PHOT 222: Quantum Photonics
LECTURE 07

Michaël Barbier, Spring semester (2024-2025)

OVERVIEW OF THE COURSE

week	topic	Serway 9th	Young
Week 1	Relativity	Ch. 39	Ch. 37
Week 2	Waves and Particles	Ch. 40	Ch. 38-39
Week 3	Wave packets and Uncertainty	Ch. 40	Ch. 38-39
Week 4	The Schrödinger equation and Probability	Ch. 41	Ch. 39
Week 5	**Midterm exam 1**		
Week 6	**Quantum particles in a potential**	**Ch. 41**	**Ch. 39**
Week 7	Harmonic oscillator		
Week 8	Tunneling through a potential barrier		
Week 9	The hydrogen atom, absorption/emission spectra		
Week 10	**Midterm exam 2**		
Week 11	Many-electron atoms		
Week 12	Pauli-exclusion principle		
Week 13	Atomic bonds and molecules		
Week 14	Crystalline materials and energy band structure		

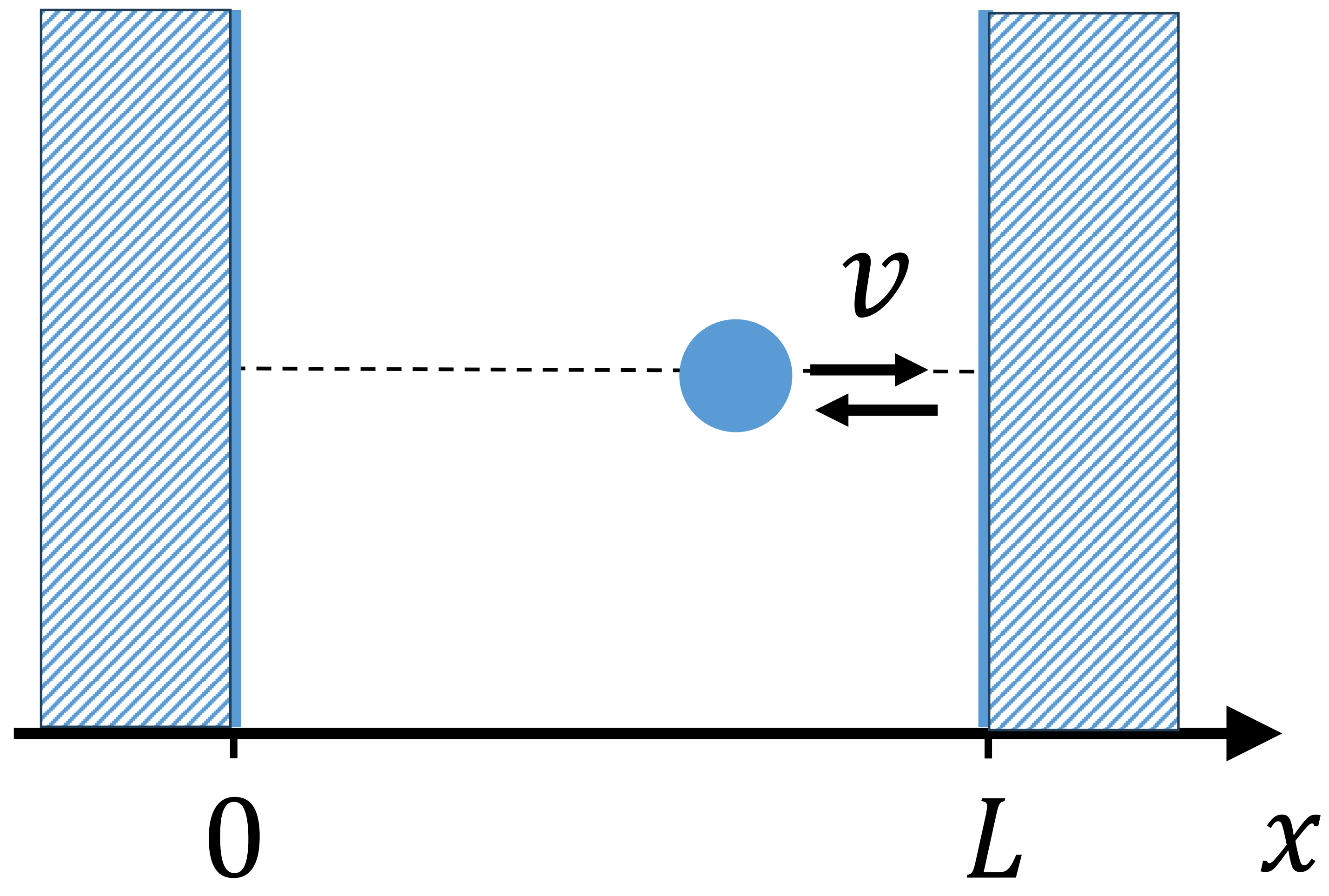
Particle in a box

CLASSICAL PARTICLE IN A BOX

- Consider a 1D box with a free particle
- Classical particle has constant velocity

$$v = \text{constant}$$

- Particle bounces back at the walls
  - Perfect elastic collision
  - Doesn't lose speed/energy
- Kinetic energy: $\mathrm{K} = \frac{1}{2}mv^2$
- Particle can exist only within the box



PARTICLE IN A BOX

- Consider a 1D box:

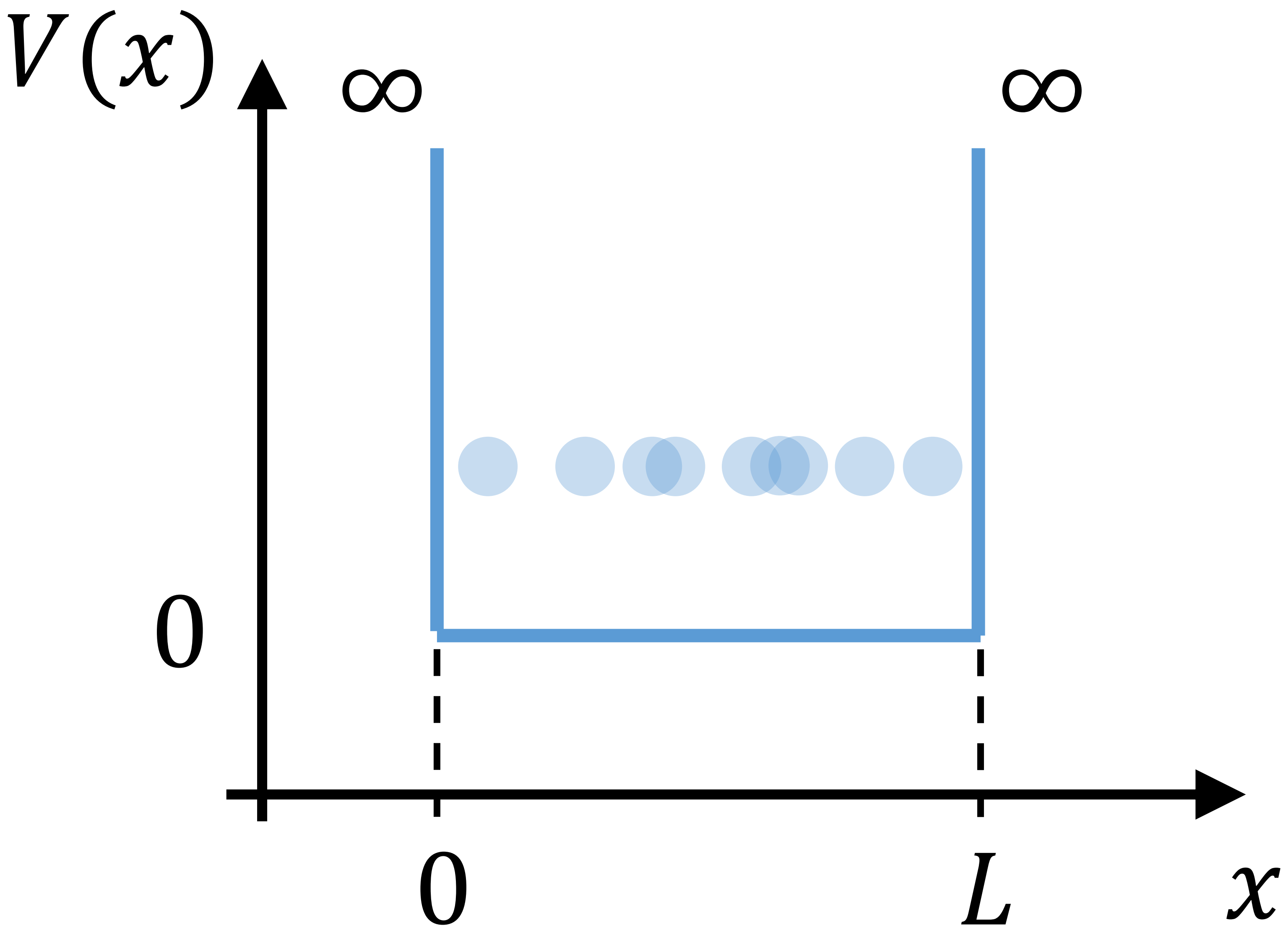
$$\Psi(\mathrm{x,y,z,t}) \rightarrow \Psi(\mathrm{x,t})$$

- Particle can exist only within the box

$$\mathrm{x} \notin [0, L] \quad \Rightarrow \quad \Psi(x,t) = 0$$

- Normalization:

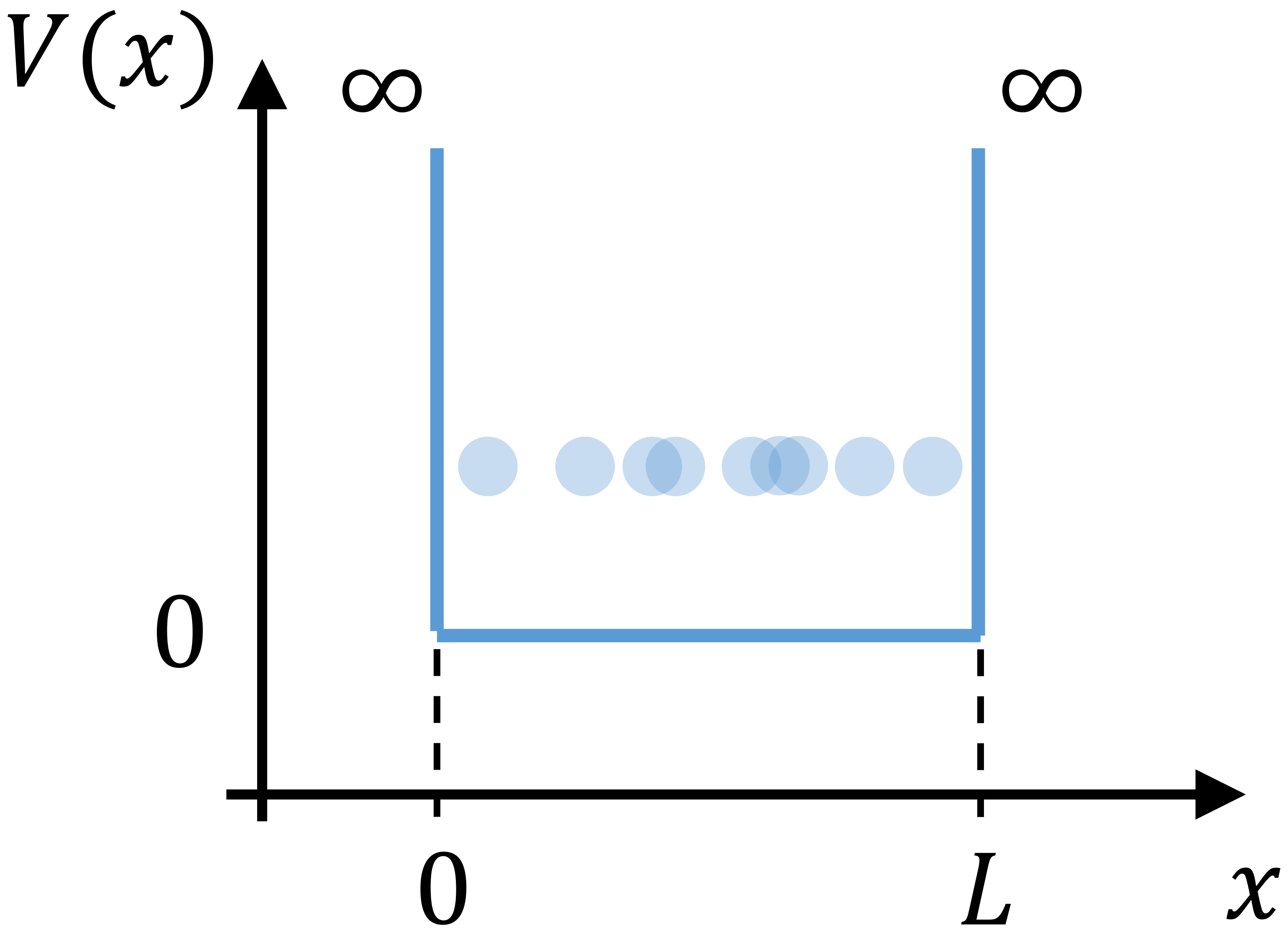
$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 = \int_0^L |\Psi(x,t)|^2 = 1$$



PARTICLE IN A BOX: WAVE FUNCTION

- Time-independent equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x) = E\,\psi(x)$$



- Particle exists only in box:

$$x \notin [0, L] \quad \Rightarrow \quad \psi(x) = 0$$

- Normalization:

$$\int_0^L \left|\psi(x)e^{-iEt/\hbar}\right|^2 = \int_0^L |\psi(x)|^2 = 1$$

PARTICLE IN A BOX: WAVE FUNCTION

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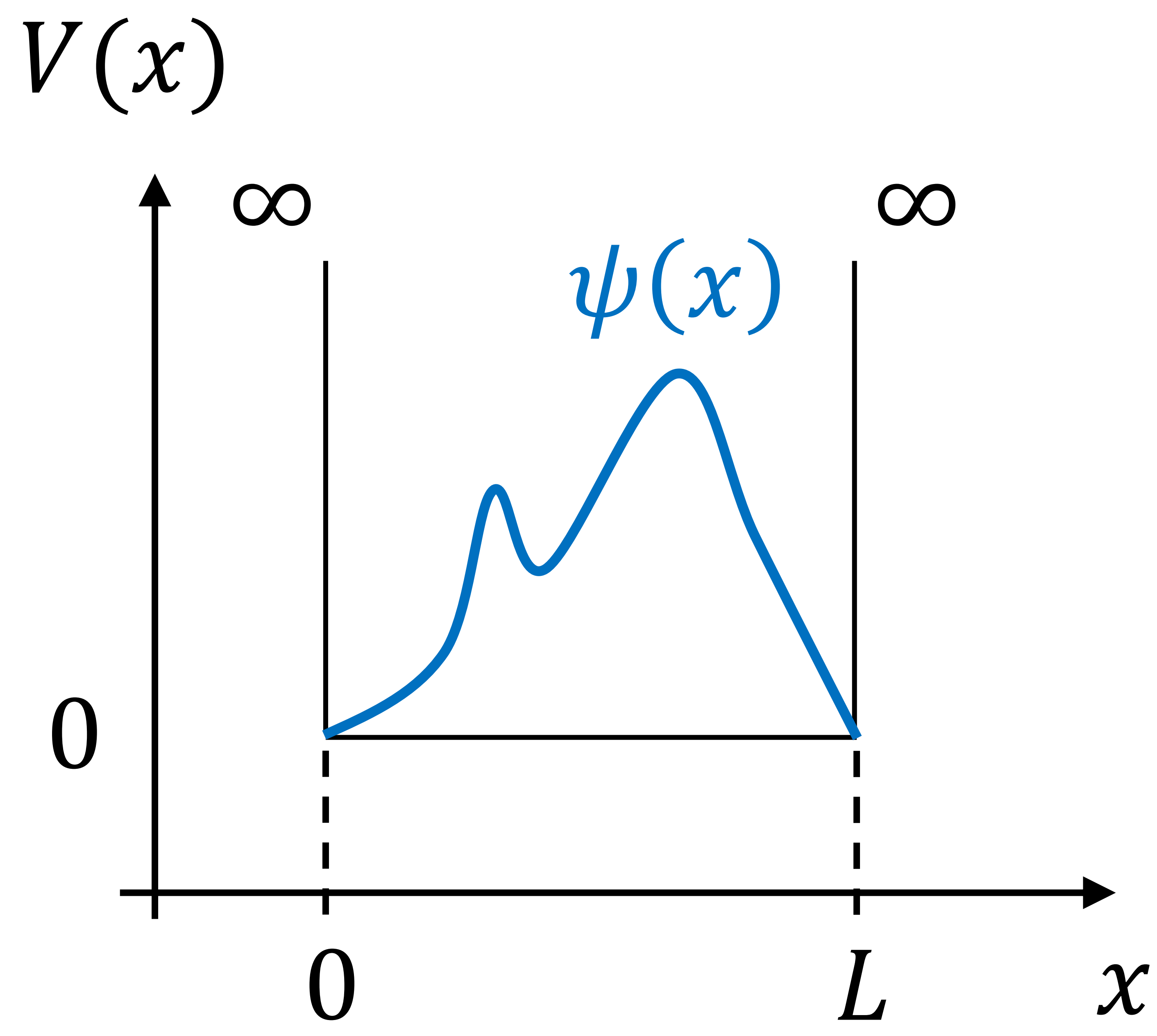

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PARTICLE IN A BOX: WAVE FUNCTION

- Time-independent equation:

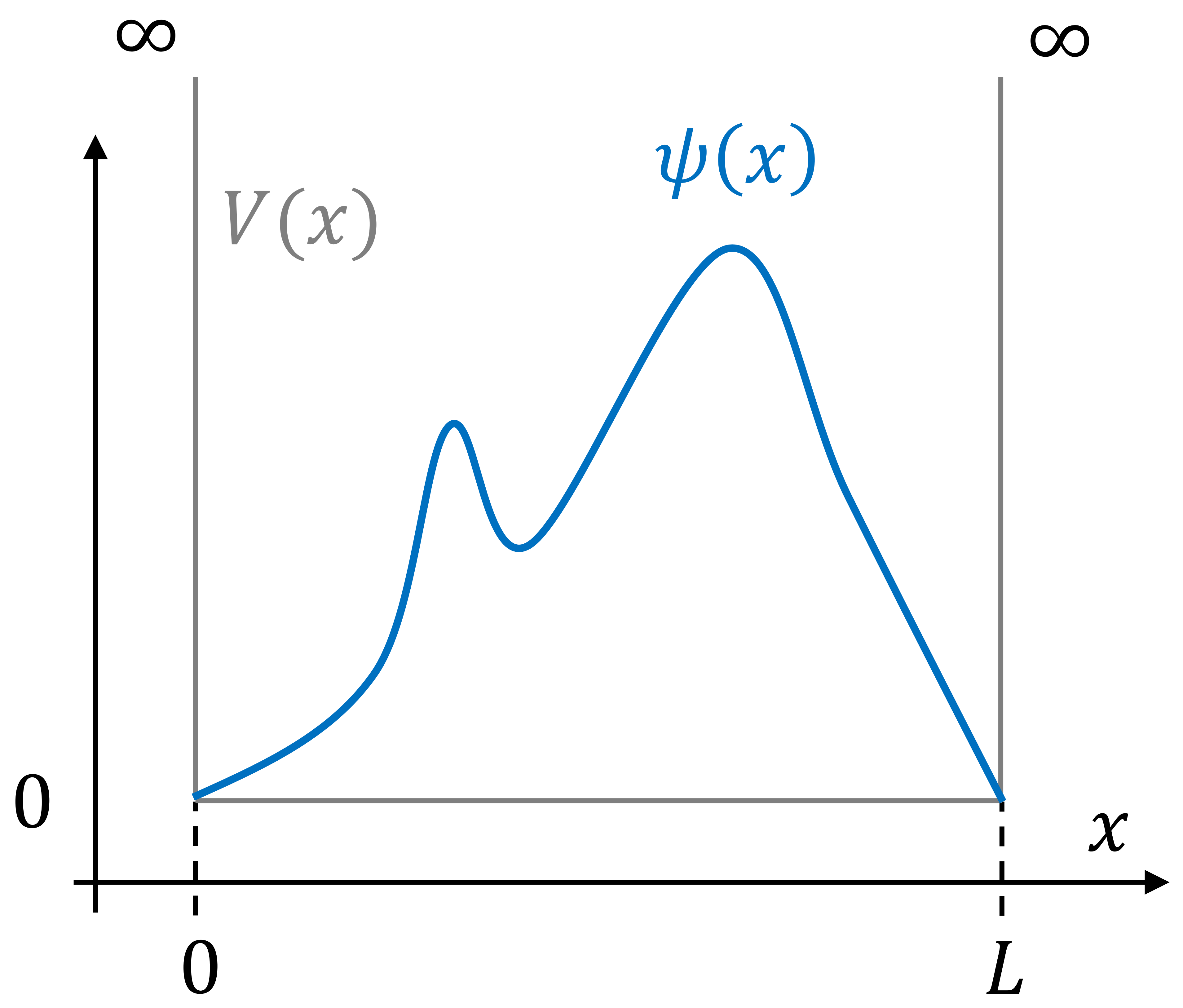
$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial \mathrm{x}^2} + U(x)\,\psi(x) = E\,\psi(x)$$

Inside the box:

$$U(x) = 0 \;\Rightarrow\; -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial \mathrm{x}^2} = E\,\psi(x)$$

Outside box:

$$U(x) = \infty \;\Rightarrow\; \psi(x) = 0$$



PARTICLE IN A BOX: WAVE FUNCTION

- Solution inside the box?

