation for the probability amplitude (wave function) $\Psi(x)$

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

time-independent SE

Remember:

- $\Psi(x)$ is generally a complex function with real & imaginary part
- $|\Psi(x)|^2 > 0$ ... prob. density

The time-independent Schrödinger equation tells us that the sum of kinetic (K) & potential (U) energy is constant:

$$E = K + U$$

→ knowing $U(x)$

→ applying boundary conditions for $\psi(x)$

$$\Downarrow$$

solution $\psi(x)$

Boundary conditions:

→ $\psi(x)$ ... continuous function

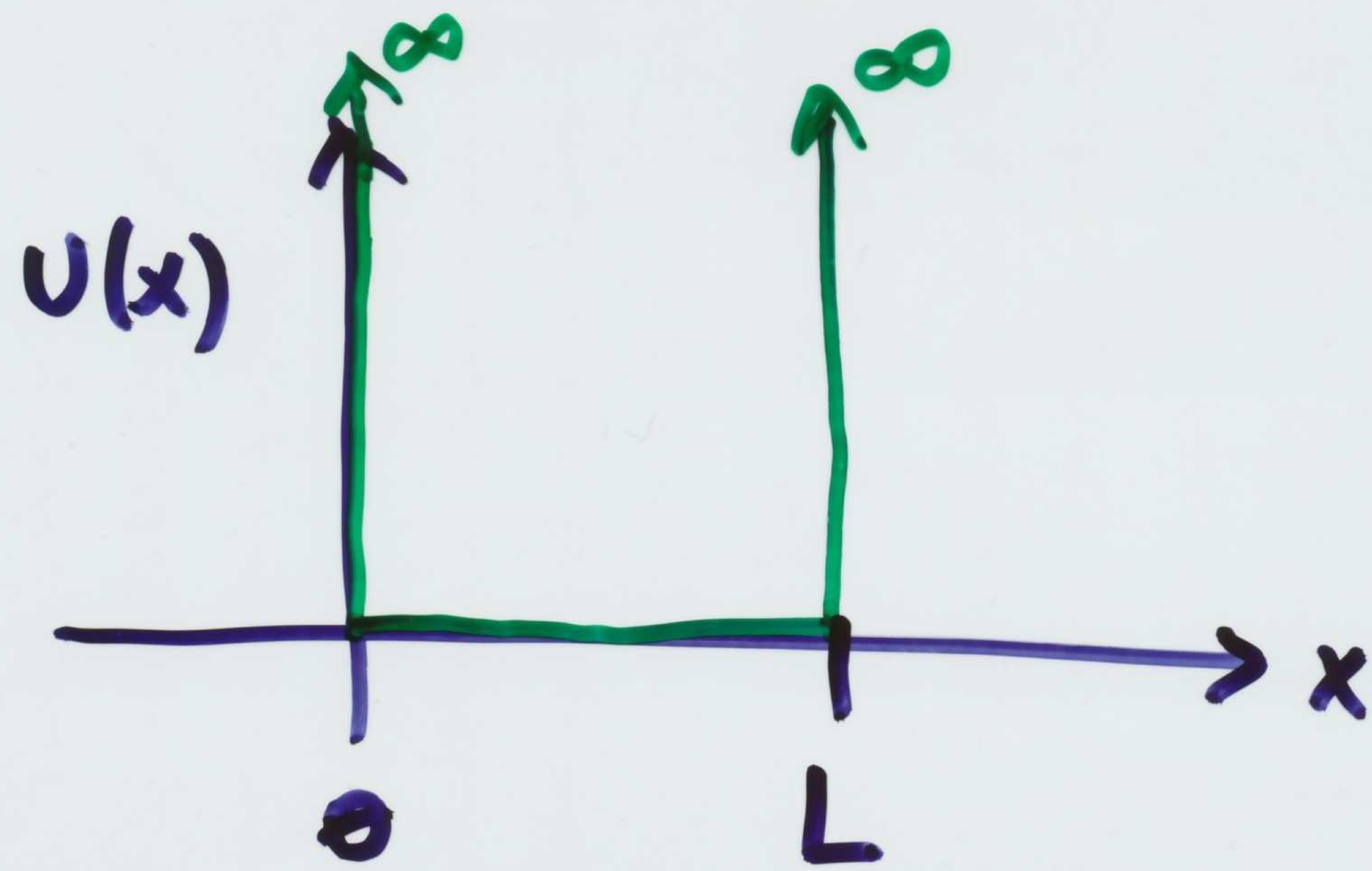
→ $\psi(x)$ ... normalized $\Rightarrow \psi(x \to \pm\infty) \to 0$

→ $\psi(x)$ ... single valued

→ if $|U(x)| < \infty \Rightarrow \frac{d\psi}{dx}$ continuous

The Schrödinger Eq. for a particle in a box

→ what is $U(x)$ for the particle in a box?



$$U(x) = \begin{cases} 0 & \{0 \le x \le L\} \\ +\infty & \left\{\begin{matrix} x < 0 \\ x > L \end{matrix}\right\} \end{cases}$$

→ only SE inside the region $0 \le x \le L$ needs to be considered

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

$$\Big\downarrow \; /\times\left(-\frac{2m}{\hbar^2}\right)$$

$$\boxed{\frac{d^2\psi}{dx^2} = k^2\psi} \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

→ general solutions:

$$\psi(x) = \cancel{A\cos kx} + B\sin kx$$

→ boundary conditions:

$$\psi(x=0) = 0 : \quad \boxed{A = 0}$$

$$\psi(x=L) = 0 : \quad \boxed{\sin kL = 0}$$

$$k_n L = n\pi \qquad n = 1, 2, 3, \ldots$$

QUANTUM NUMBER

$$\Big\downarrow \text{follows steps}$$

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