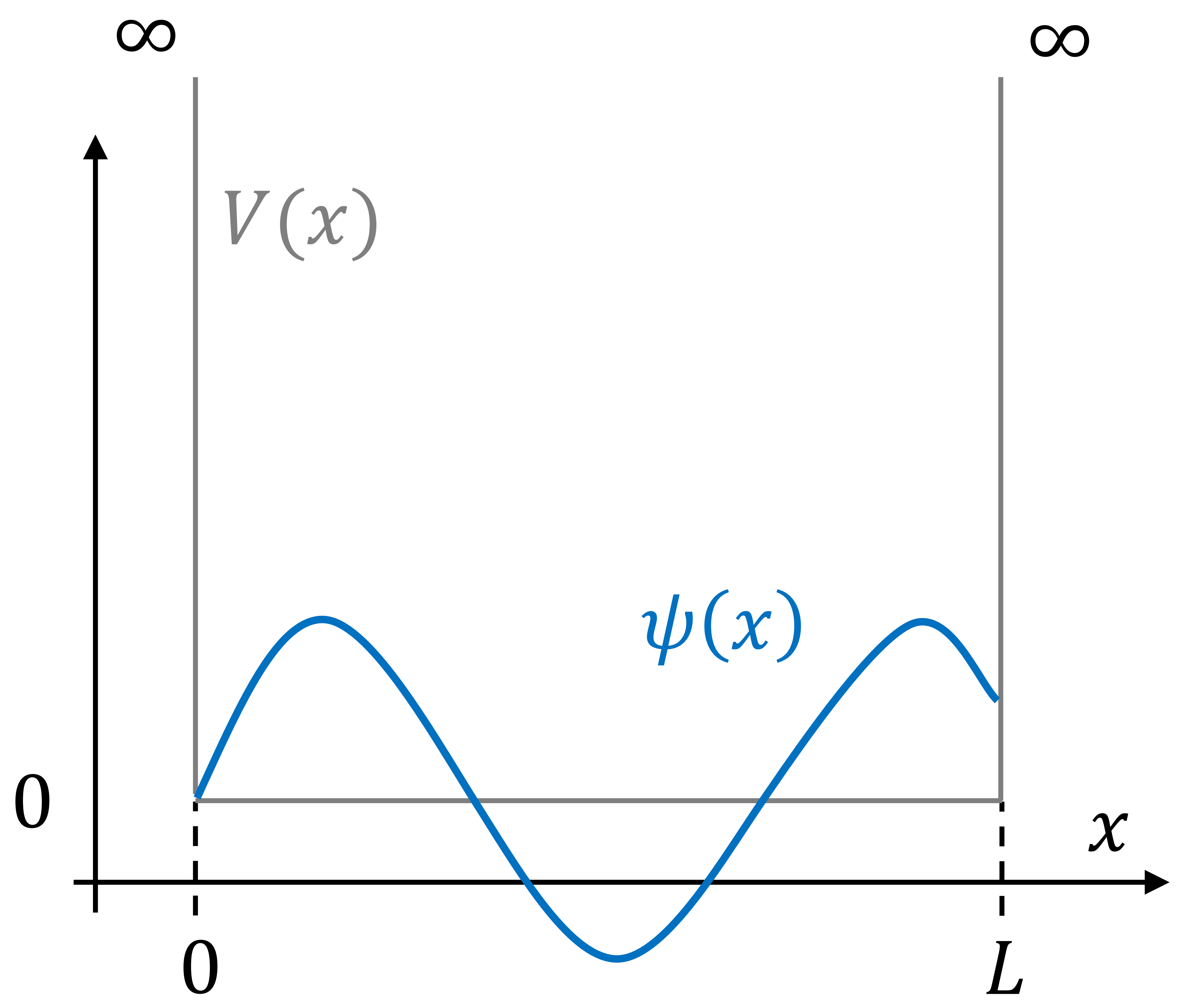
$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} = E\,\psi(x)$$

- Inside ⇨ free particle solution:

$$\psi(x) = A\,e^{ikx}, \qquad E = \frac{\hbar^2 k^2}{2m}$$

Or:

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



PARTICLE IN A BOX: WAVE FUNCTION

- Solution inside the box?

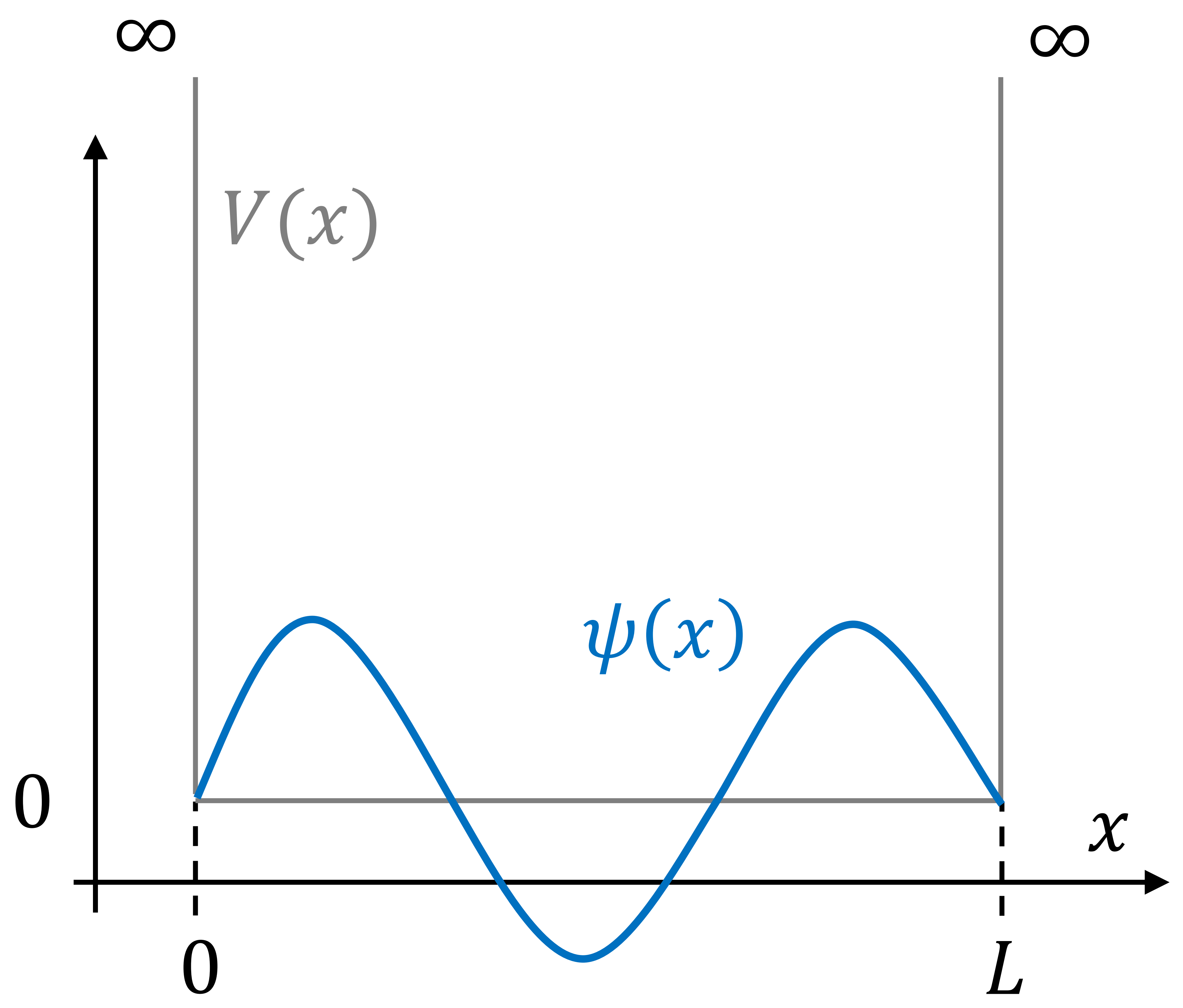
$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} = E\,\psi(x)$$

- Inside ⟹ free particle solution:

$$\begin{cases} \psi(x) = A\sin(kx) + B\cos(kx) \\ E = \dfrac{\hbar^2 k^2}{2m} \end{cases}$$

- Boundary conditions

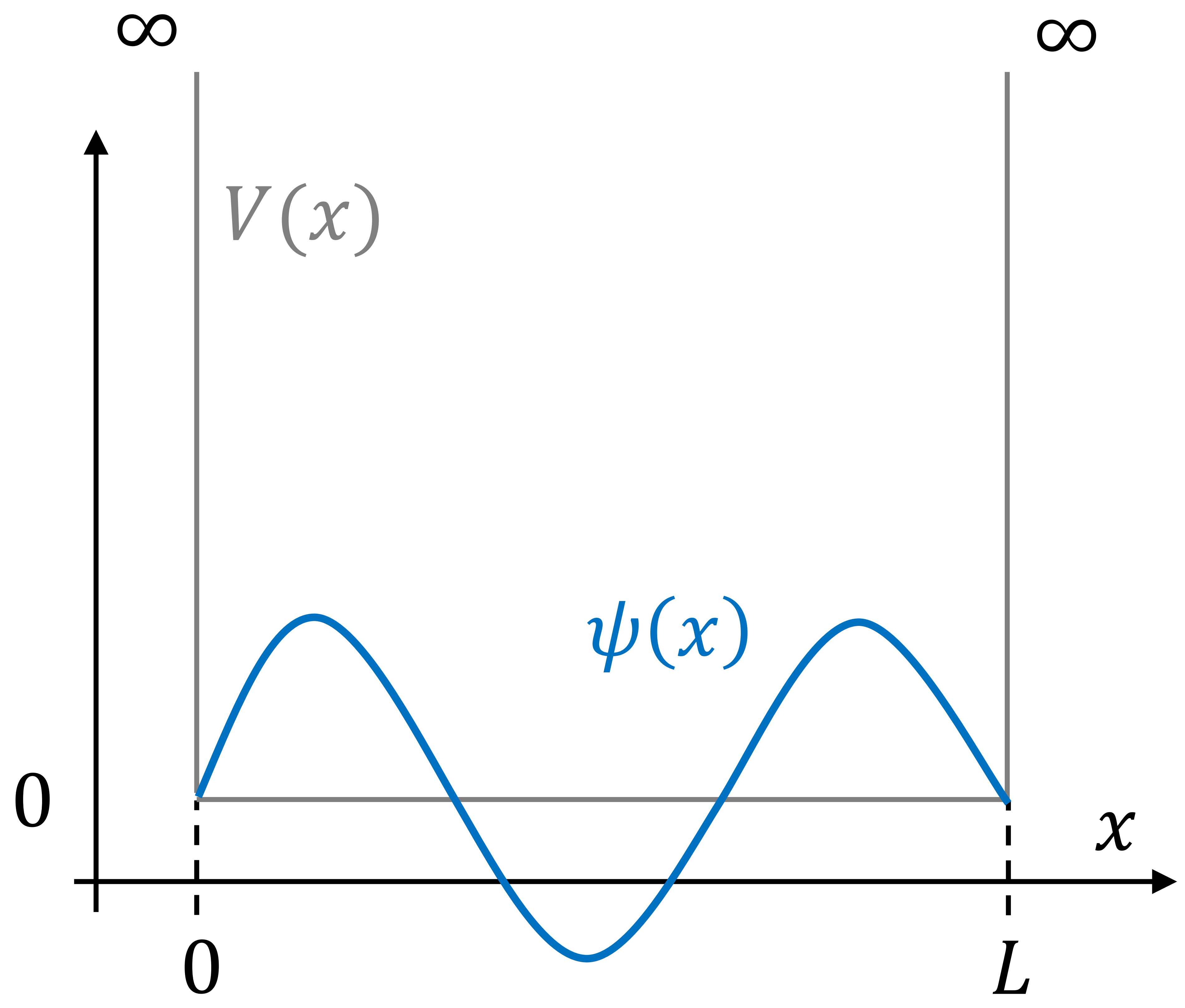
$$\psi(0) = 0 \quad \text{and} \quad \psi(L) = 0$$



PARTICLE IN A BOX: WAVE FUNCTION

- Inside free particle solution:

$$\begin{cases} \psi(x) = A\sin(kx) + B\cos(kx) \\ E = \dfrac{\hbar^2 k^2}{2m} \\ \psi(0) = 0 \quad \text{and} \quad \psi(L) = 0 \end{cases}$$



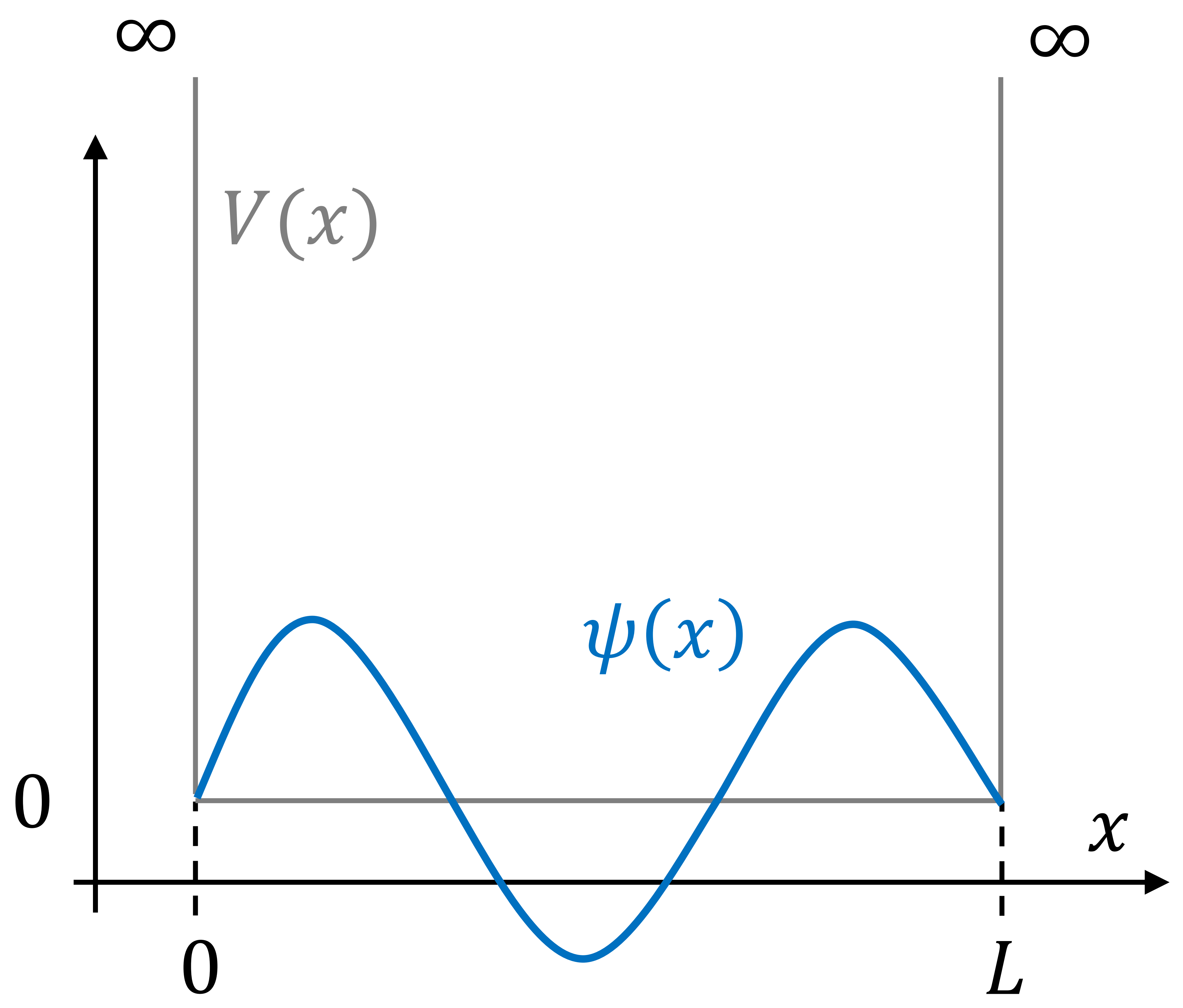
PARTICLE IN A BOX: WAVE FUNCTION

- Inside free particle solution:

$$\begin{cases} \psi(x) = A\sin(kx) + \cancel{B\cos(kx)} \\ E = \dfrac{\hbar^2 k^2}{2m} \\ \psi(0) = 0 \quad \text{and} \quad \psi(L) = 0 \end{cases}$$

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

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



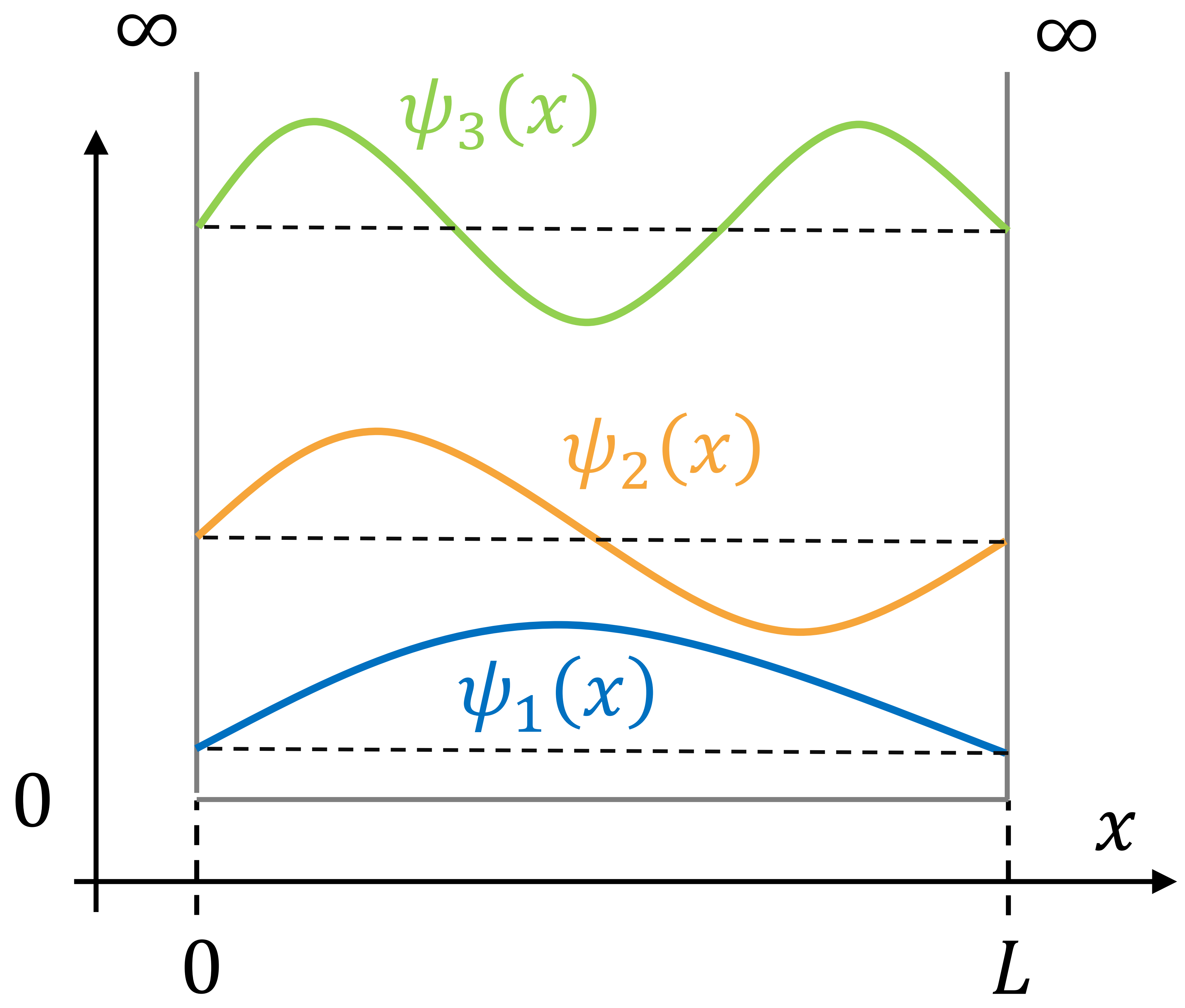
PARTICLE IN A BOX: WAVE FUNCTION

- Inside free particle solution:

$$\begin{cases} \psi(x) = A\sin(kx) \\ E = \dfrac{\hbar^2 k^2}{2m} \\ \psi(0) = 0 \quad \text{and} \quad \psi(L) = 0 \end{cases}$$

$$\Rightarrow \quad \psi_n(L) = A_n \sin(k_n L) = 0$$

$$k_n = \frac{n\pi}{L}, \qquad E_n = \frac{\hbar^2 k_n^2}{2m}$$



PARTICLE IN A BOX: WAVE FUNCTION

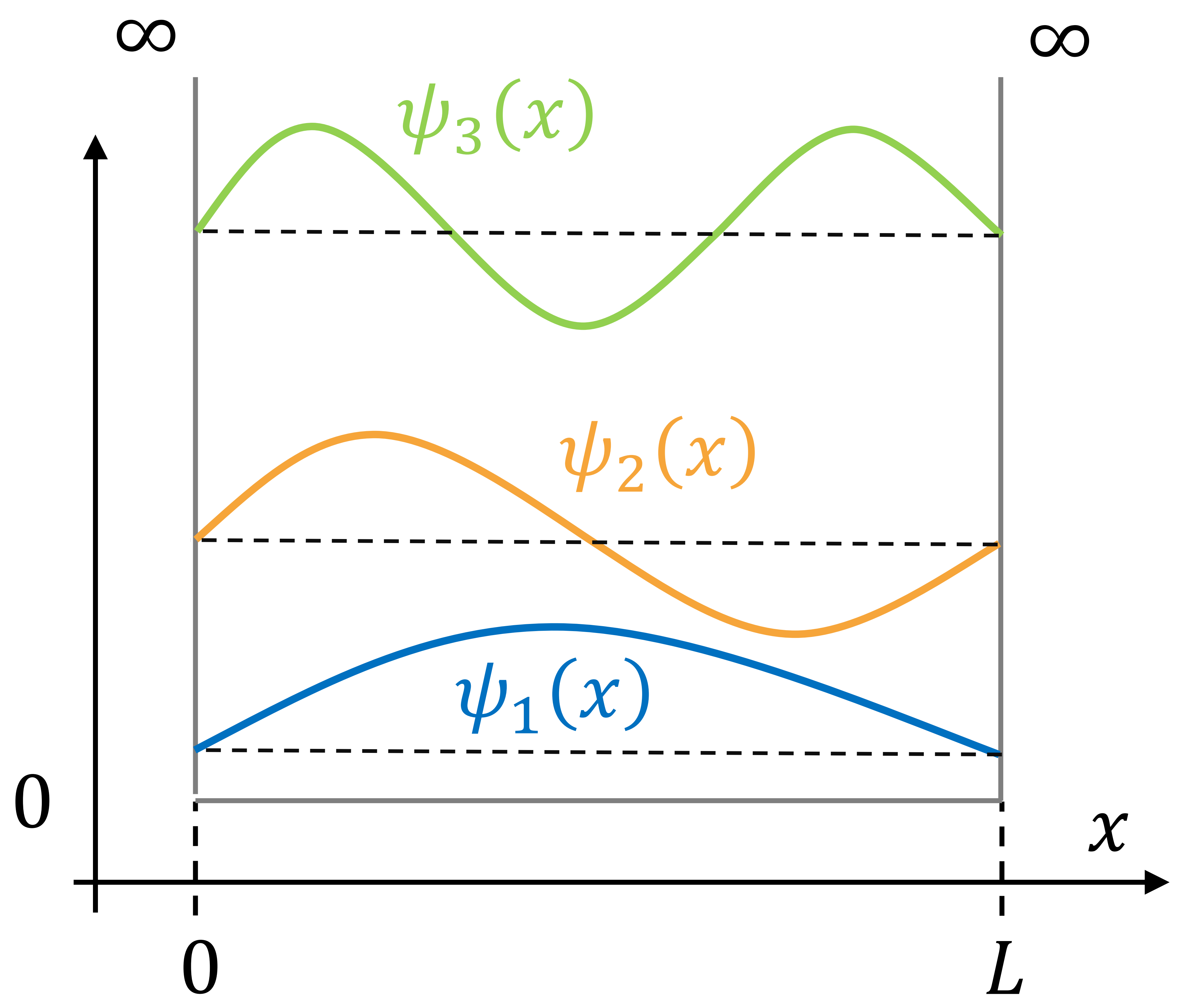
- Solutions:

$$\begin{cases} \psi_n(x) = A_n \sin(k_n x) = 0 \\ k_n = \dfrac{n\pi}{L}, \qquad E_n = \dfrac{\hbar^2 k_n^2}{2m} \end{cases}$$

- Normalization constant $A_n = ?$

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

$$\Rightarrow \quad A_n = \sqrt{\frac{2}{L}}$$



PARTICLE IN A BOX: SOLUTIONS

Wave function solutions

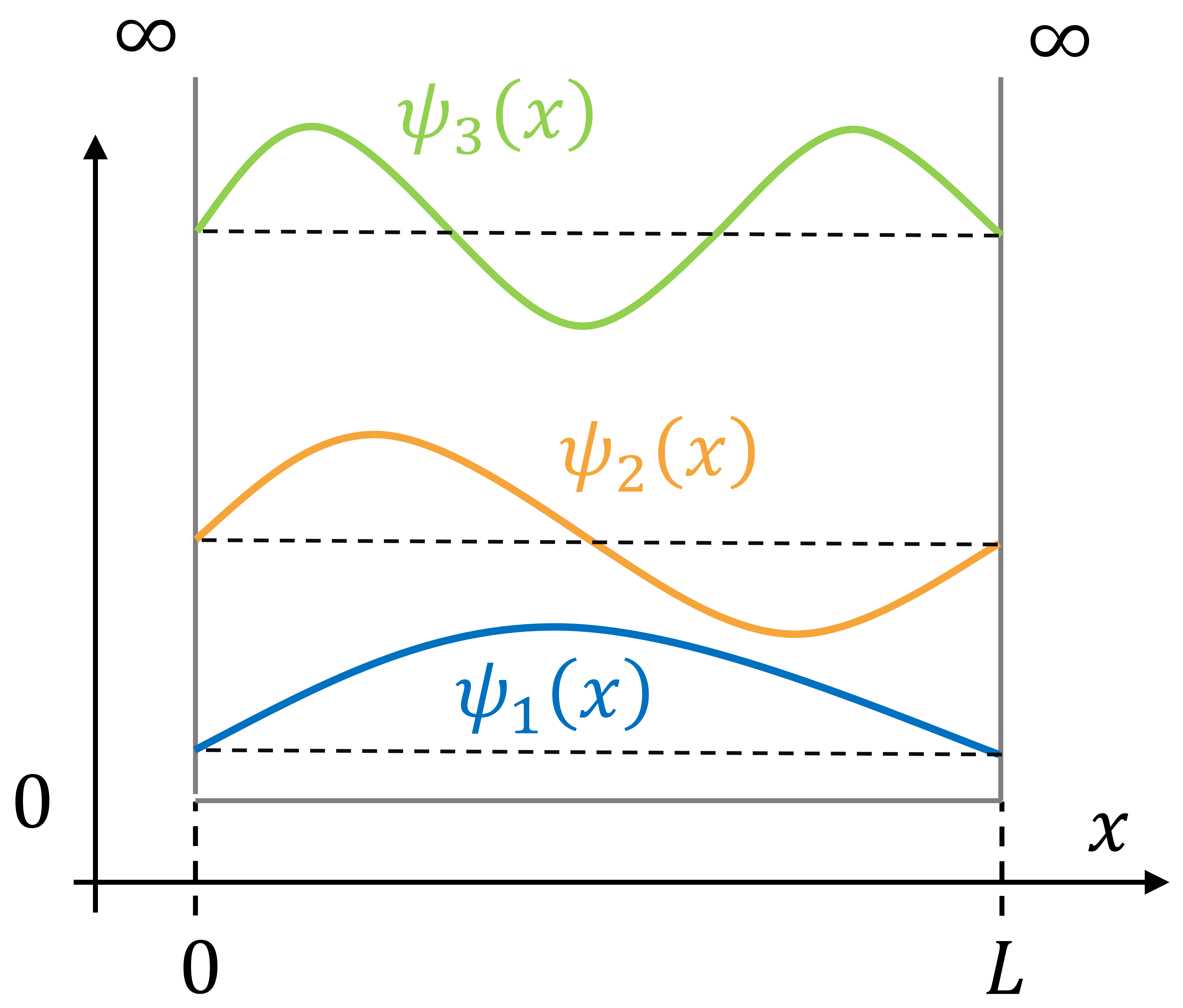
$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x)$$

Wave number

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

Energy

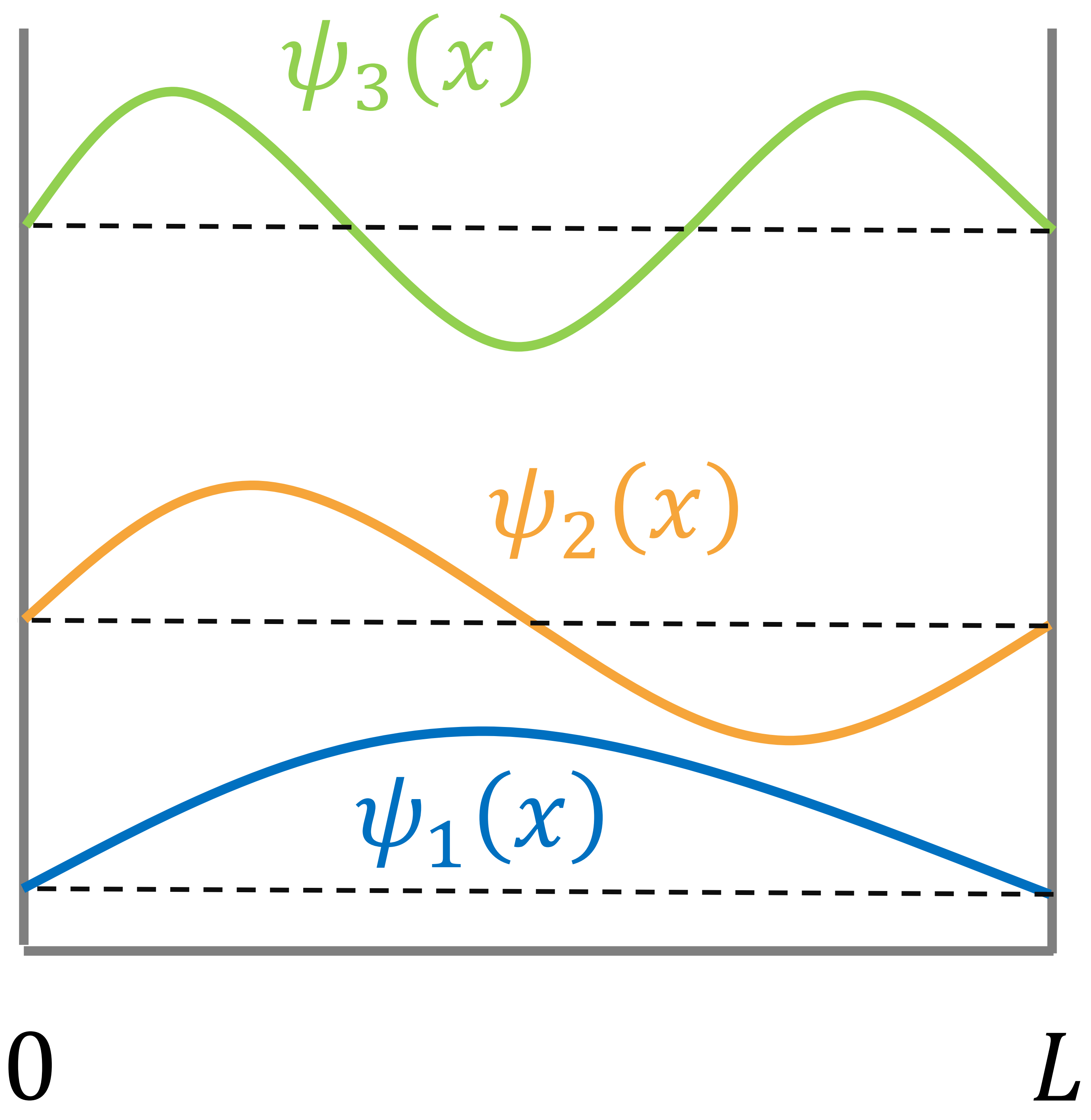
$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

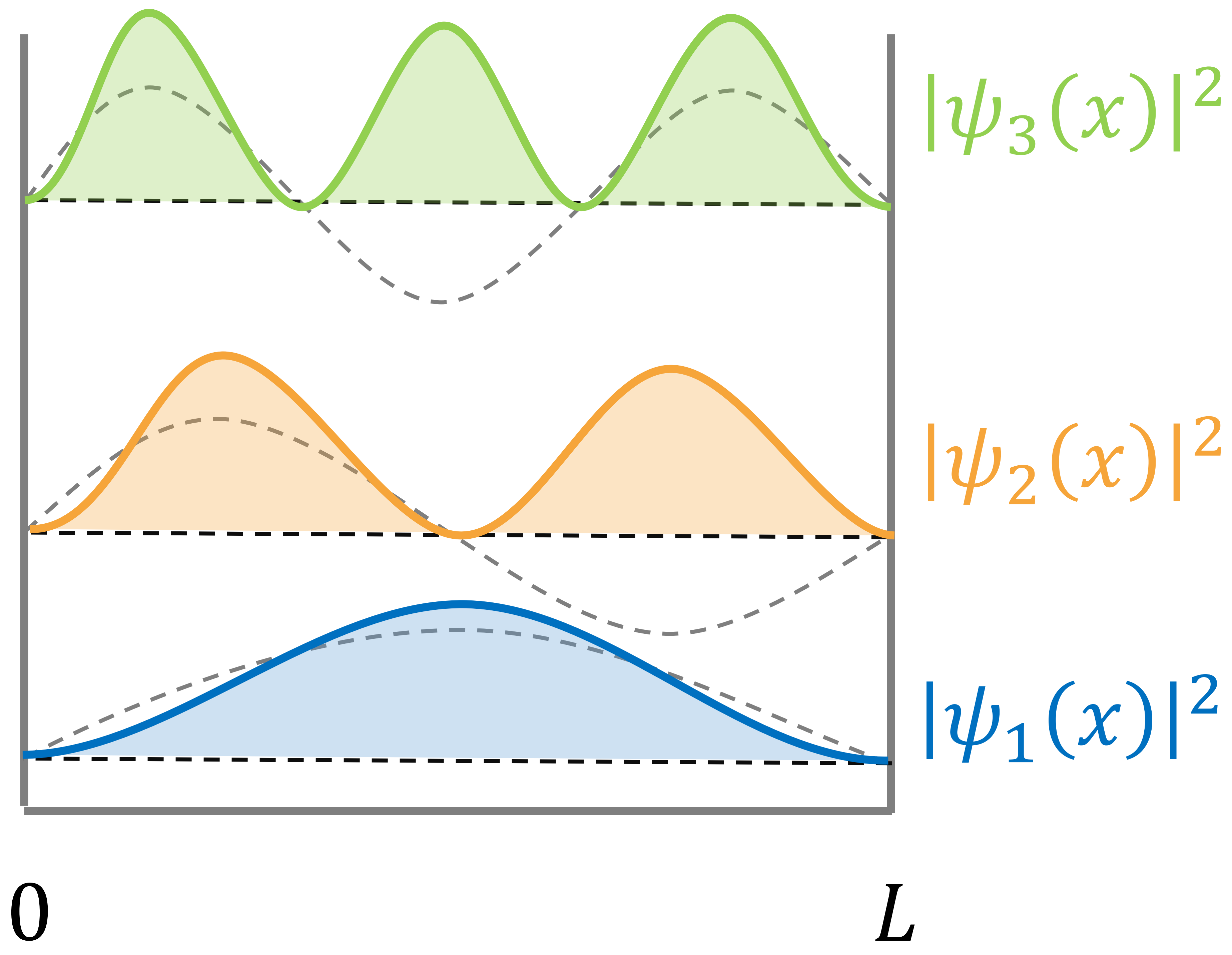


PARTICLE IN A BOX: SOLUTIONS

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

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

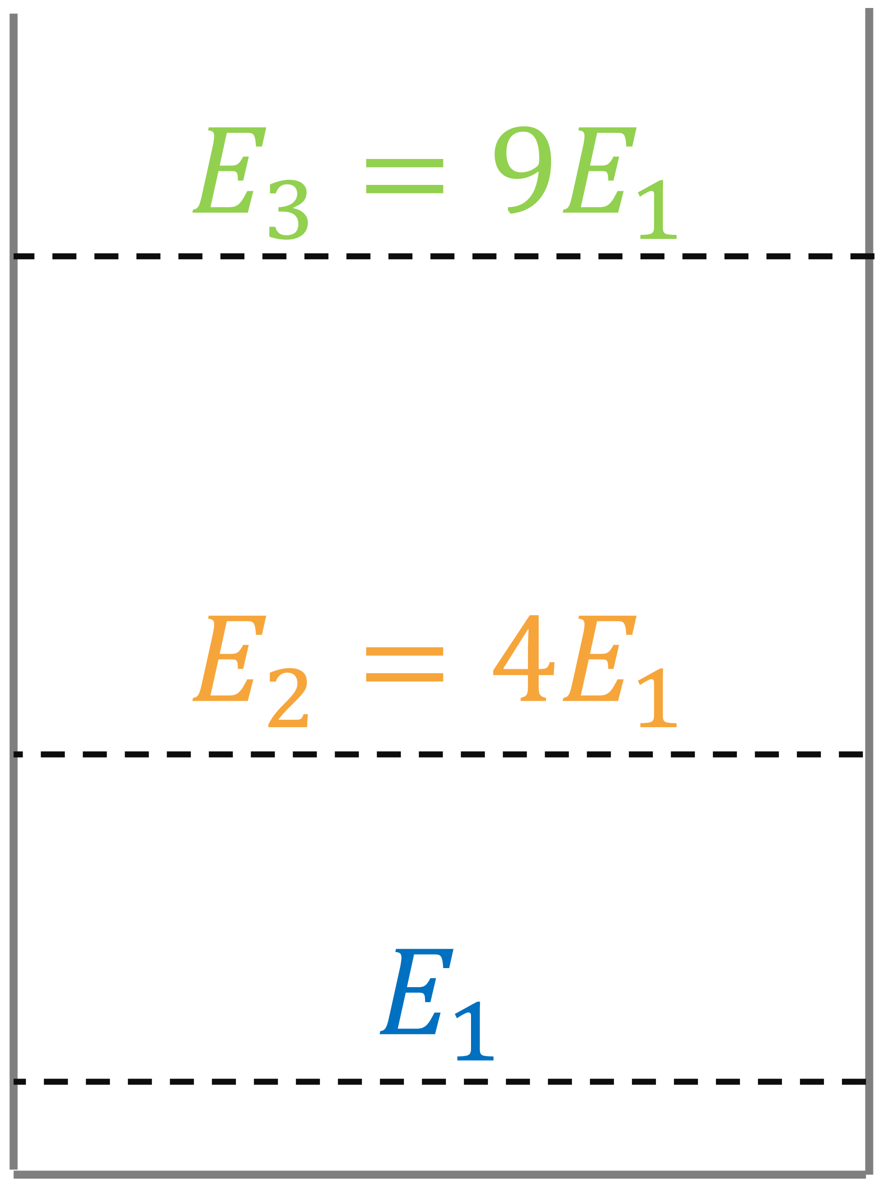




PARTICLE IN A BOX: ENERGIES

Energy-levels proportional with n^2

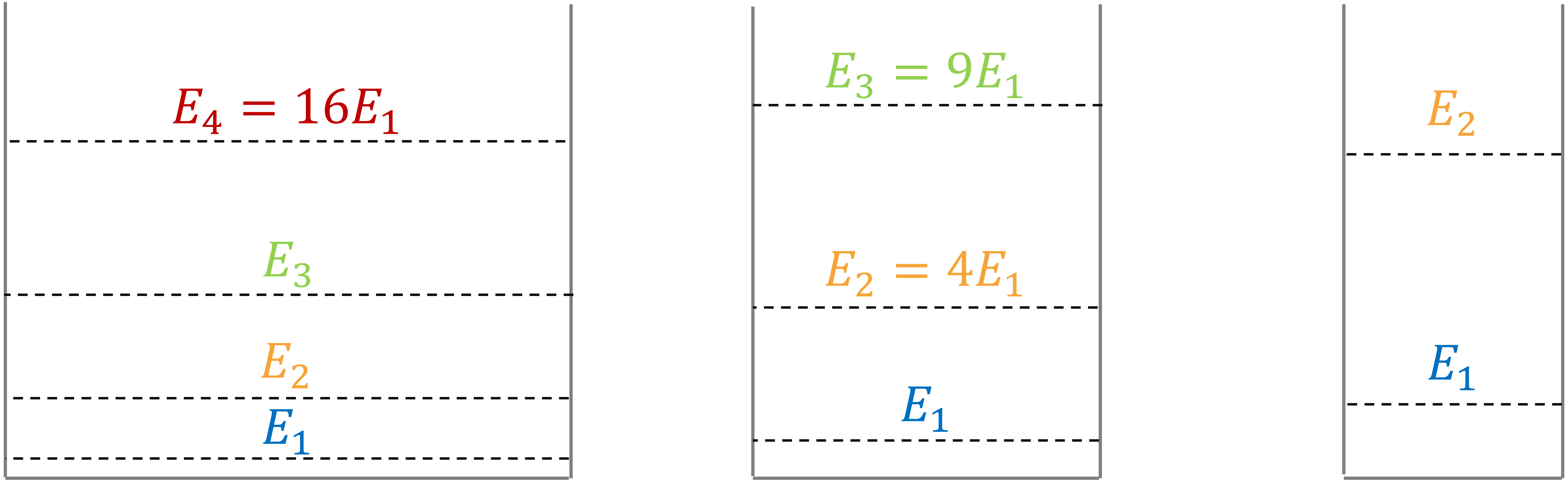
$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}, \qquad E_1 = \frac{\hbar^2 \pi^2}{2mL^2}, \qquad E_n = n^2 E_1$$



PARTICLE IN A BOX: ENERGIES

Energy-levels proportional with $\frac{1}{L^2}$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}, \qquad E_1 = \frac{\hbar^2 \pi^2}{2mL^2}, \qquad E_n = n^2 E_1$$

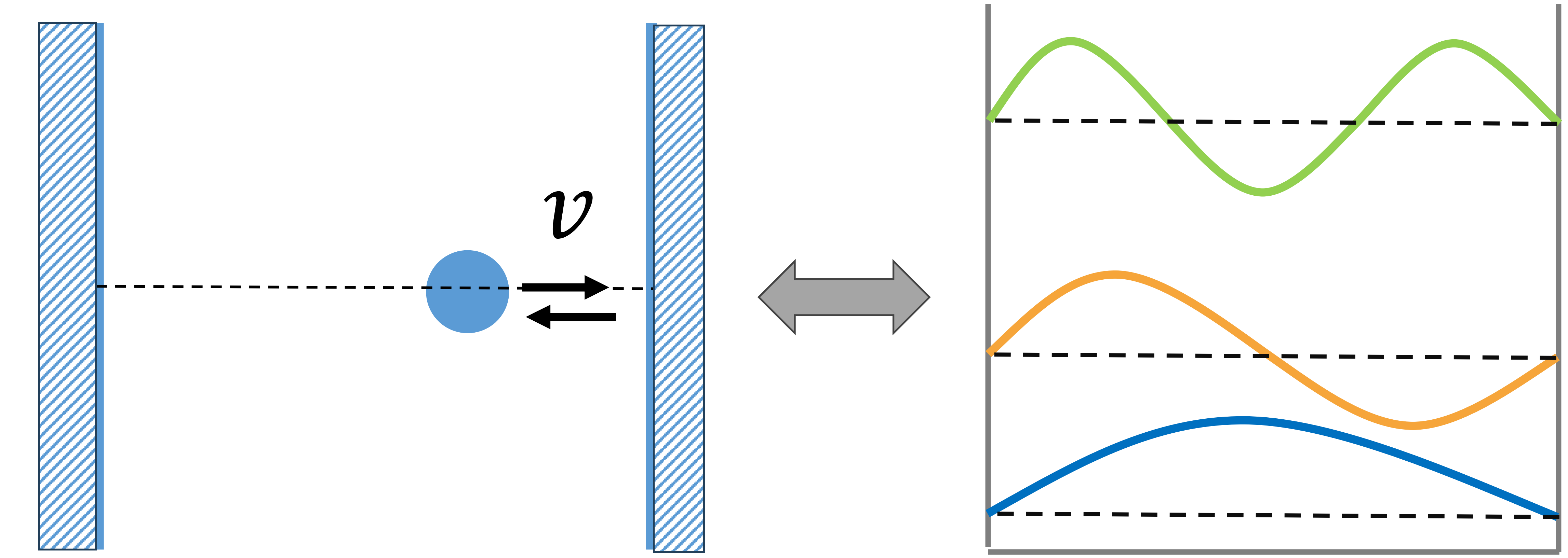


PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

- 1924: De Broglie: particle-wave duality

De Broglie momentum: $p = \frac{h}{\lambda}$

De Broglie energy: $E = \hbar\omega$

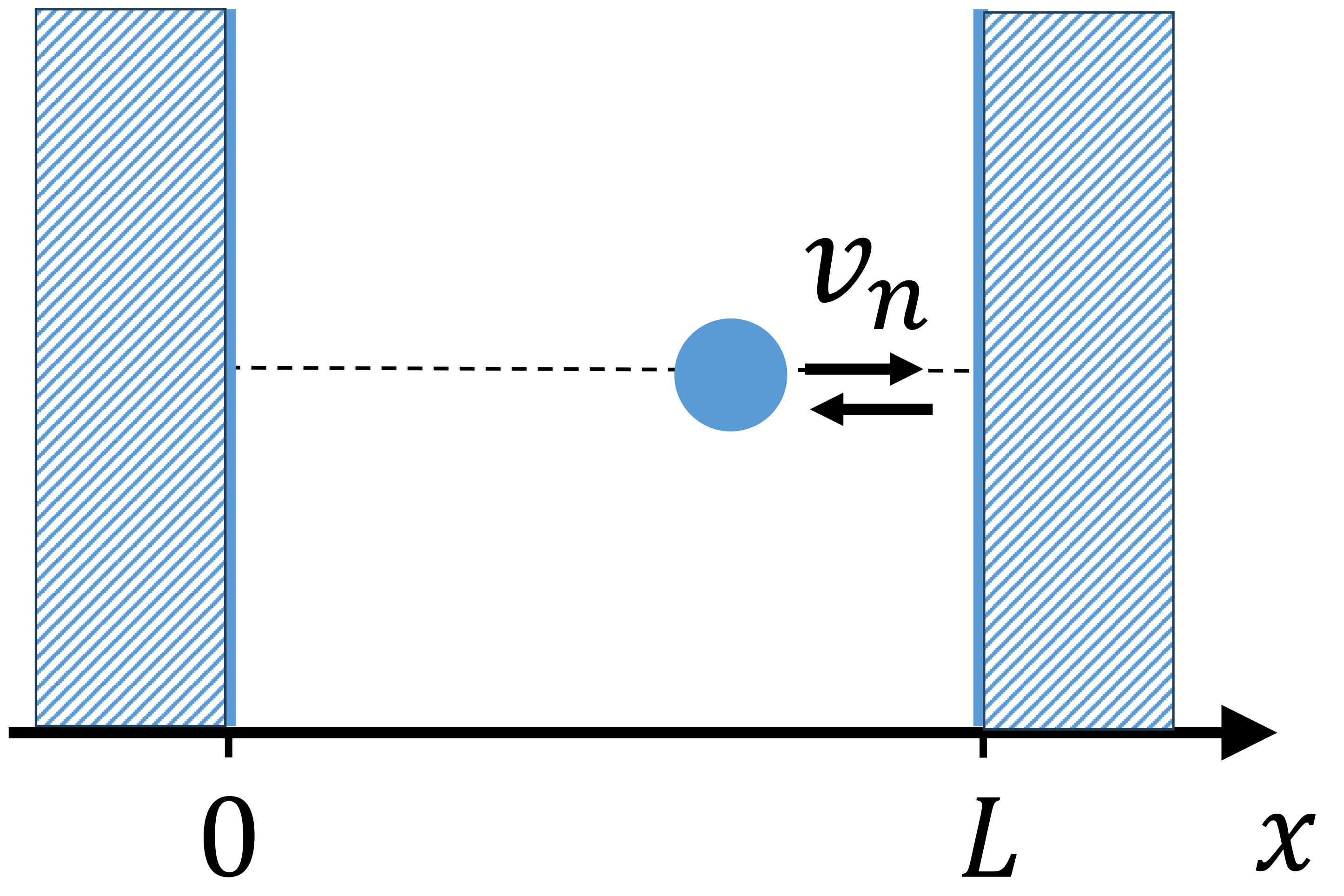


(Duke) Louis de Broglie

Picture from Wikipedia

PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

Energy	wave number	wavelength
$E_n = \dfrac{\hbar^2 k_n^2}{2m}$,	$k_n = \dfrac{n\pi}{L}$,	$\lambda_n = \dfrac{2\pi}{k_n} = \dfrac{2L}{n}$

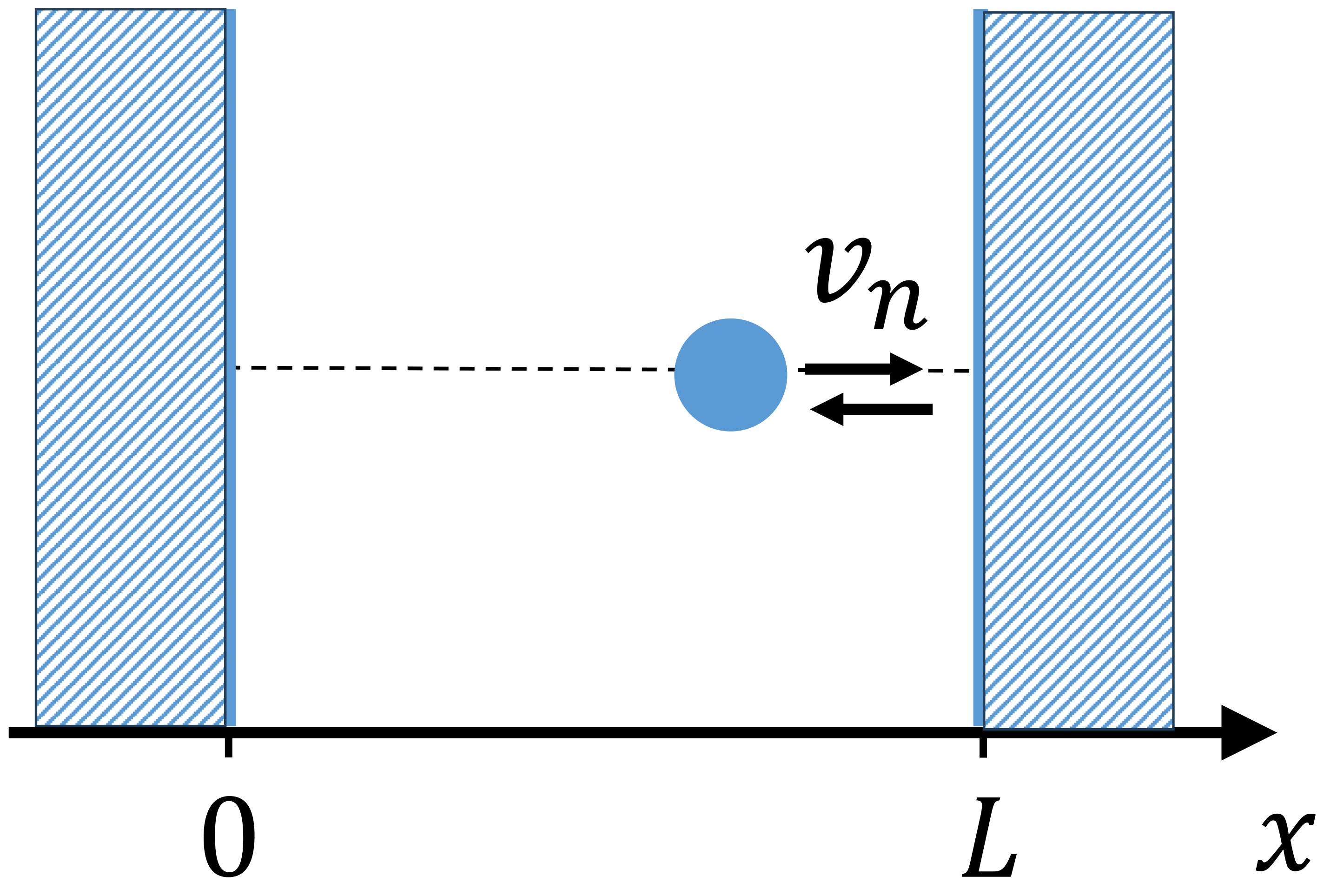


$$p_n = \frac{h}{\lambda_n} \Rightarrow p_n = \hbar k_n$$ **de Broglie momentum**

$$E_n = \hbar\omega \Rightarrow E_n = \frac{p_n^2}{2m} = \frac{1}{2} m v_n^2$$ **de Broglie energy**

PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

$$\begin{cases} p_n = \dfrac{h}{\lambda_n} \quad \Rightarrow \quad p_n = \hbar k_n = \dfrac{\hbar n \pi}{L} \\ \Downarrow \\ E_n = \hbar\omega \quad \Rightarrow \quad E_n = \dfrac{p_n^2}{2m} = \dfrac{1}{2} m v_n^2 \end{cases}$$



- Minimum momentum/speed: $v_1 = \dfrac{p_1}{m} = \dfrac{\hbar\pi}{mL}$
- Discontinuous energy spectrum, velocity jumps? $E_n = \dfrac{\hbar^2\pi^2 n^2}{2mL^2} = \dfrac{p_n^2}{2m} = \dfrac{1}{2} m v_n^2$

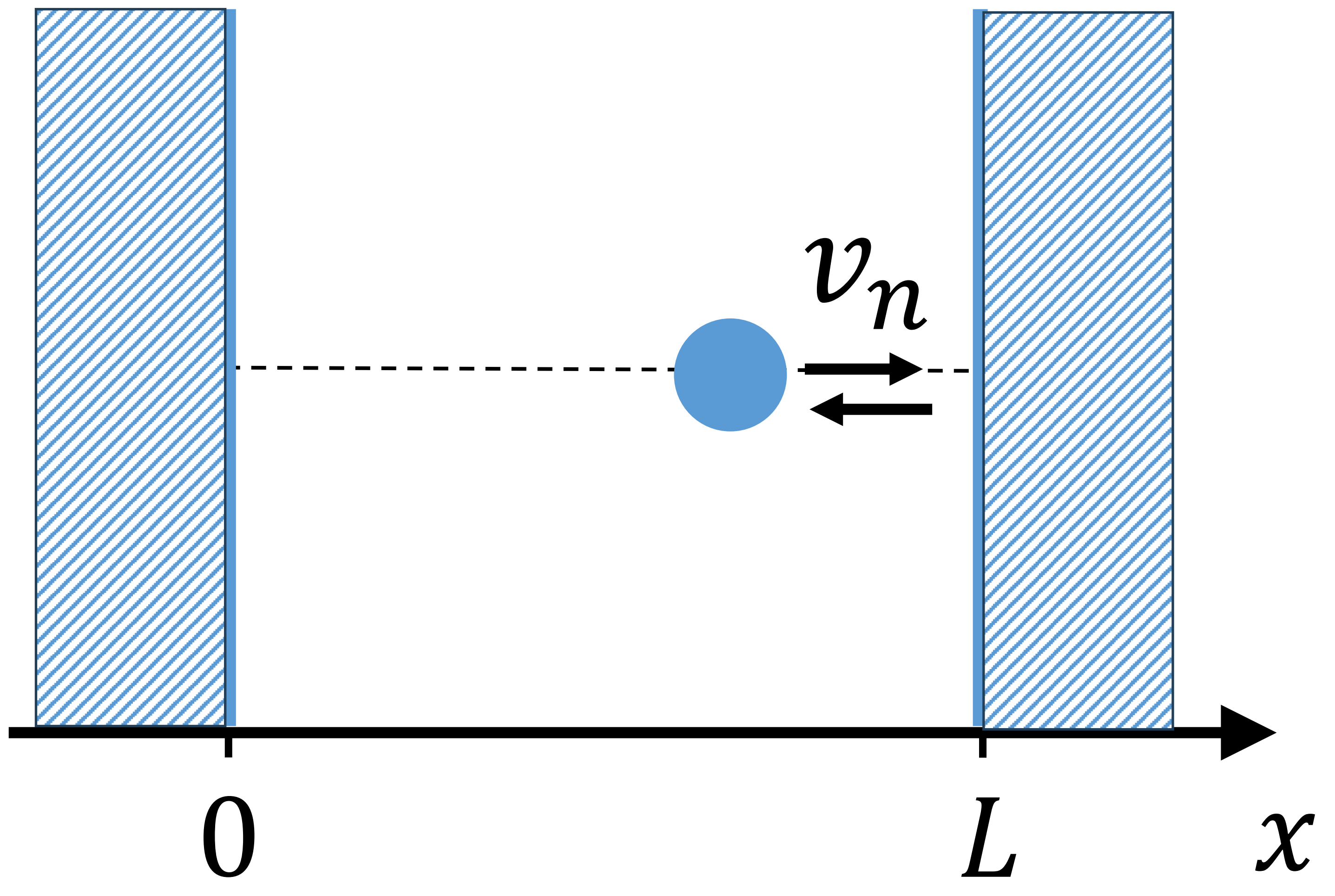
PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

$$\begin{cases} p_n = \dfrac{h}{\lambda_n} \\[2em] E_n = \hbar\omega \end{cases}$$

$$p_n = \frac{h}{\lambda_n} \Rightarrow p_n = \hbar k_n = \frac{\hbar n\pi}{L}$$

$$\Downarrow$$

$$E_n = \hbar\omega \Rightarrow E_n = \frac{p_n^2}{2m} = \frac{1}{2}mv_n^2$$



Minimum momentum/speed:

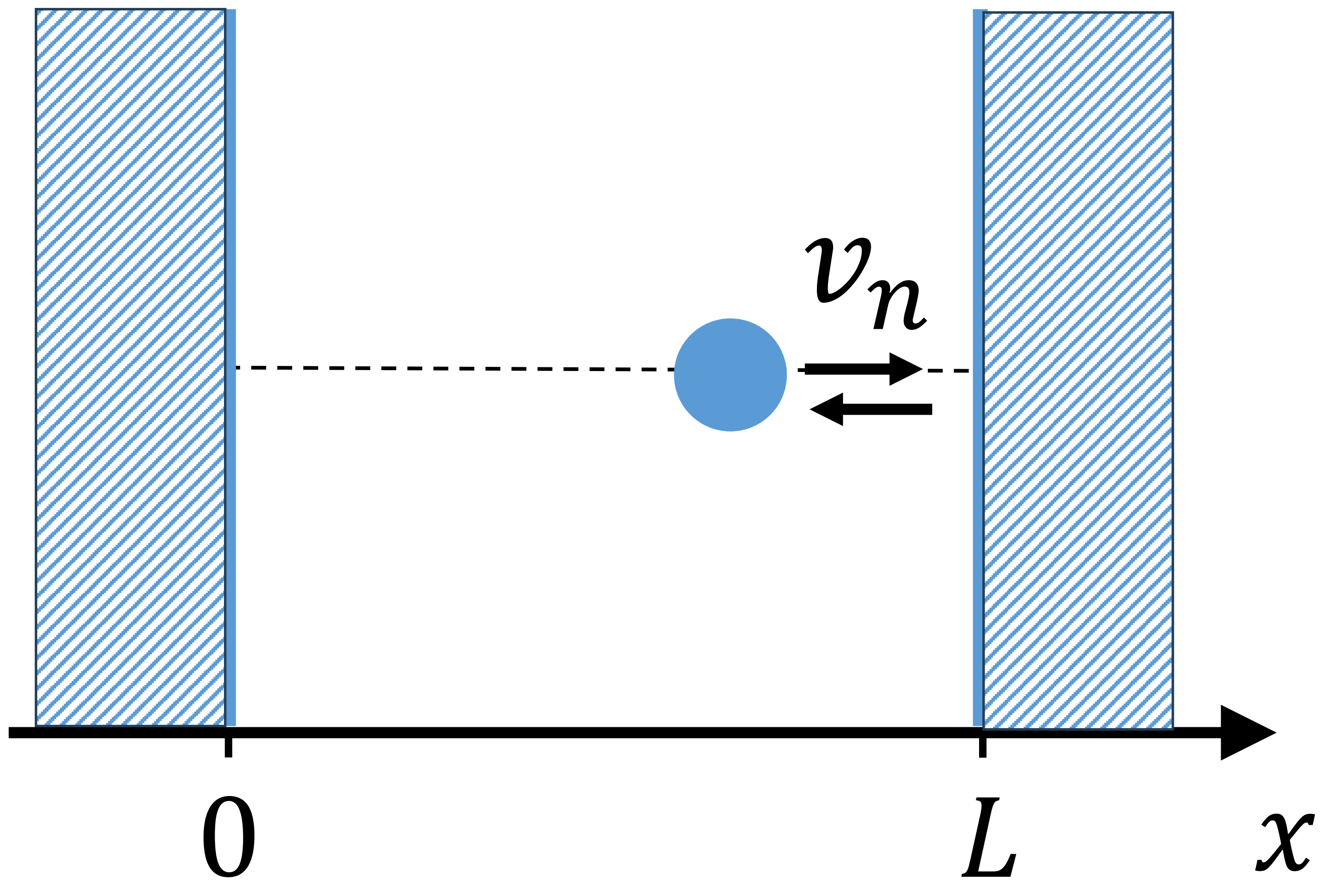
Electron in box size 0.2 nm:

$$\boldsymbol{v_1} = \frac{p_1}{m} = \frac{\hbar\pi}{mL} = \frac{6.63\times10^{-34}\ \mathrm{J\cdot s}}{2\cdot 9.11\times10^{-31}\ \mathrm{kg}\cdot 0.2\times10^{-9}\ \mathrm{m}}$$

$$\approx \frac{33}{18}\times10^{6}\ \mathrm{m/s} \approx \boldsymbol{2\times10^{6}\ \mathrm{m/s}}$$

PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

$$\begin{cases} p_n = \dfrac{h}{\lambda_n} & \Rightarrow \quad p_n = \hbar k_n = \dfrac{\hbar n \pi}{L} \\ & \Downarrow \\ E_n = \hbar\omega & \Rightarrow \quad E_n = \dfrac{p_n^2}{2m} = \dfrac{1}{2} m v_n^2 \end{cases}$$



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Tennisball in box size 20 m:
(0.05 kg)

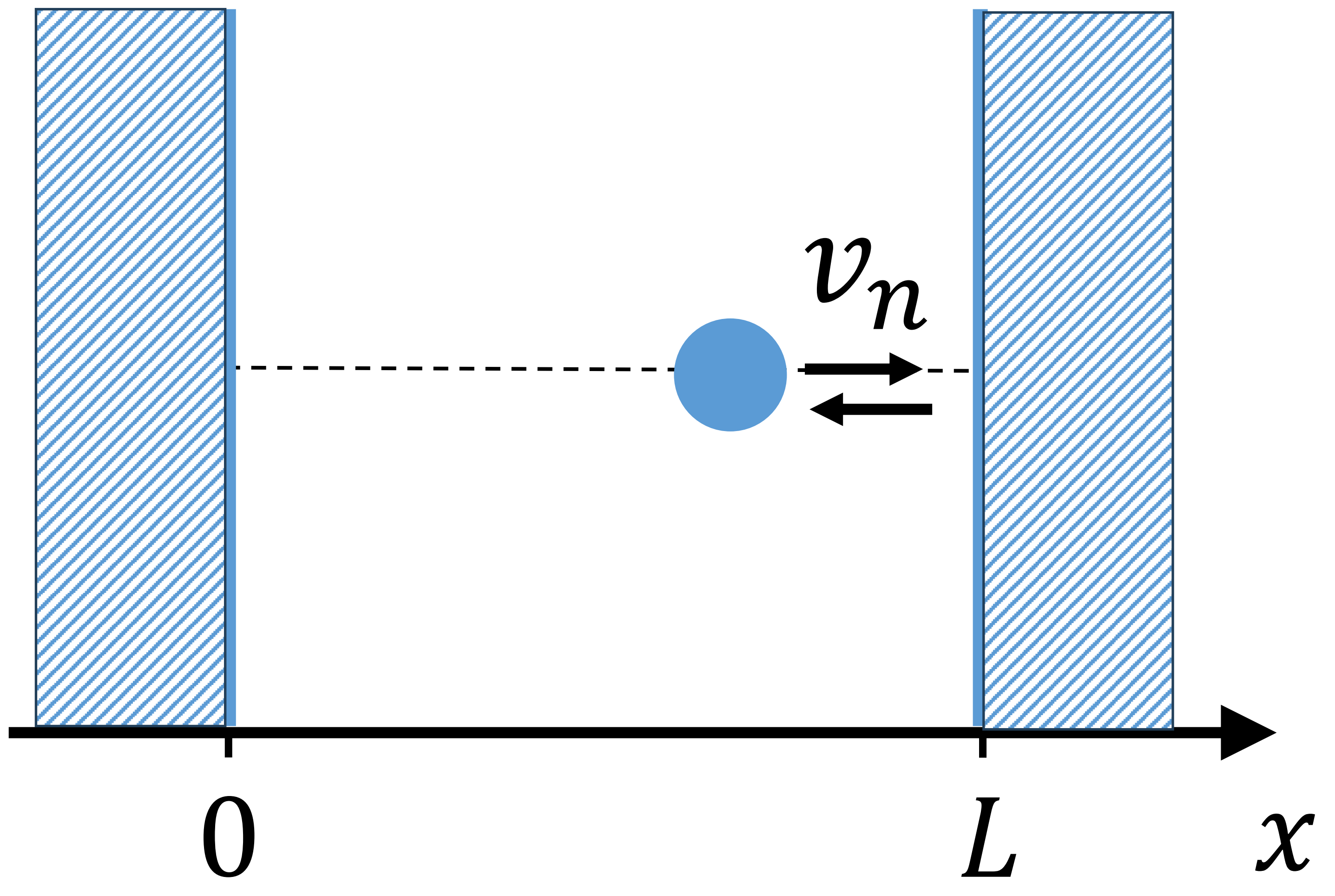
$$\boldsymbol{v_1} = \frac{p_1}{m} = \frac{\hbar\pi}{mL} = \frac{6.63 \times 10^{-34}\ \mathrm{J \cdot s}}{2 \cdot 0.05\ \mathrm{kg} \cdot 20\ \mathrm{m}} \approx \mathbf{3.3 \times 10^{-34}\ \frac{m}{s}}$$

PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

$$\begin{cases} p_n = \dfrac{h}{\lambda_n} \\ E_n = \hbar\omega \end{cases}$$

$$p_n = \frac{h}{\lambda_n} \Rightarrow p_n = \hbar k_n = \frac{\hbar n \pi}{L}$$

$$E_n = \hbar\omega \Rightarrow E_n = \frac{p_n^2}{2m} = \frac{1}{2} m v_n^2$$



Energy jumps:

Electron in box size 0.2 nm:

$$\boldsymbol{E_n} = \frac{\hbar^2\pi^2 n^2}{2mL^2} = \frac{(6.63 \times 10^{-34}\ \mathrm{J \cdot s})^2}{8 \cdot 9.11 \times 10^{-31}\ \mathrm{kg} \cdot (2 \times 10^{-10}\ \mathrm{m})^2}$$

$$\approx \frac{10}{73} \times 10^{-17}\ \mathrm{J} \approx \frac{1.5 \times 10^{-18}}{1.6 \times 10^{-19}}\ \mathrm{eV} \approx \mathbf{9.4\ eV}$$

PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

$$p_n = \frac{h}{\lambda_n} \Rightarrow p_n = \hbar k_n = \frac{\hbar n \pi}{L}$$

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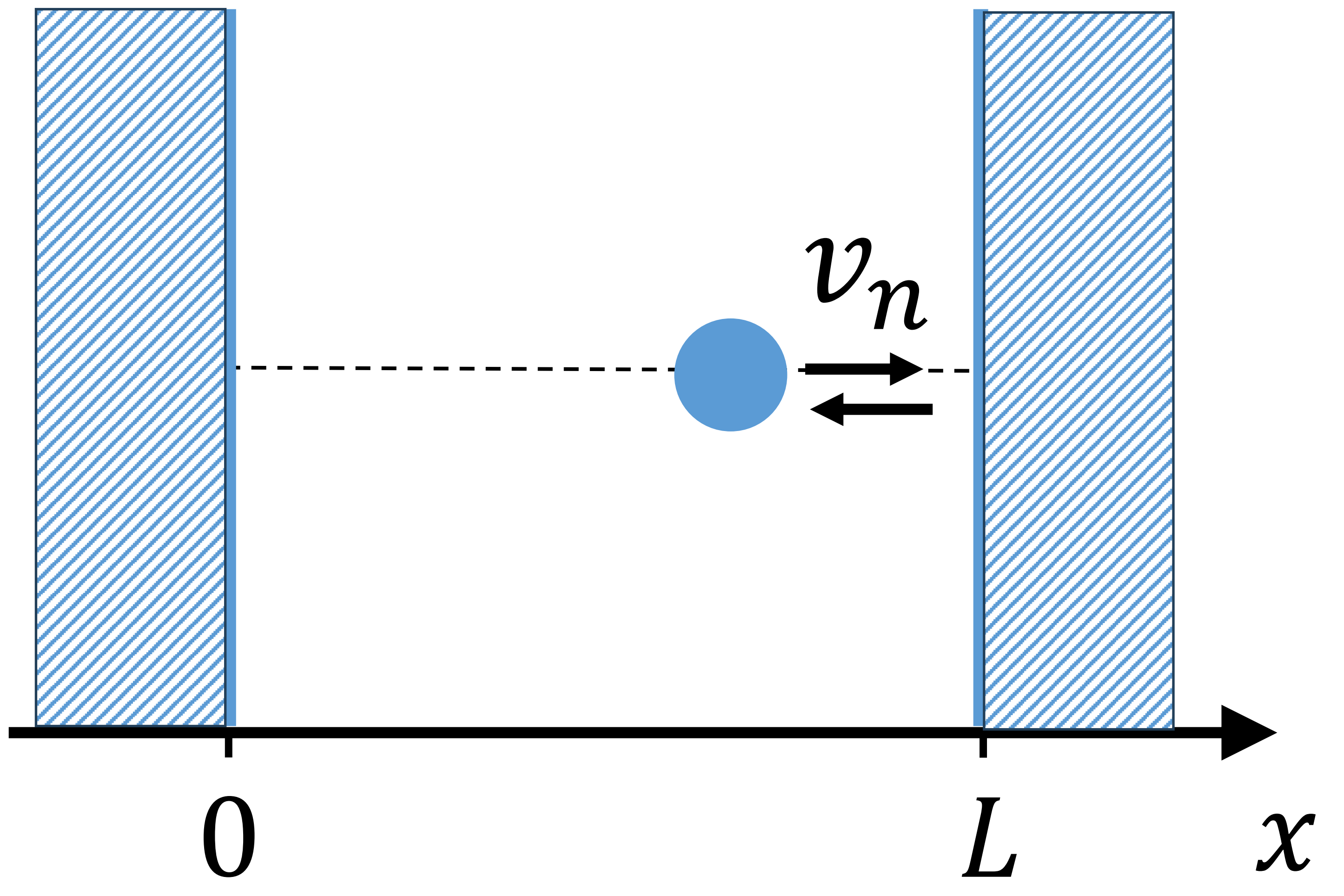

Energy jumps:

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Tennisball in box size 20 m:
(0.05 kg)

$$\boldsymbol{E_1} = \frac{\hbar^2\pi^2 n^2}{2mL^2} = \frac{(6.63 \times 10^{-34}\ \mathrm{J \cdot s})^2}{8 \cdot 0.05\ \mathrm{kg} \cdot 400\ \mathrm{m}} \approx \frac{2.7 \times 10^{-35}}{1.6 \times 10^{-19}}\ \mathrm{eV}$$

$$\approx \mathbf{1.7 \times 10^{-15}\ eV}$$

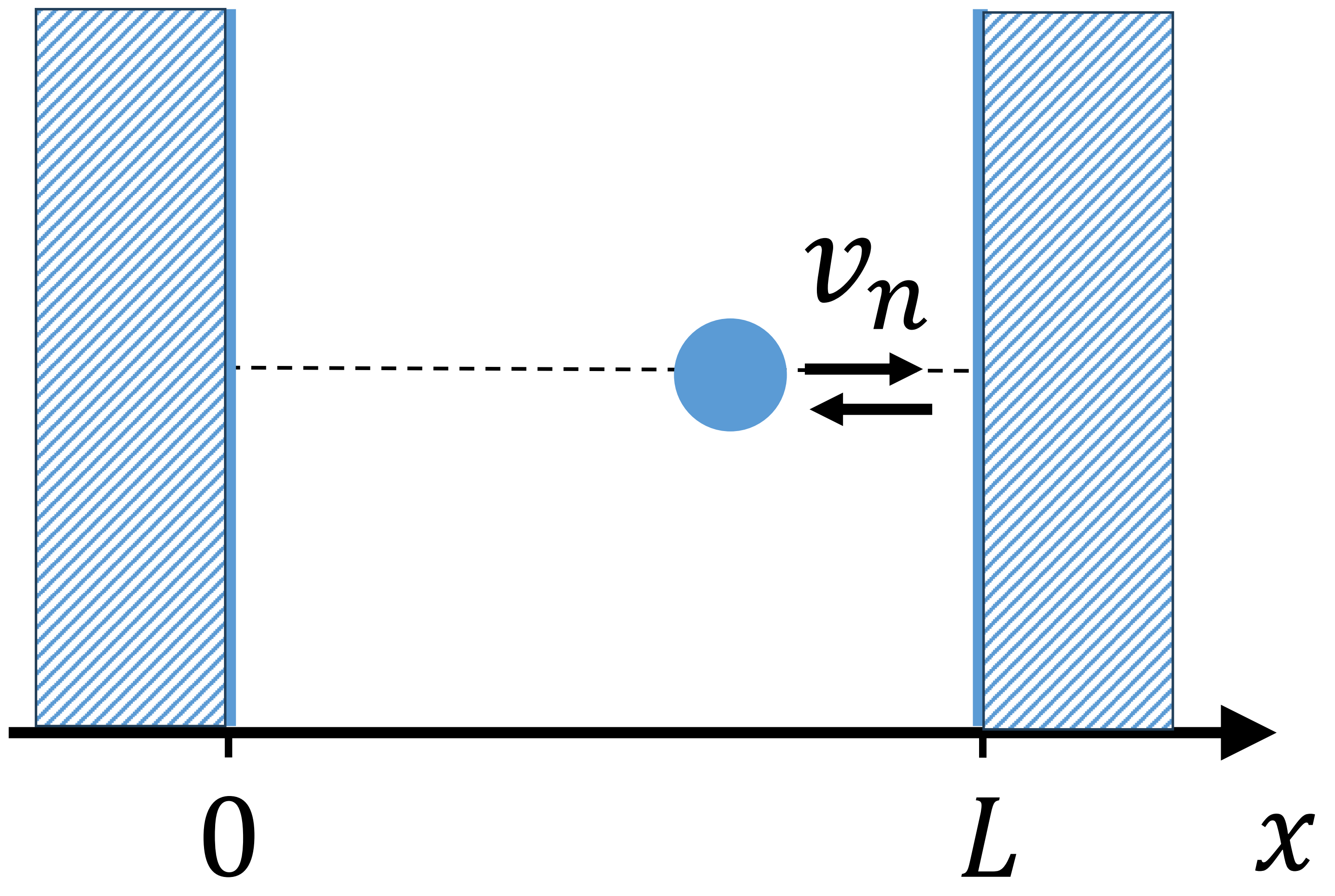
PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

$$\begin{cases} p_n = \dfrac{h}{\lambda_n} \\[2ex] E_n = \hbar\omega \end{cases}$$

$$\Rightarrow \quad p_n = \hbar k_n = \frac{\hbar n \pi}{L}$$

$$\Downarrow$$

$$\Rightarrow \quad E_n = \frac{p_n^2}{2m} = \frac{1}{2} m v_n^2$$



- **Quantum size effects** due **confinement** to small box
- **Classical mechanics valid** for **Macroscopic objects**
  - large mass and larger box
  - Minimum momentum/speed very small
  - Continuous energy spectrum

PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

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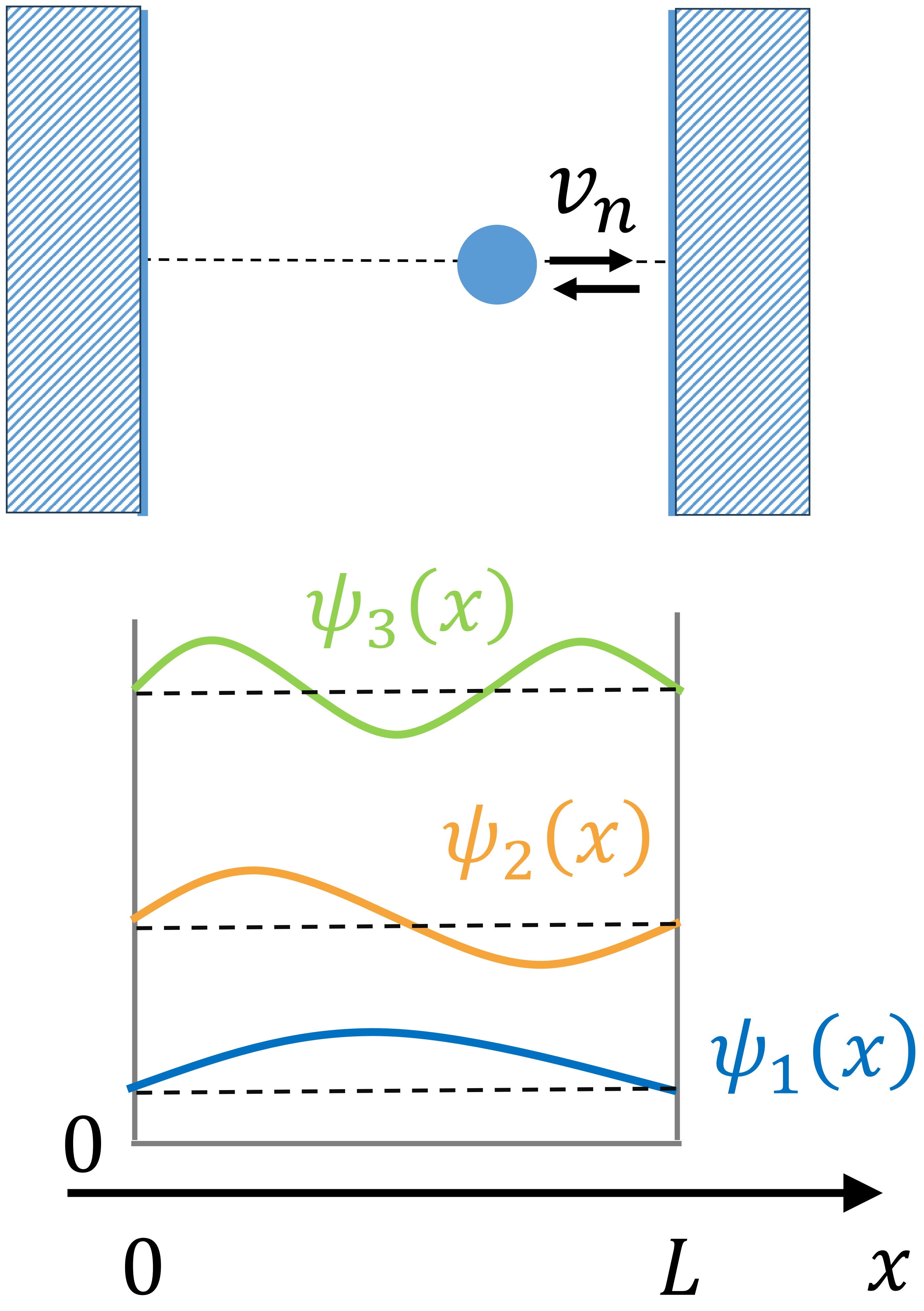

- Explain **all** quantum effects via de Broglie?
- What about position & velocity of particles?

PARTICLE IN A BOX: DE BROGLIE -- WAVE AND PARTICLE

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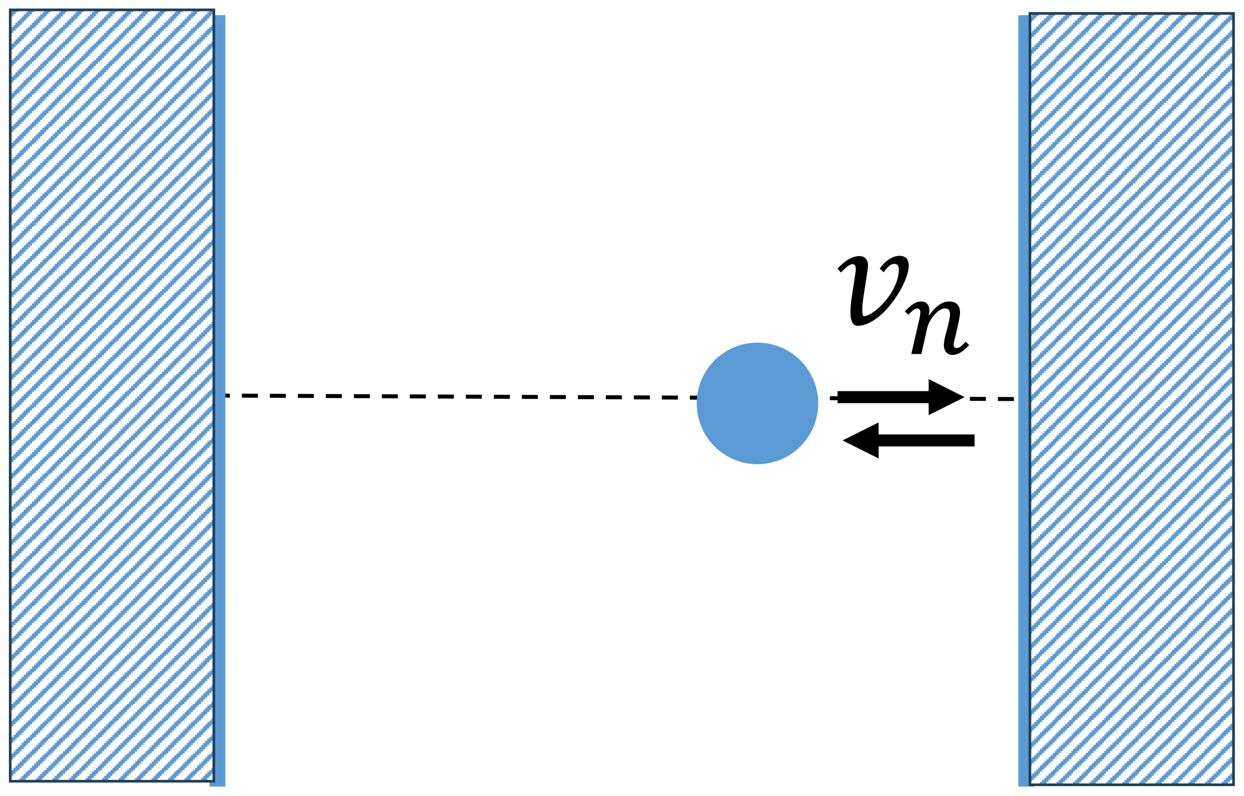
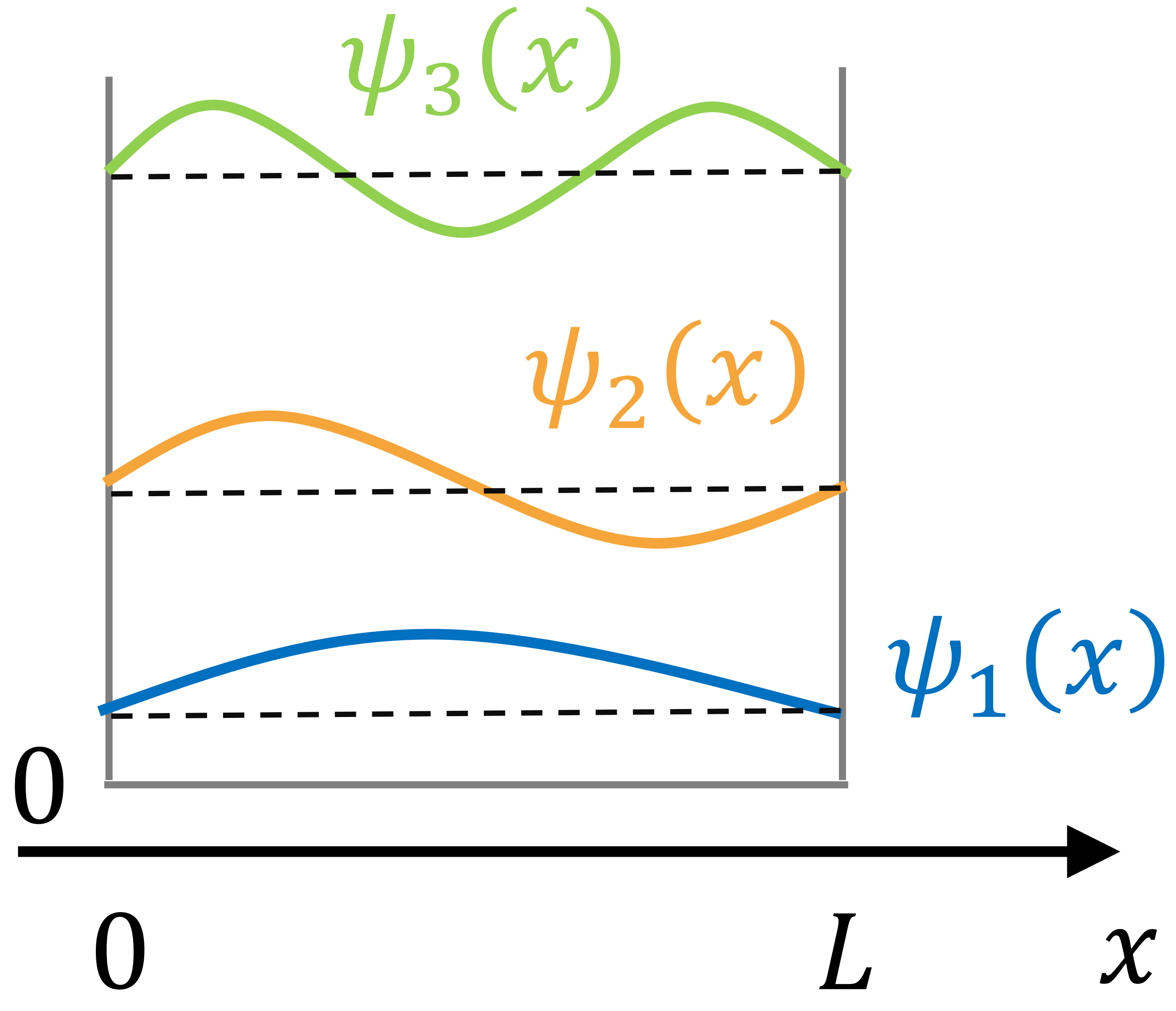


Energy: time dependency?
$\Theta(t) = e^{-iE_n t/\hbar}$

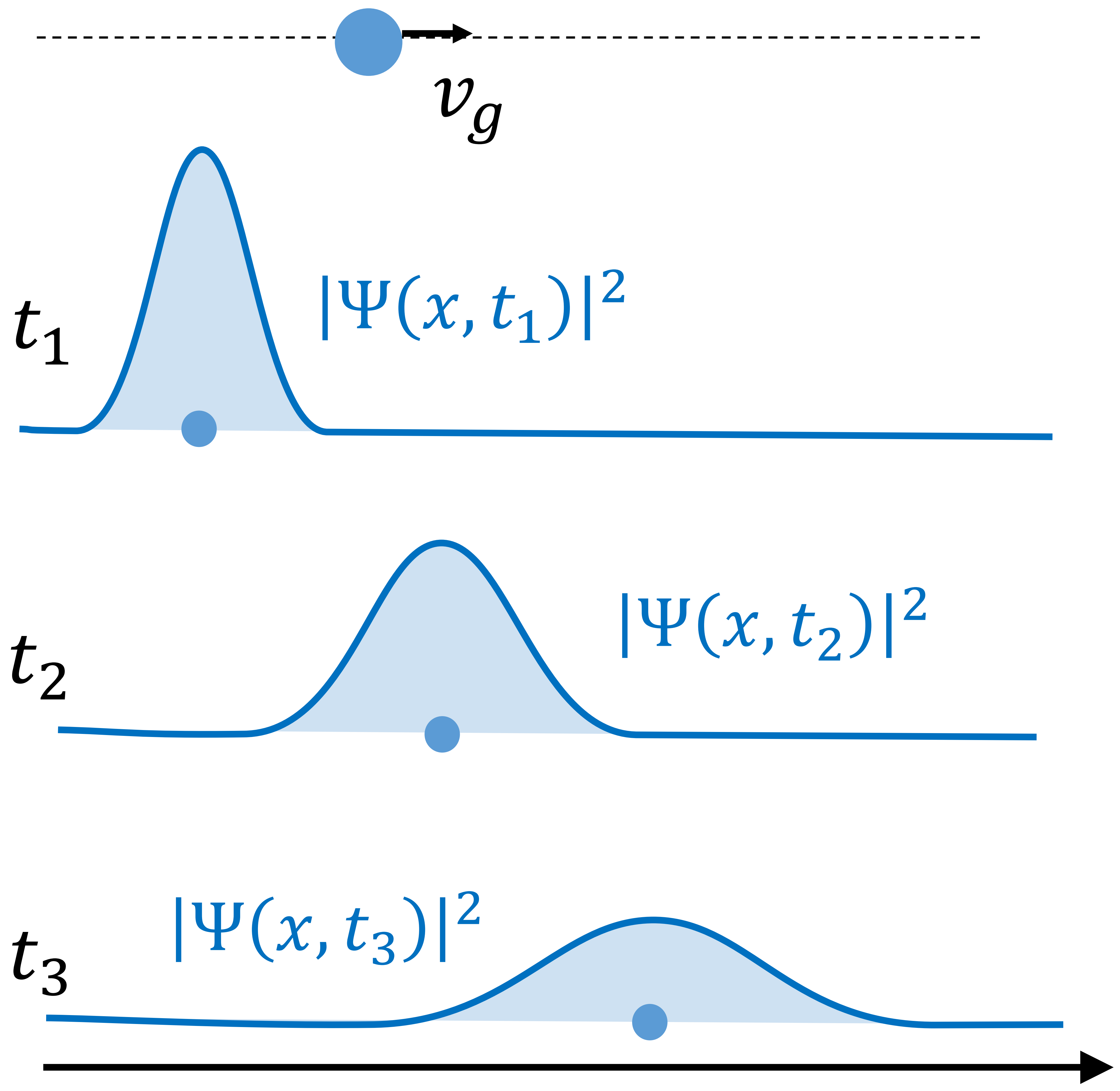
what is the velocity of probability ?



- Explain **all** quantum effects via de Broglie?
- What about position & velocity of particles?

PARTICLE IN A BOX: SUPERPOSITION

- Probability density goes beyond particle view of de Broglie
- Free particles → Wave packets with group velocity
- Uncertainty spreads in time



PARTICLE IN A BOX: SUPERPOSITION

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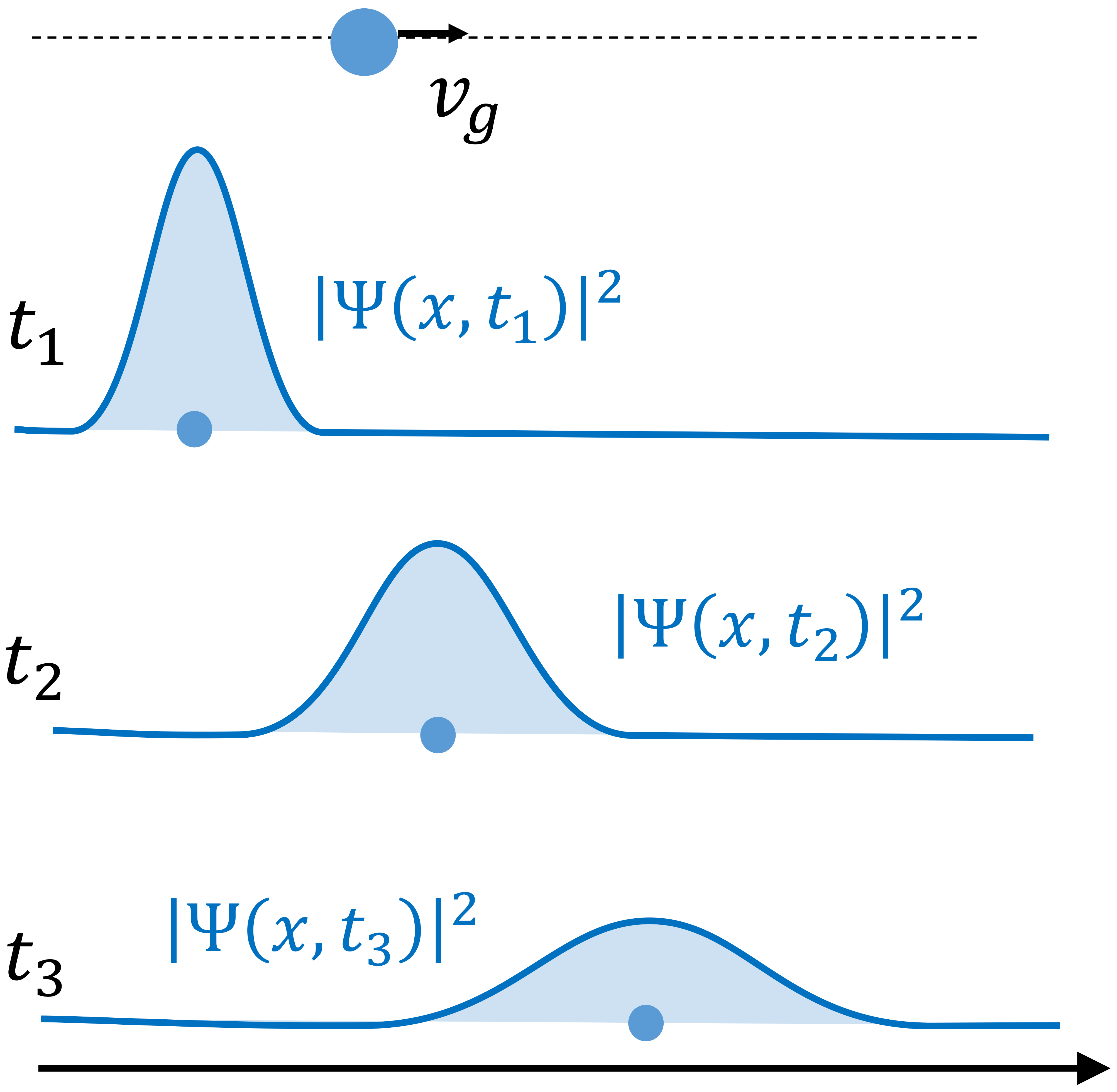
- Free particles → Wave packets with group velocity
- Uncertainty spreads in time

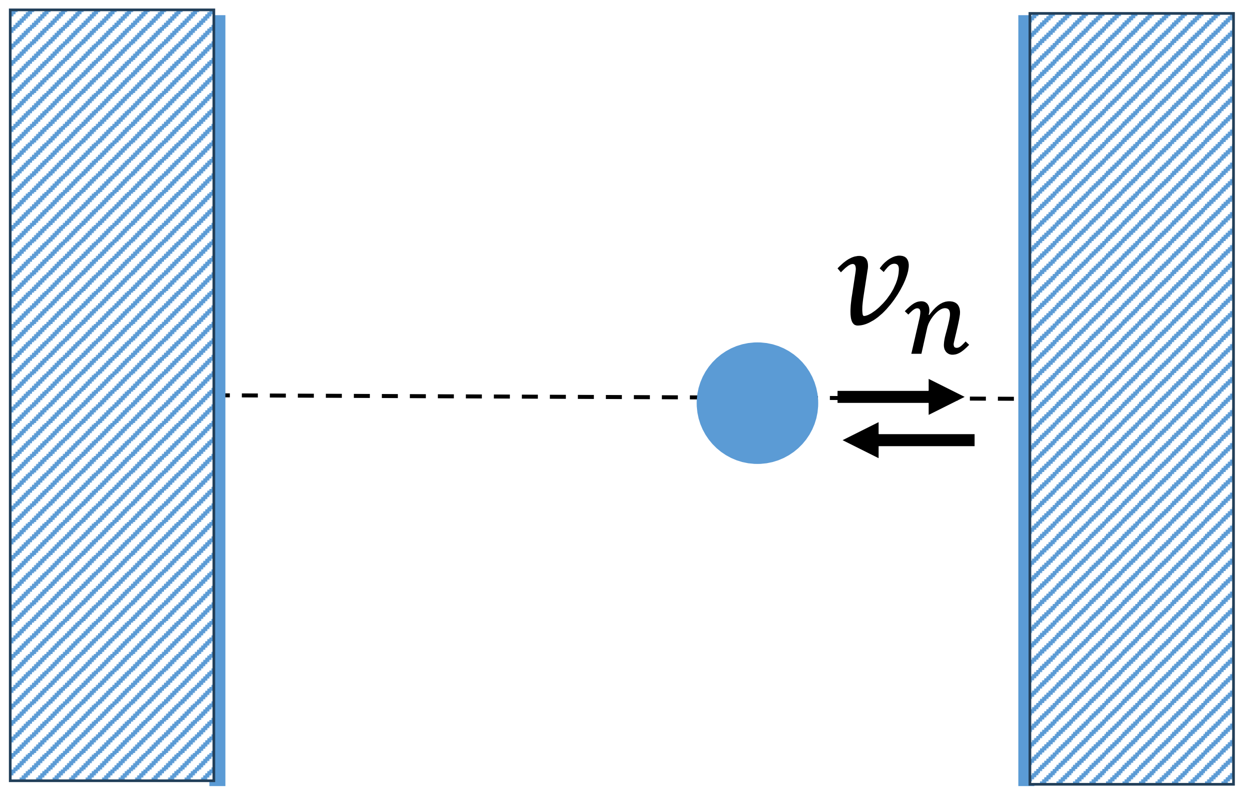
What about superposition of waves for confined particle?

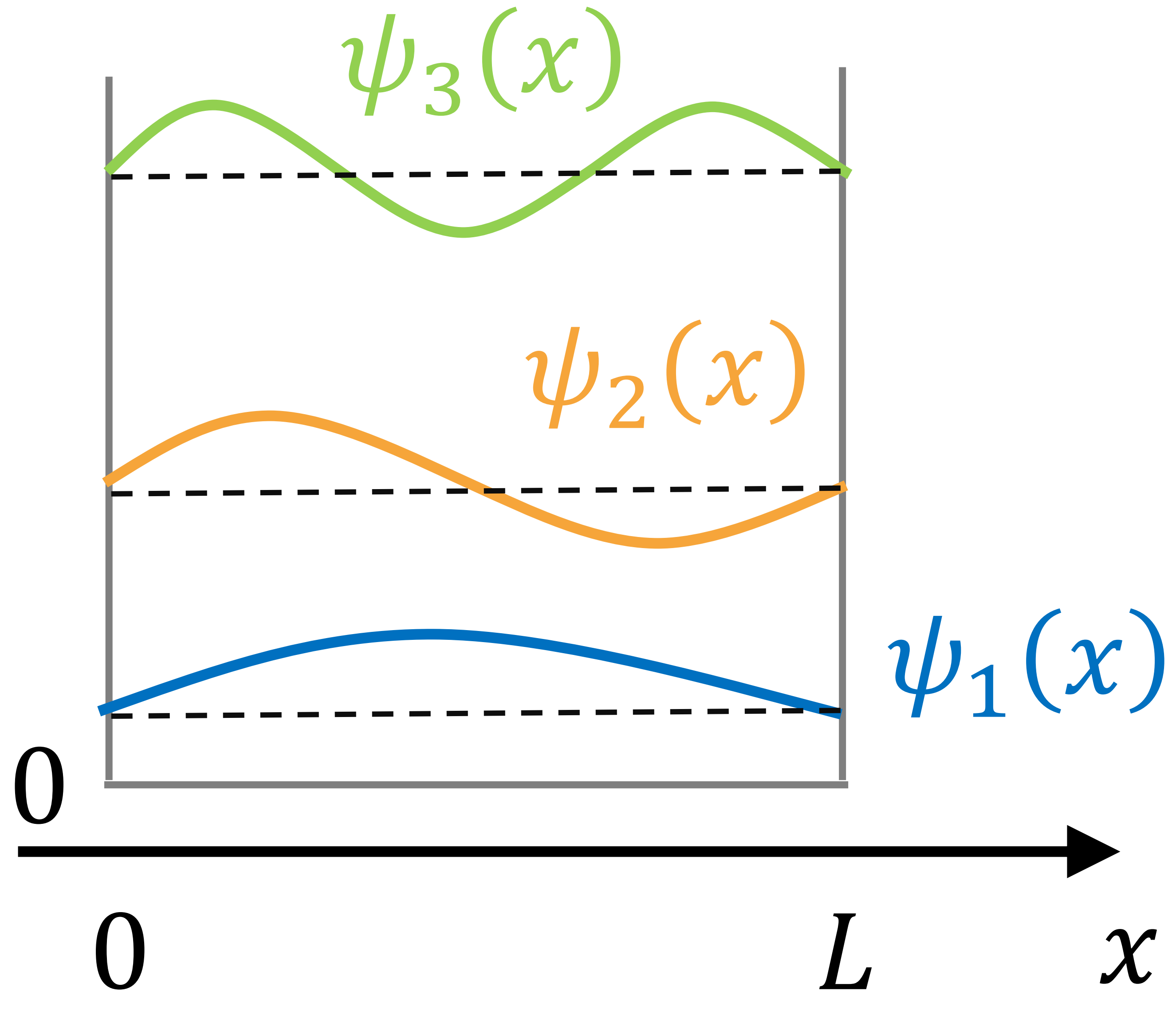
Behavior of probability density?



PARTICLE IN A BOX: SUPERPOSITION

- Particle in a box:
  - Solutions standing waves: $\psi_n \;\rightarrow\; E_n, k_n$
  - Superposition of standing waves





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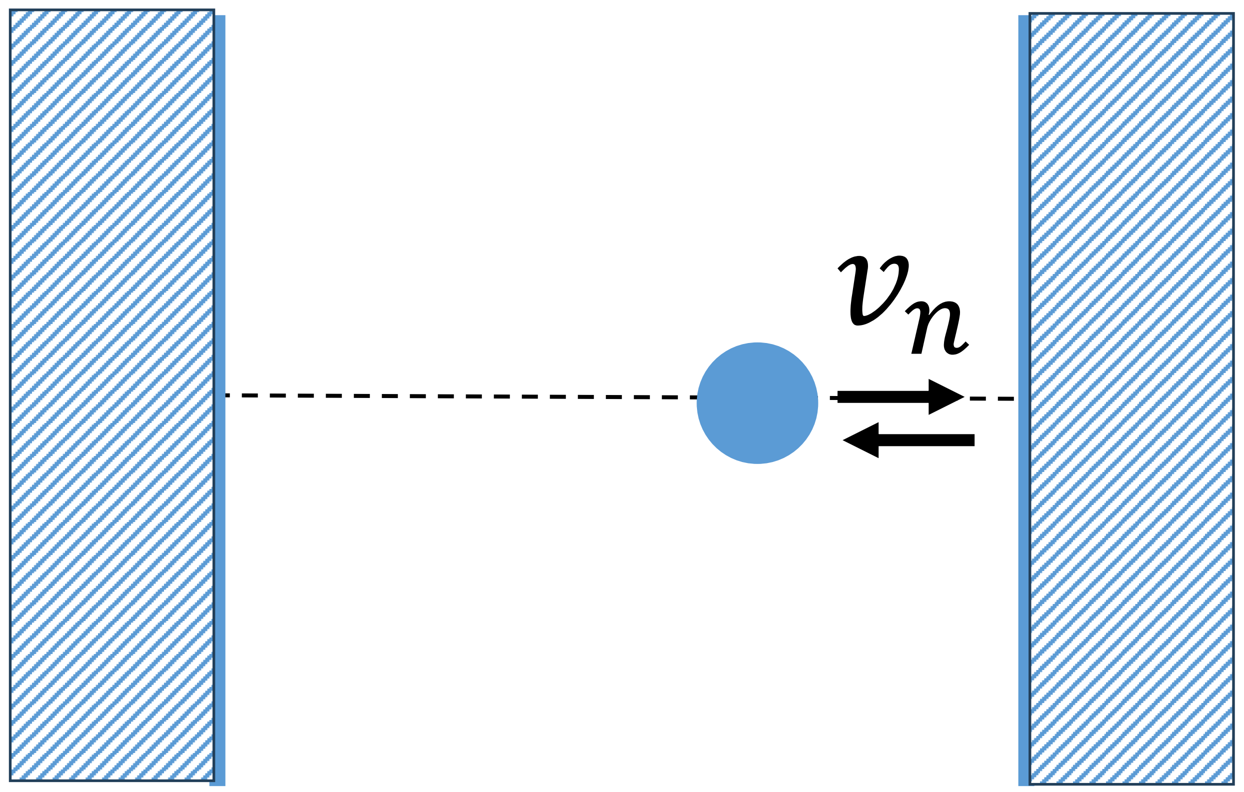
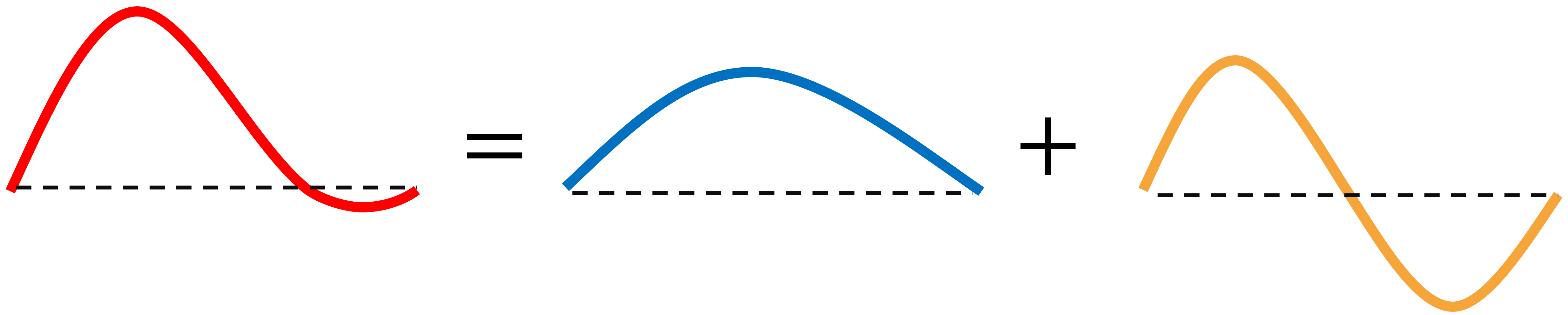
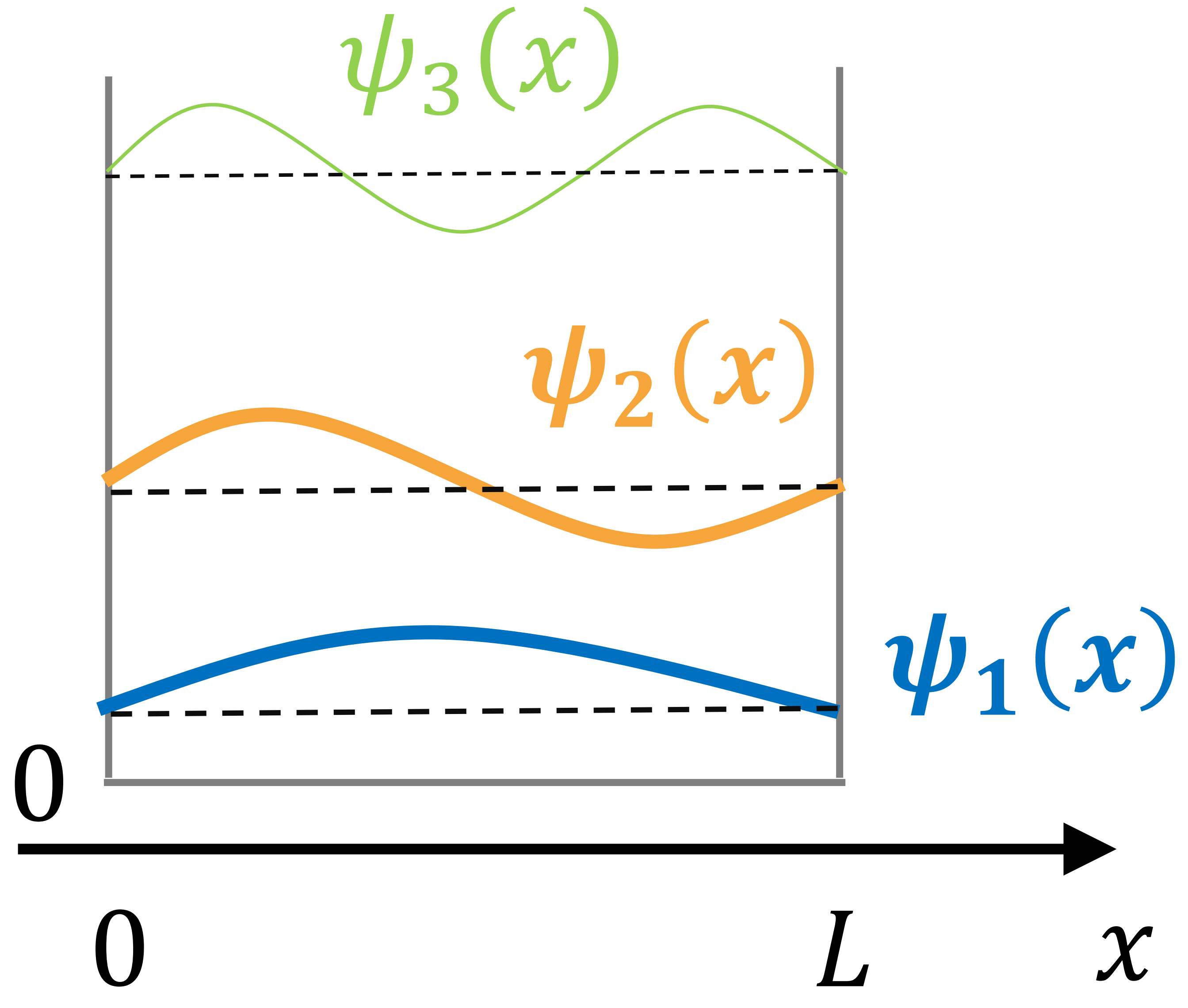


- Example superposition:

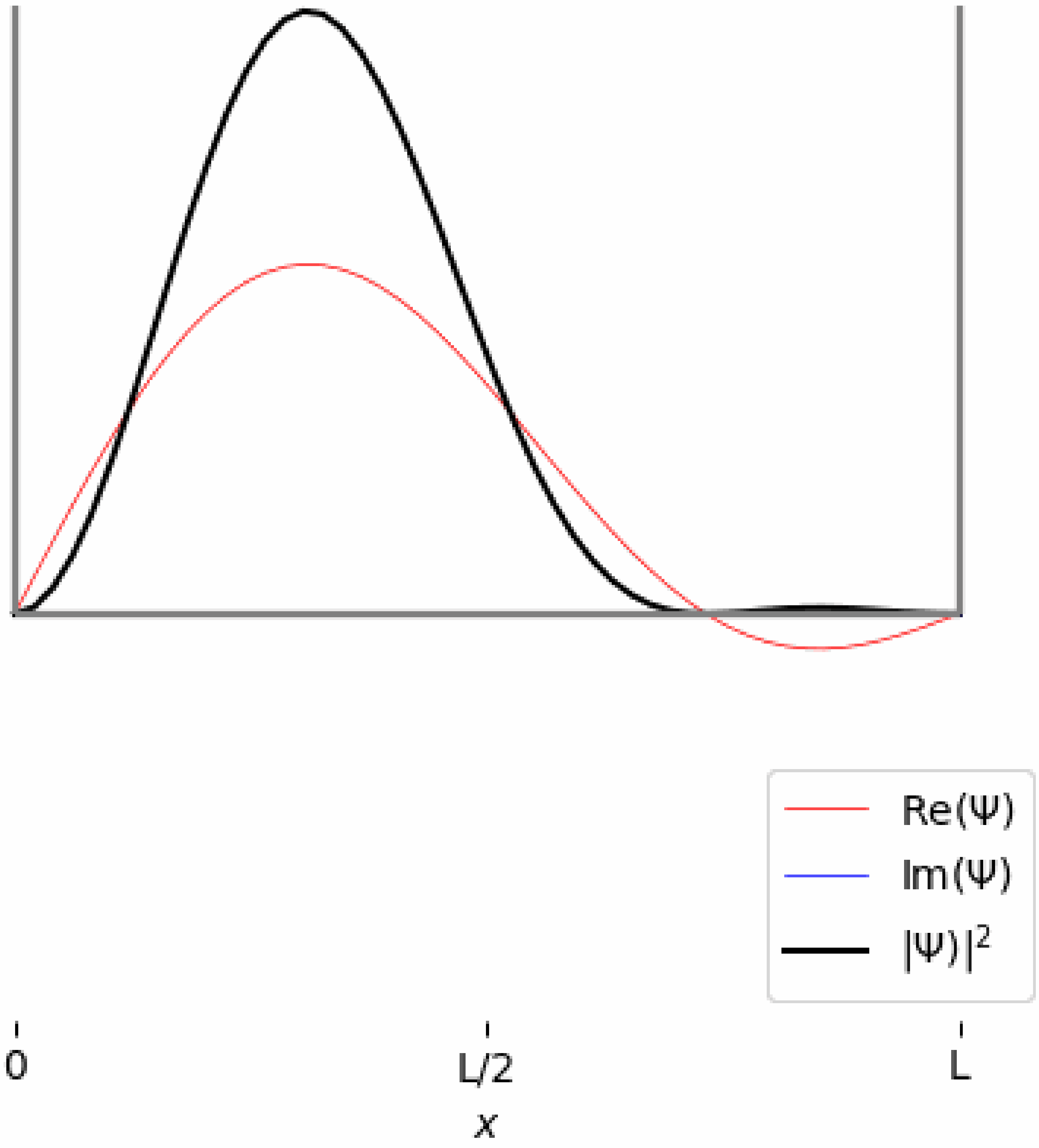
$$\Psi(x,t) = \psi_1(x)\, e^{\frac{iE_1 t}{\hbar}} + \psi_2(x)\, e^{\frac{i4E_1 t}{\hbar}}$$





PARTICLE IN A BOX: SUPERPOSITION

- Particle in a box:
  - Solutions standing waves: $\psi_n \rightarrow E_n, k_n$
  - Superposition of standing waves



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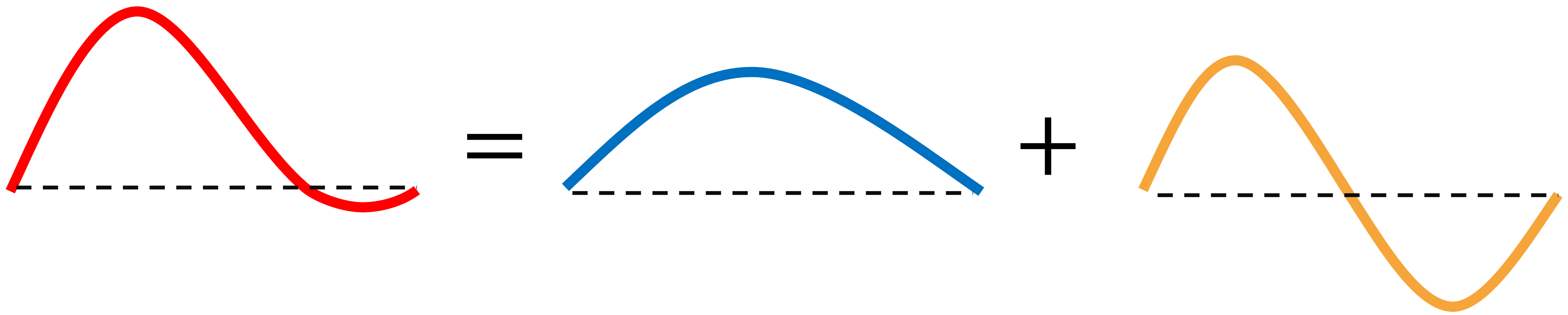
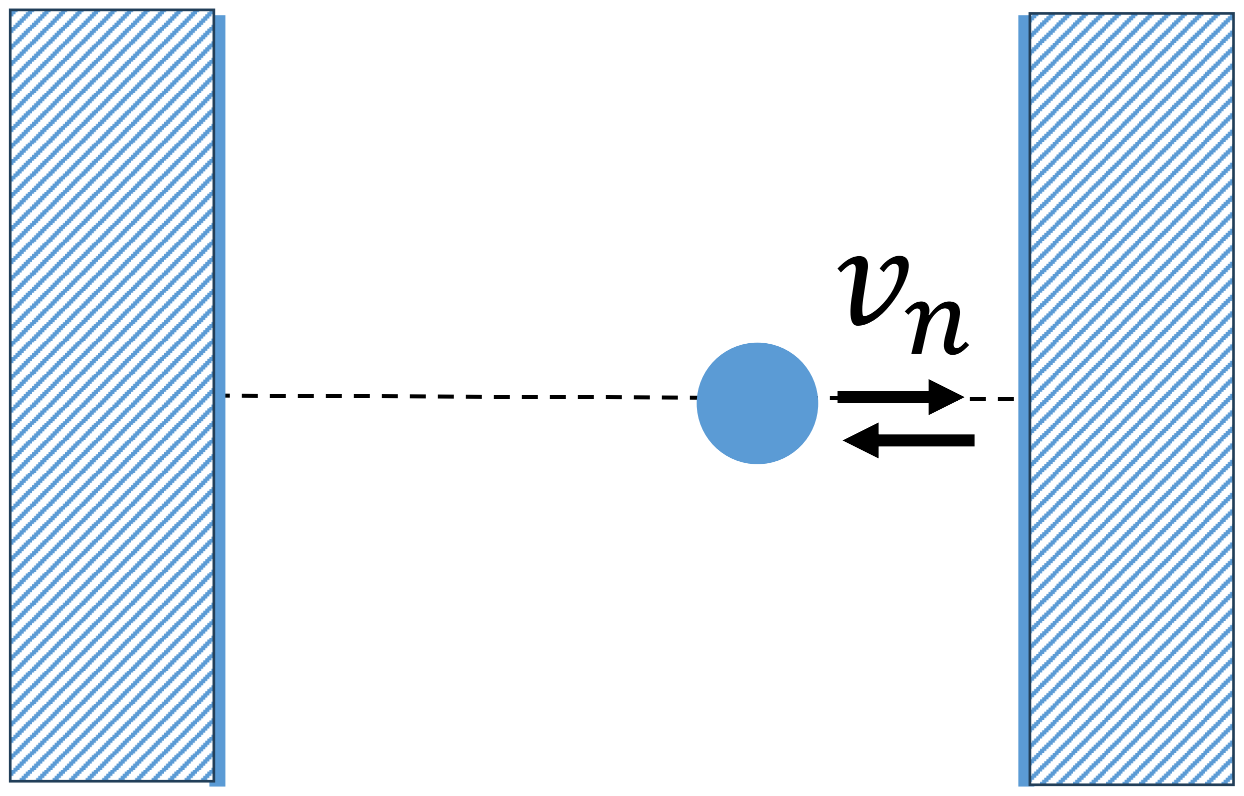


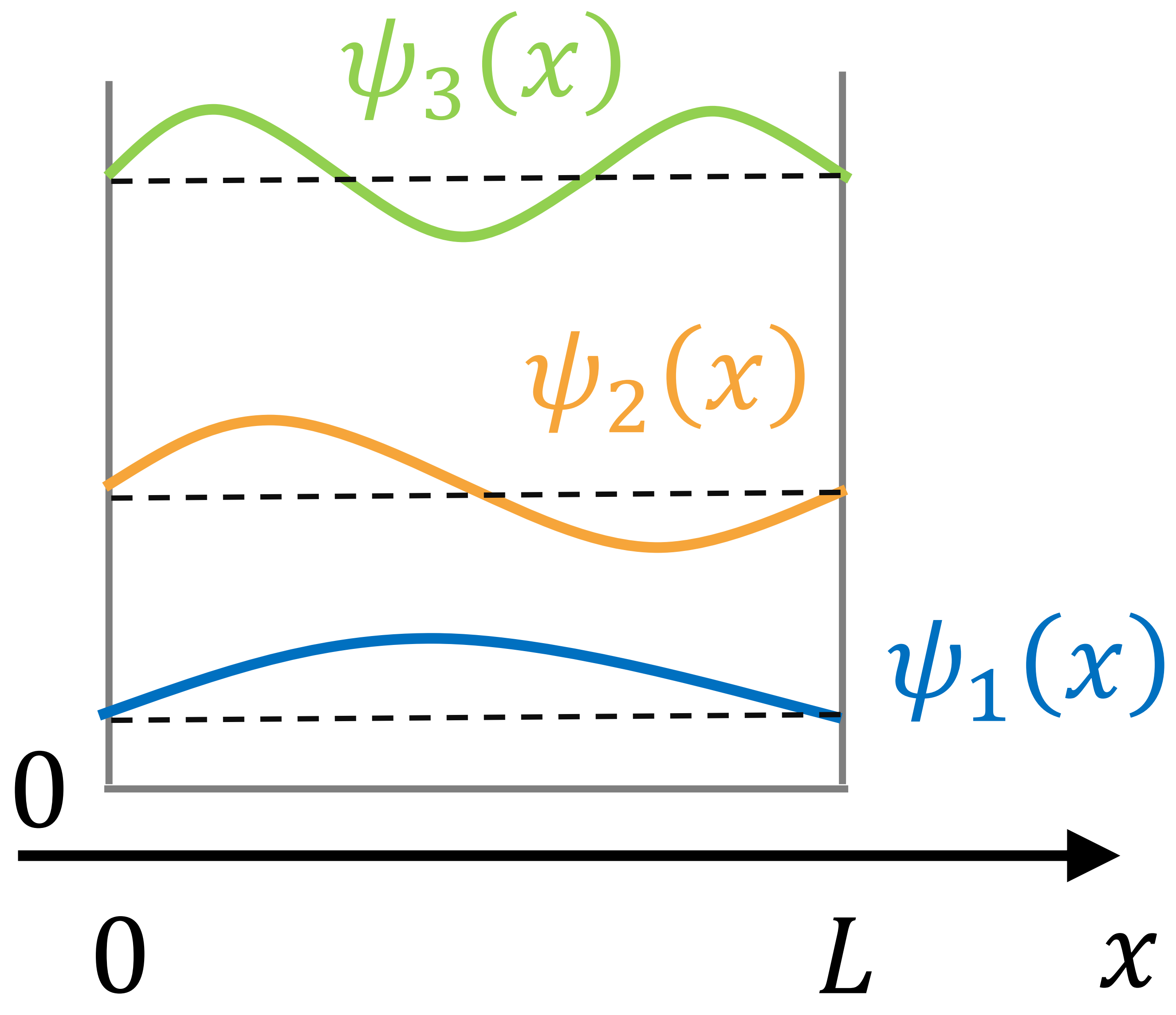
PARTICLE IN A BOX: UNCERTAINTY

- Particle view: uniform probability
- Probability density goes beyond particle view of de Broglie
- Uncertainty relation:

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

- Small box: Δx is small so uncertainty on momentum is large
- Classical mechanics for large objects





SUMMARY PARTICLE IN A BOX

- Classical mechanics for large objects in large boxes

- Macroscopic objects
  - large mass and larger box
  - Small minimum momentum/speed
  - Continuous energy spectrum

- Small box & quantum particles
  - Energy quantization
  - Higher “classical” kinetic energy due to spatial constraints

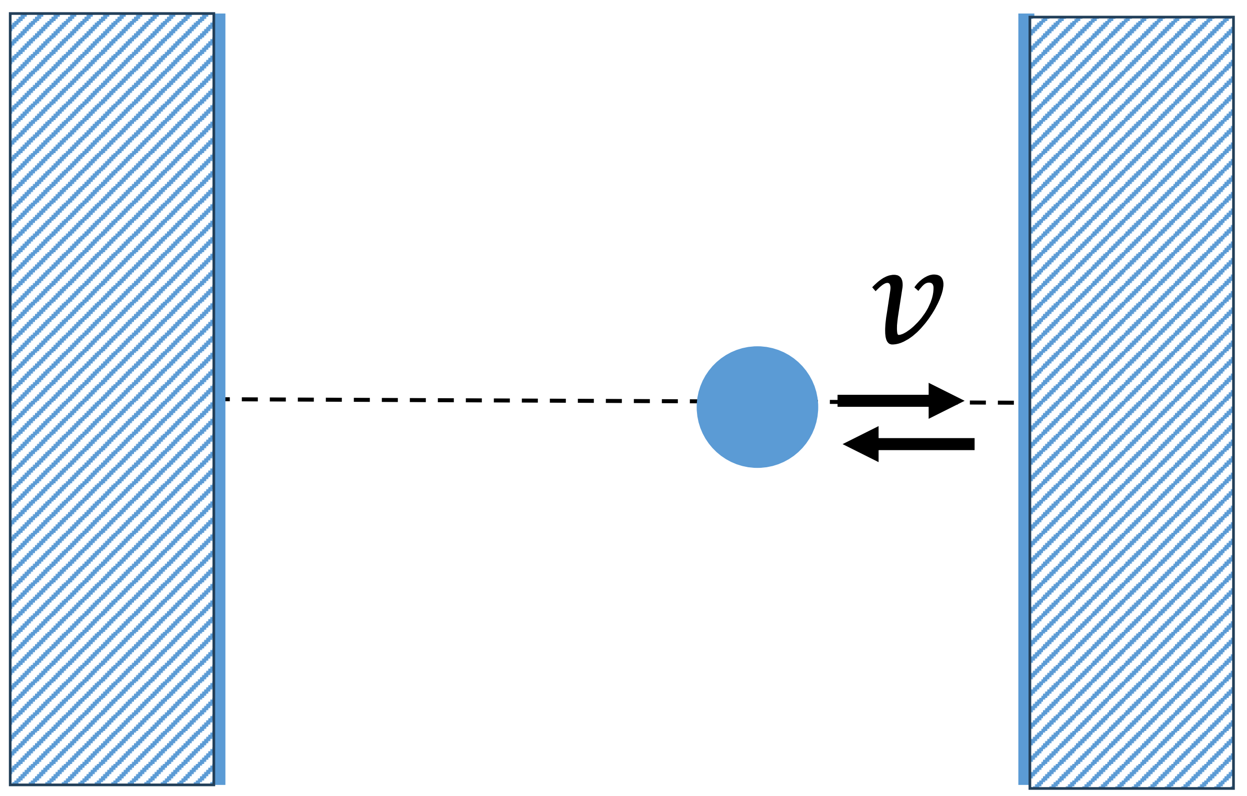
particle in a **infinite well** or **a box**

Particle in a **finite well**

INFINITE WELL = PARTICLE IN A BOX

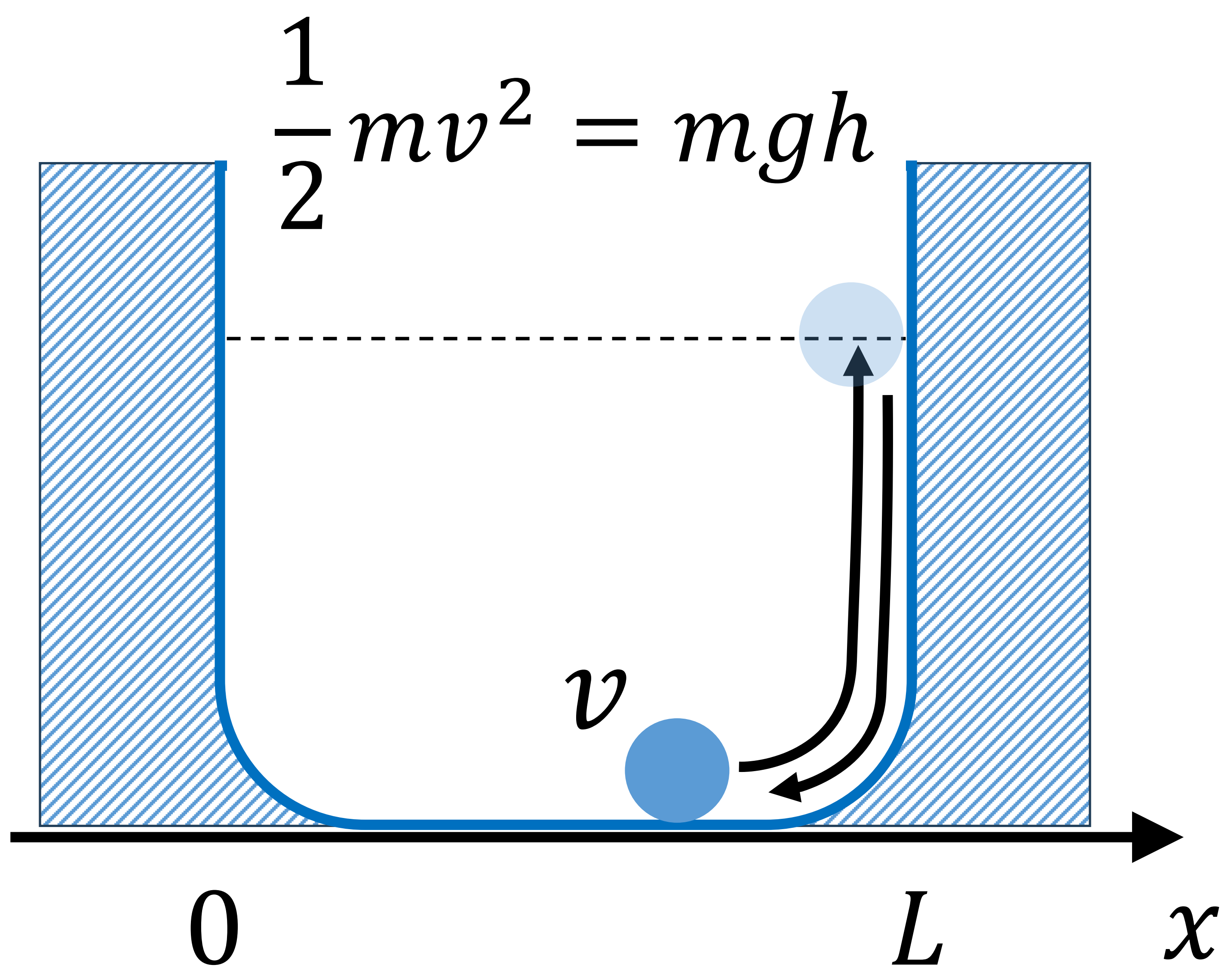
Particle in a box model:

- Particle bounces back at the walls
  - Perfect elastic collision
  - Doesn't lose speed/energy



Alternative model: well with infinite walls:

- Particle rolls up and down (without resistance)
- Kinetic energy converts in potential energy and back: $E = K + V$



THE CLASSICAL FINITE WELL

(1) If energy lower than the walls:

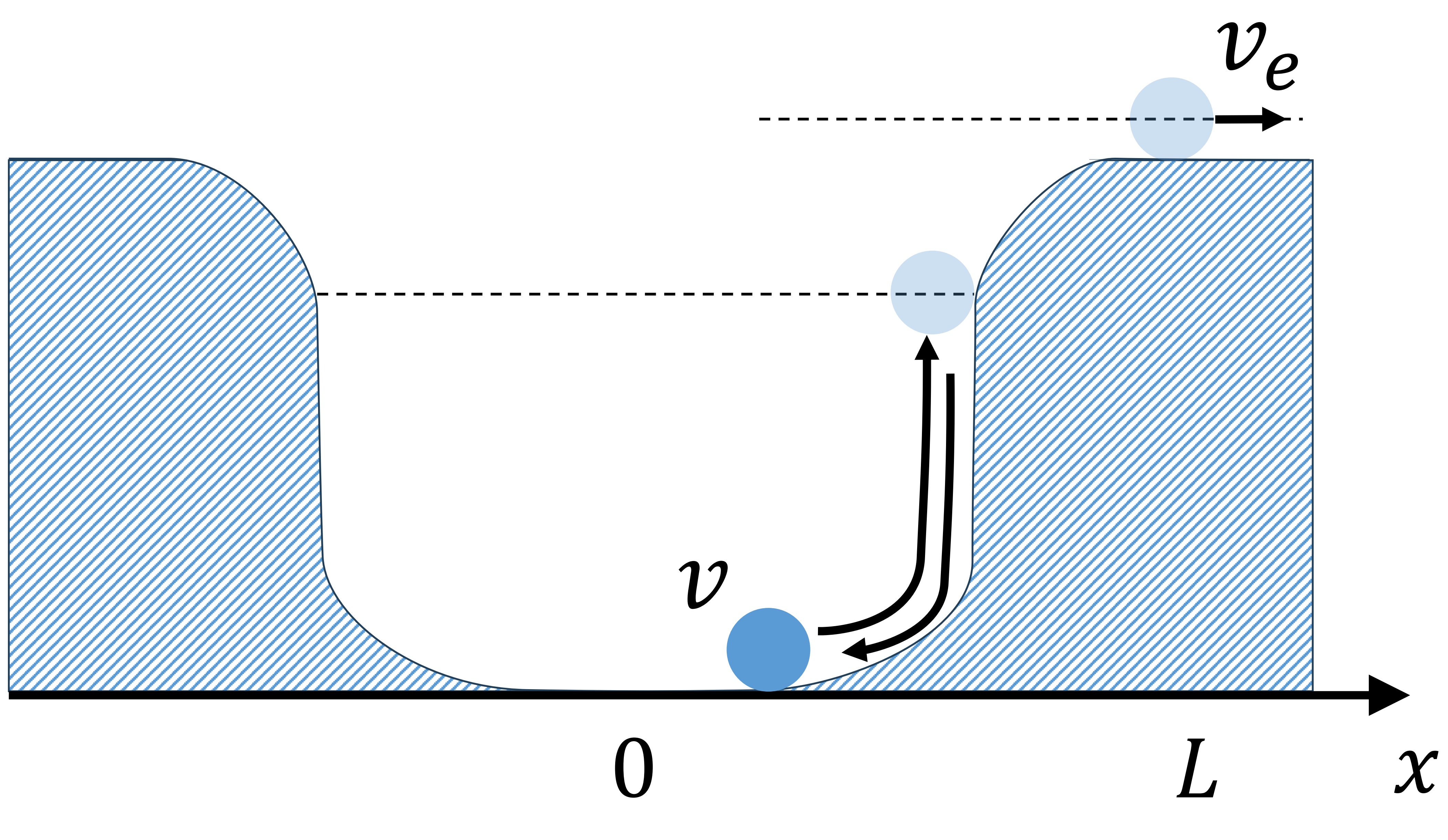
- Particle rolls up and down (without resistance)

$$\frac{1}{2}mv^2 = mgh + \frac{1}{2}mv_e^2$$

(2) If energy larger than the wall:

- Particle escapes the well
- Velocity inside v higher than after rolling up wall v_e
- Part kinetic energy K converts

in potential energy $V = mgh$



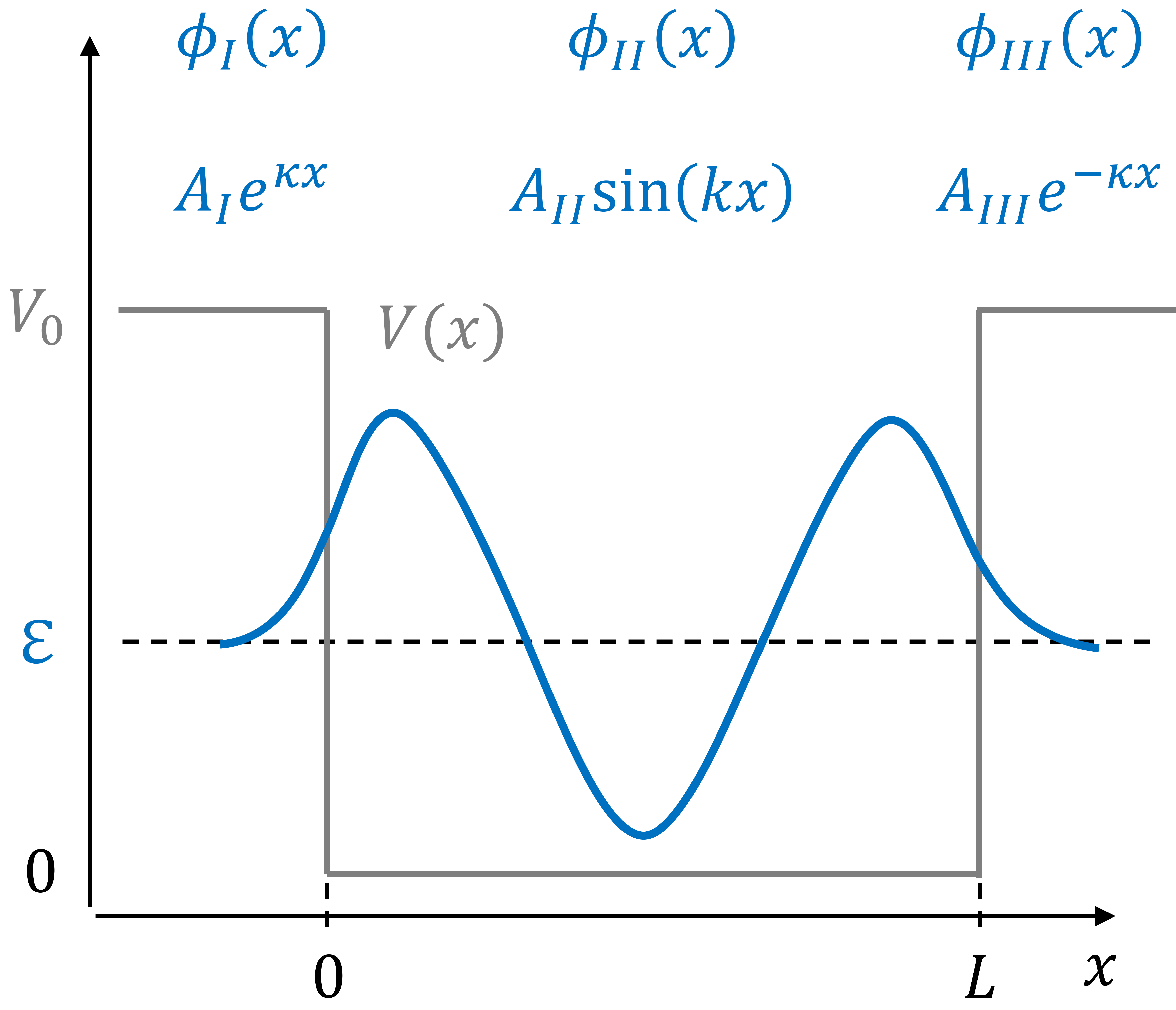
THE QUANTUM FINITE WELL

(1) If energy lower than walls:

- Wave function ϕ penetrates
- Evanescent waves in wall: exponentially decaying

$$\begin{cases} \phi_I(x) = A_I e^{\kappa x} \\ \phi_{II}(x) = A_{II}\sin(kx) \\ \phi_{III}(x) = A_{III} e^{-\kappa x} \end{cases}$$

With $\kappa = \sqrt{2m(V_0 - \mathcal{E})}/\hbar$ and $k = \sqrt{2m\mathcal{E}}/\hbar$



THE QUANTUM FINITE WELL

(1) If energy lower than walls:

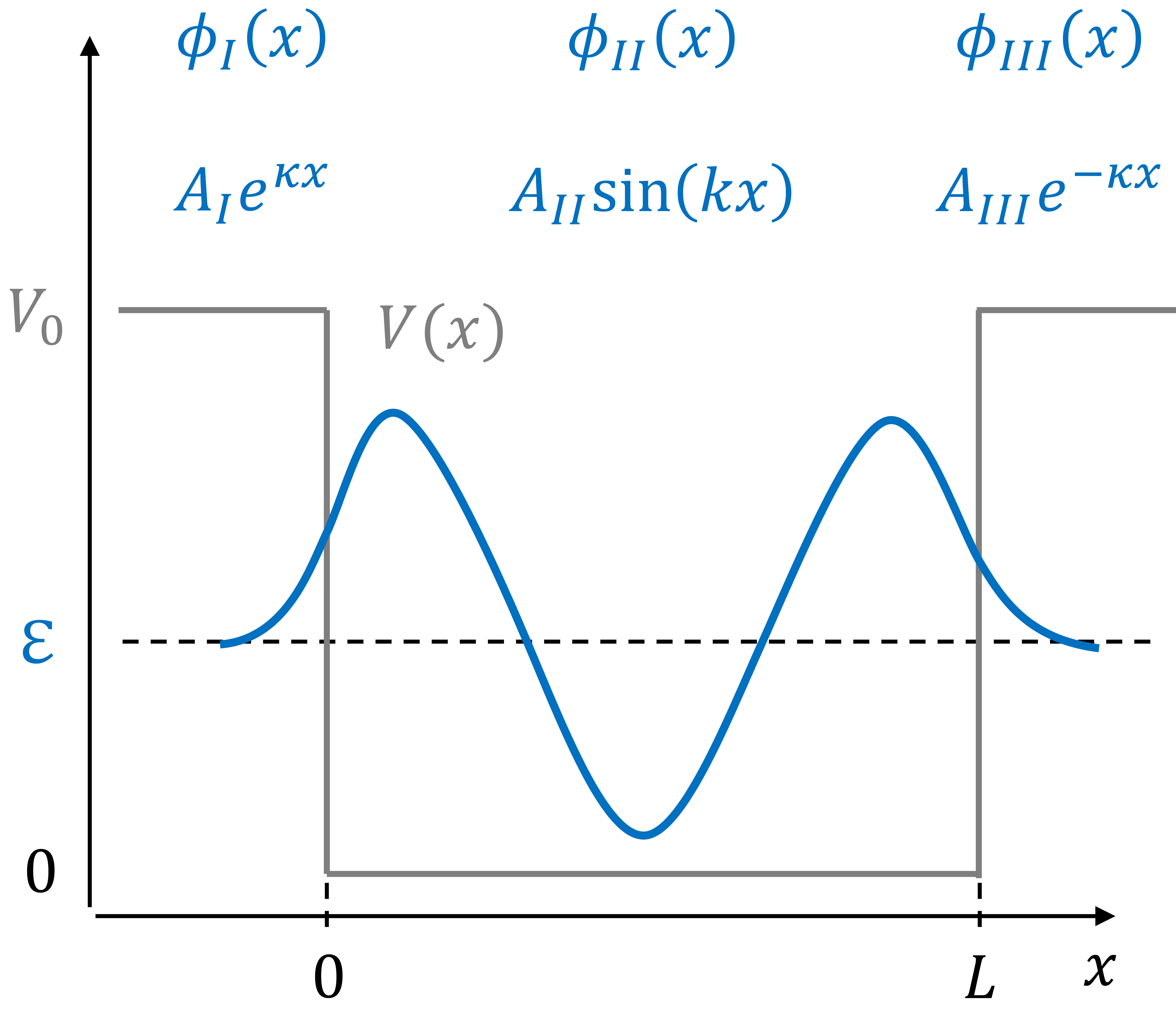
- Discrete energies $\mathcal{E}_n$ and wave numbers
- Boundary conditions lead to the final wave functions ϕ_n:

Continuity wave function

$$\phi_I(0) = \phi_{II}(0)$$
$$\phi_{II}(L) = \phi_{III}(L)$$

Continuity derivative:

$$\phi'_I(0) = \phi'_{II}(0)$$
$$\phi'_{II}(L) = \phi'_{III}(L)$$



THE QUANTUM FINITE WELL

(2) If energy larger than walls:

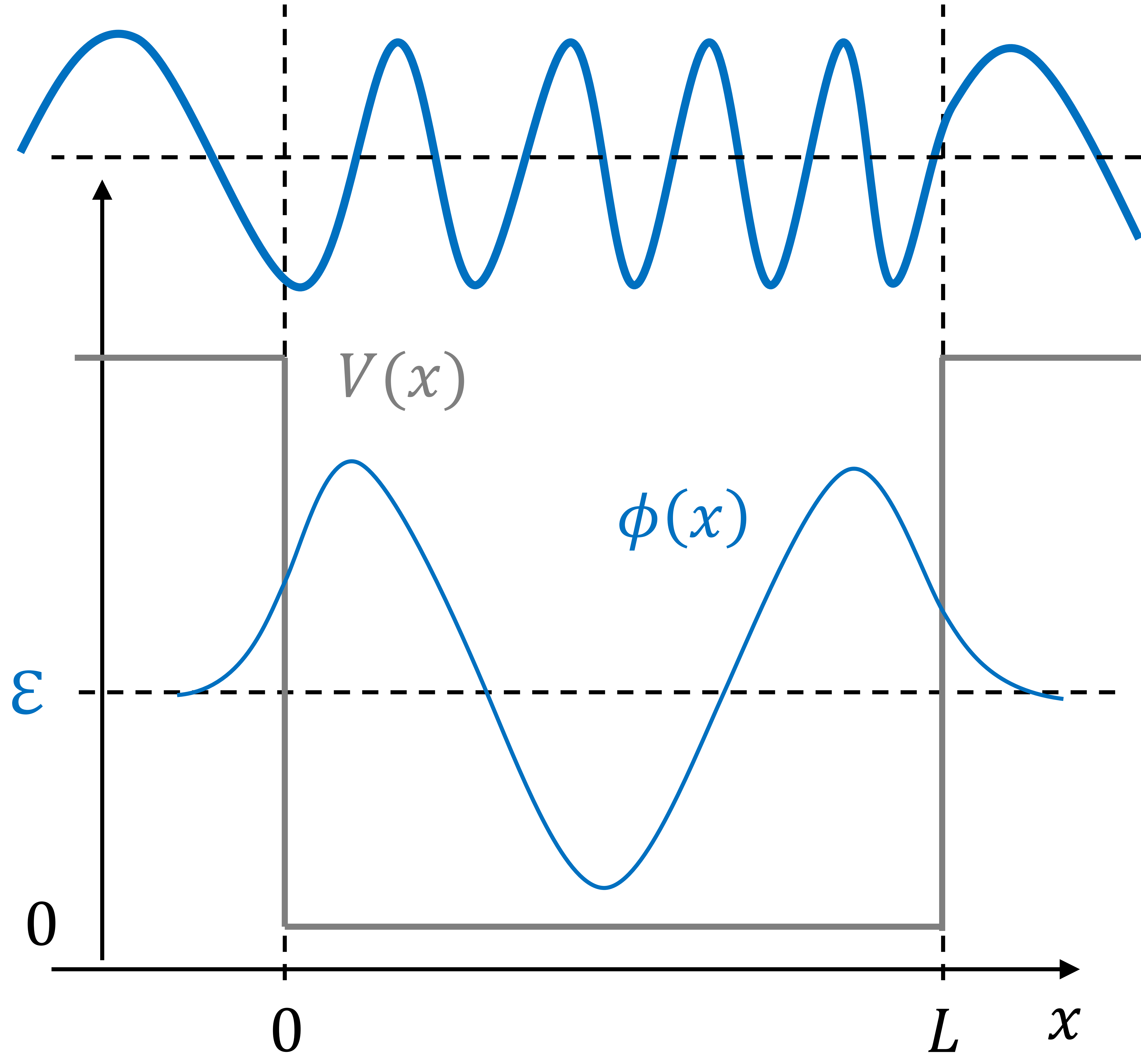
- Wave-like solutions in both well and barrier region

$$\phi_I(x) = A_I e^{ik_0 x} + B_I e^{-ik_0 x}$$
$$\phi_{II}(x) = A_{II} e^{ikx} + B_{II} e^{-ikx}$$
$$\phi_{III}(x) = A_{III} e^{ik_0 x} + B_{III} e^{-ik_0 x}$$

- Wave number k inside well larger than k_0 outside well:

$k_0 = \sqrt{2m(\mathcal{E} - V_0)}/\hbar$ and

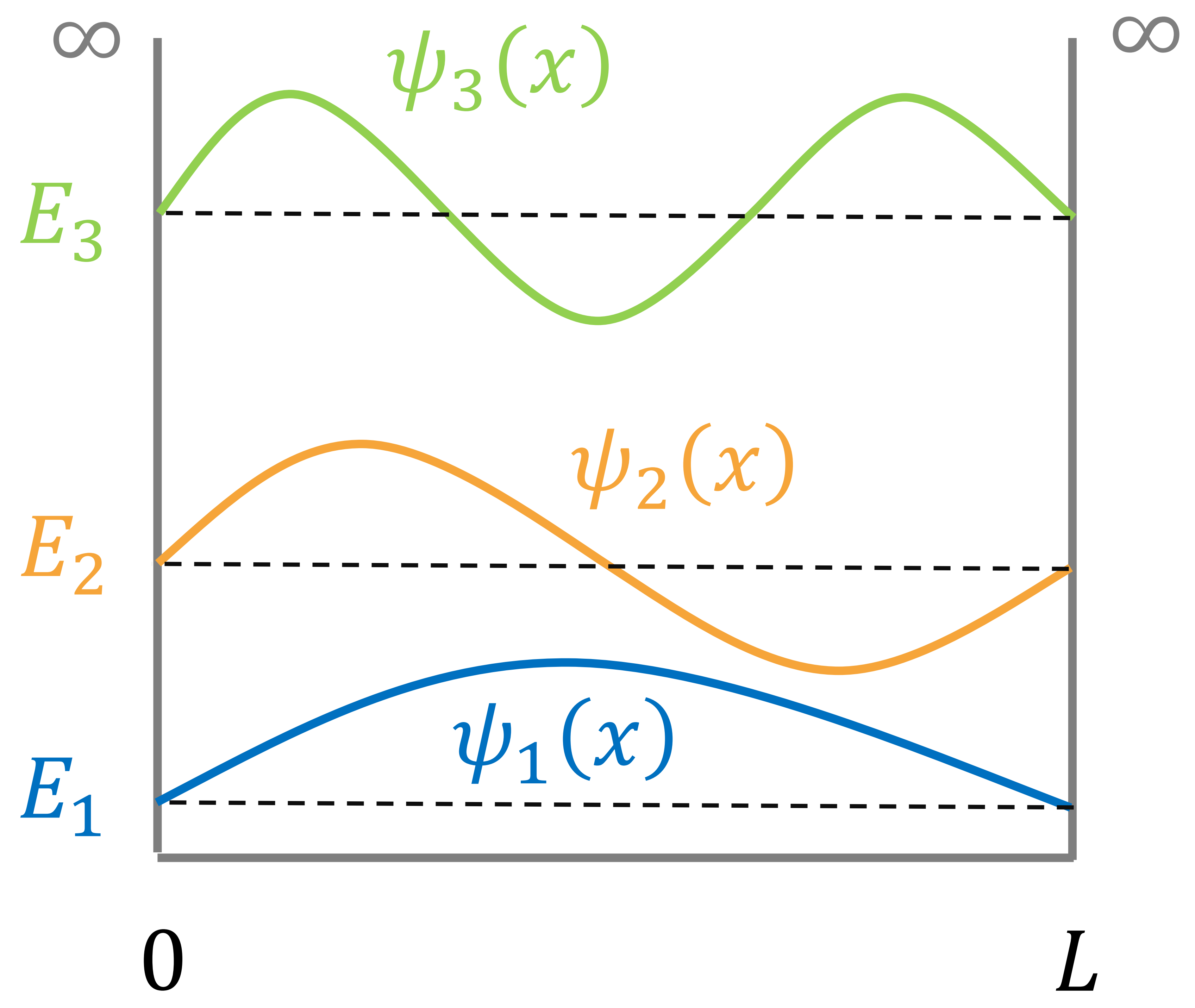
$k = \sqrt{2m\mathcal{E}}\,/\hbar$



INFINITE VERSUS FINITE WELL

Infinite well (box)

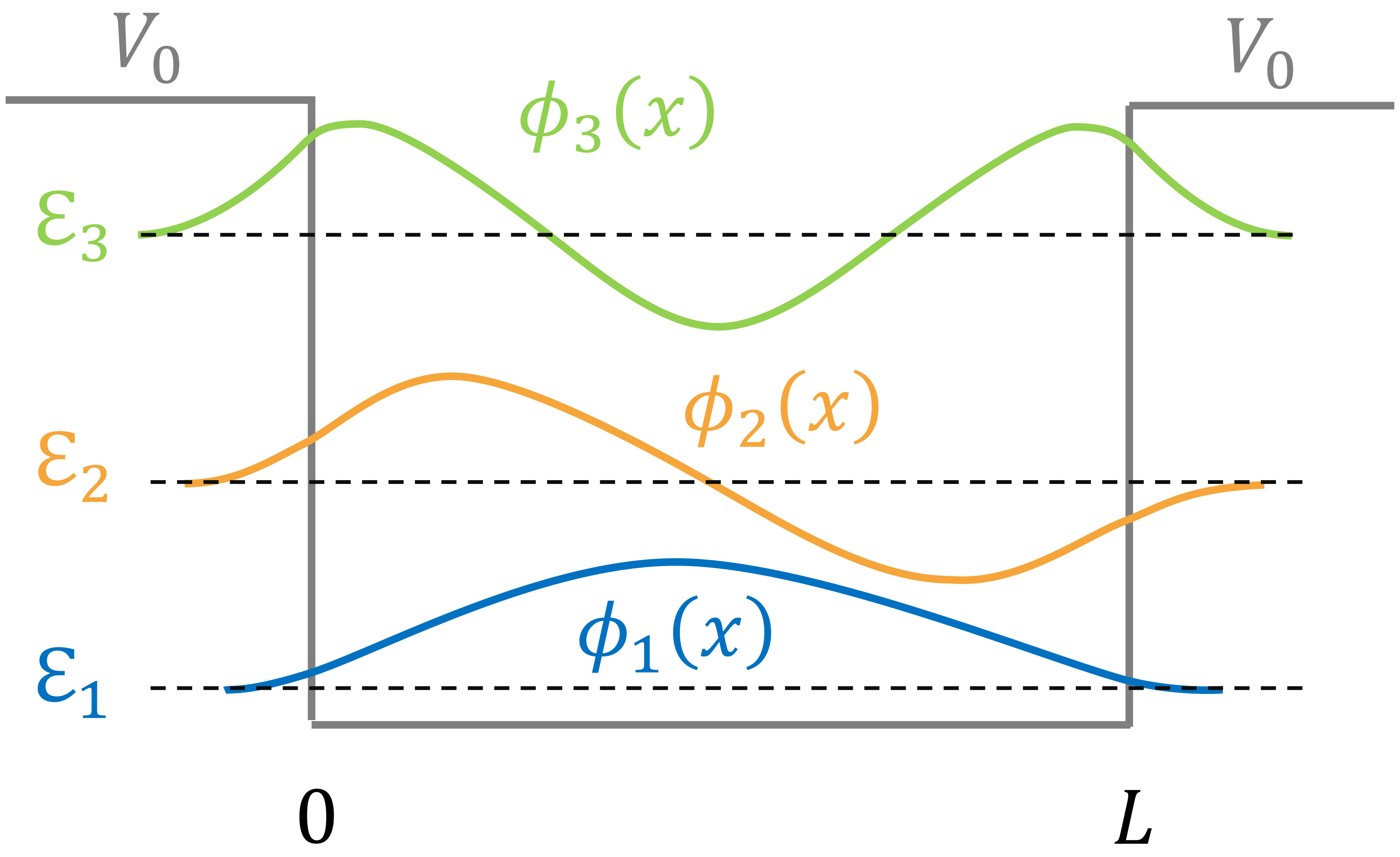
$$\psi_n(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{n\pi x}{L}\right), \qquad E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}$$



Finite well

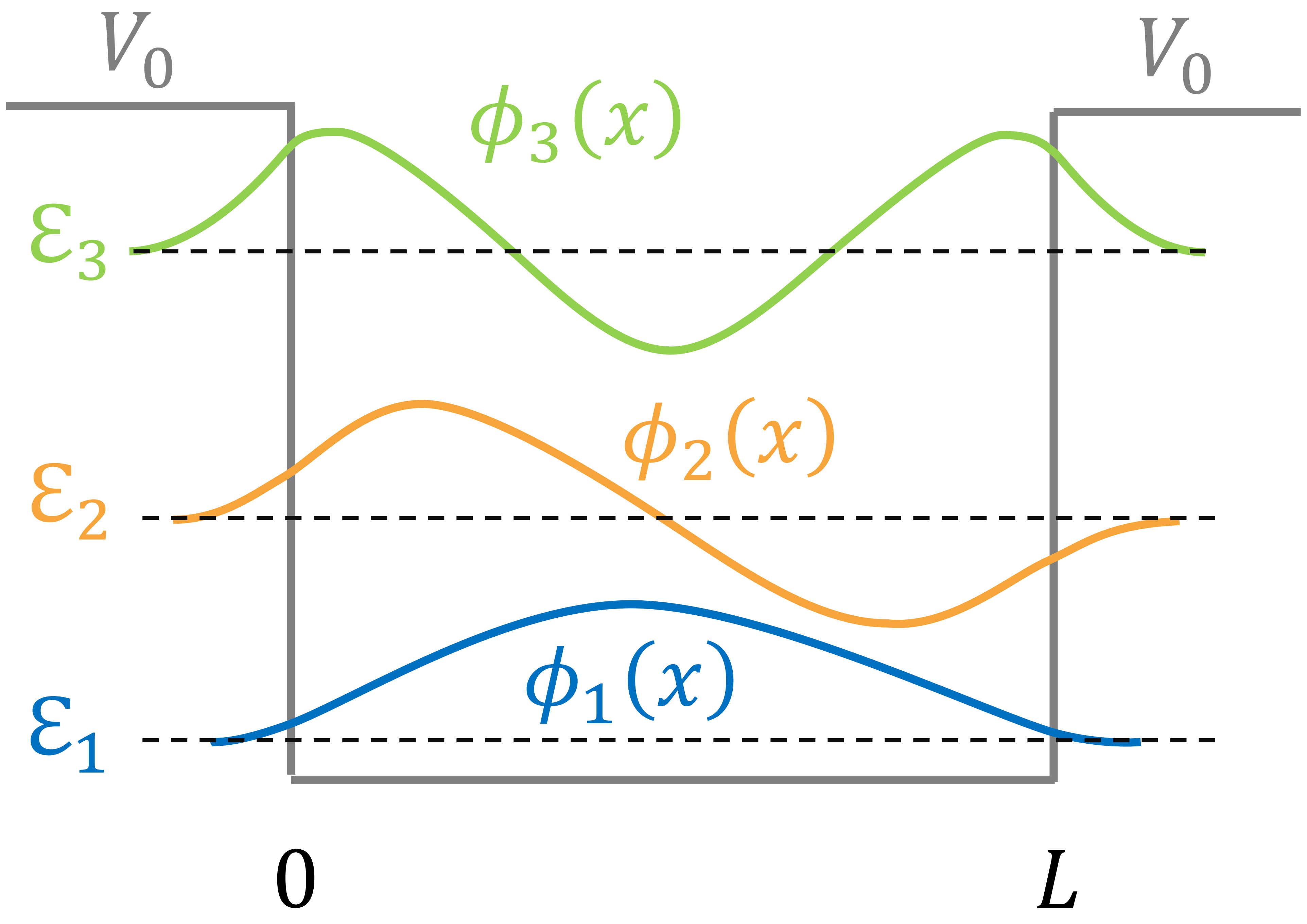
- Standing waves $\phi_n(x)$ penetrate the walls
- Energies $\mathcal{E}_n$ lower since $\phi_n(x)$ less confined

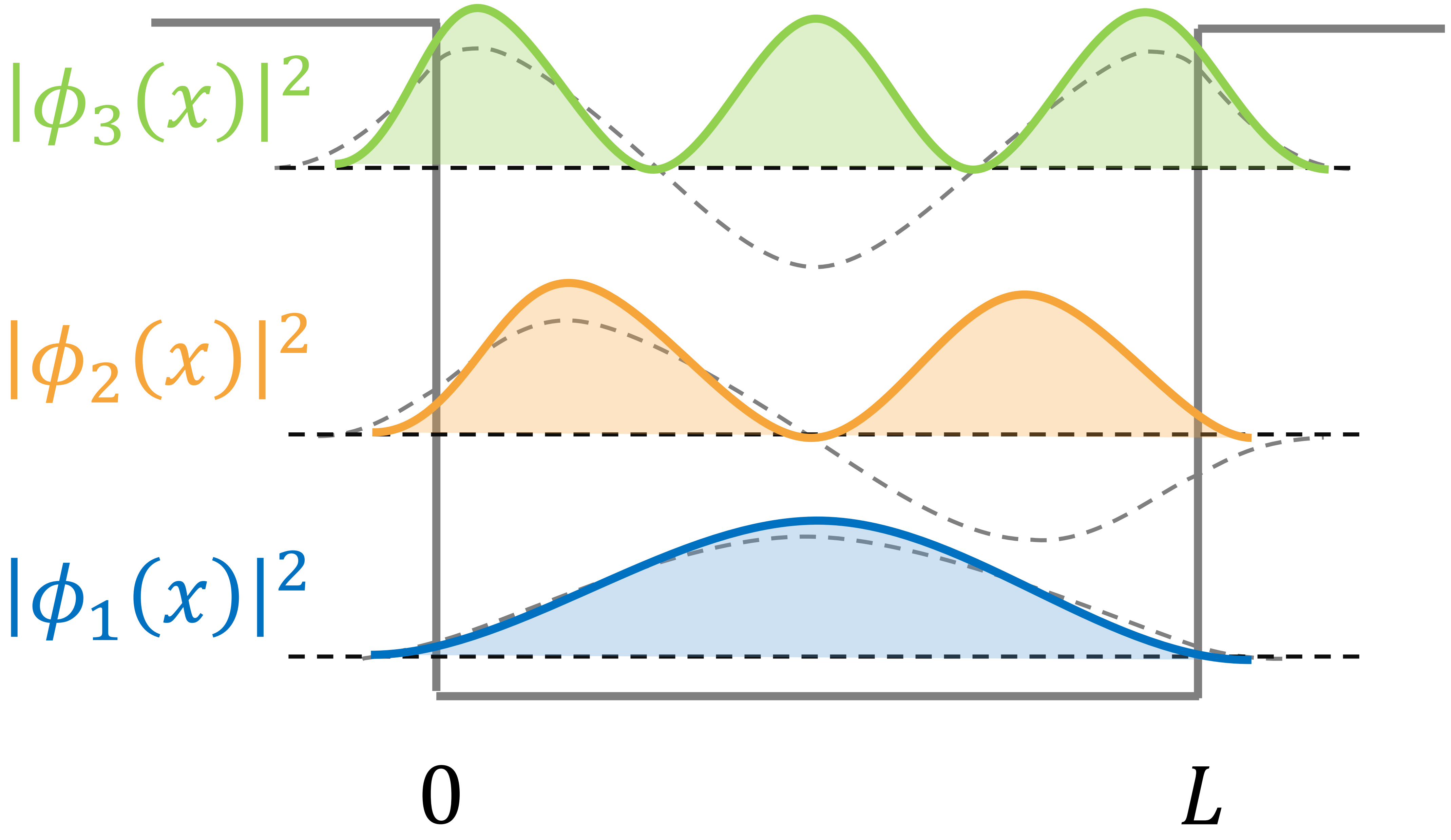
$$\phi_n(x) \approx \psi_n(x)\,,\ \mathcal{E}_n < E_n$$



FINITE WELL: PROBABILITY DENSITY FUNCTION

- Nonzero probability for particle to be outside well
- Exponential decay of ϕ_n (and probability $|\phi_n|^2$) outside well
- Penetration larger for highest energy level in well

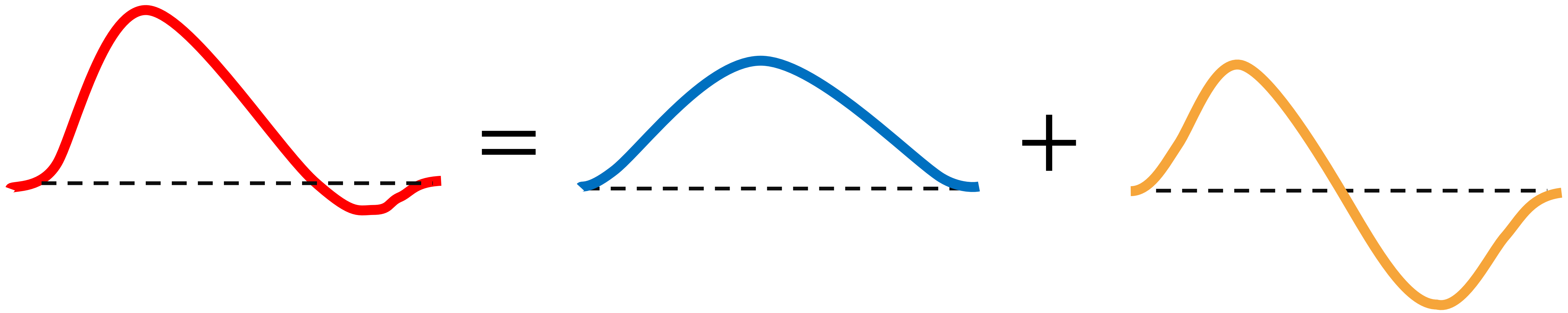


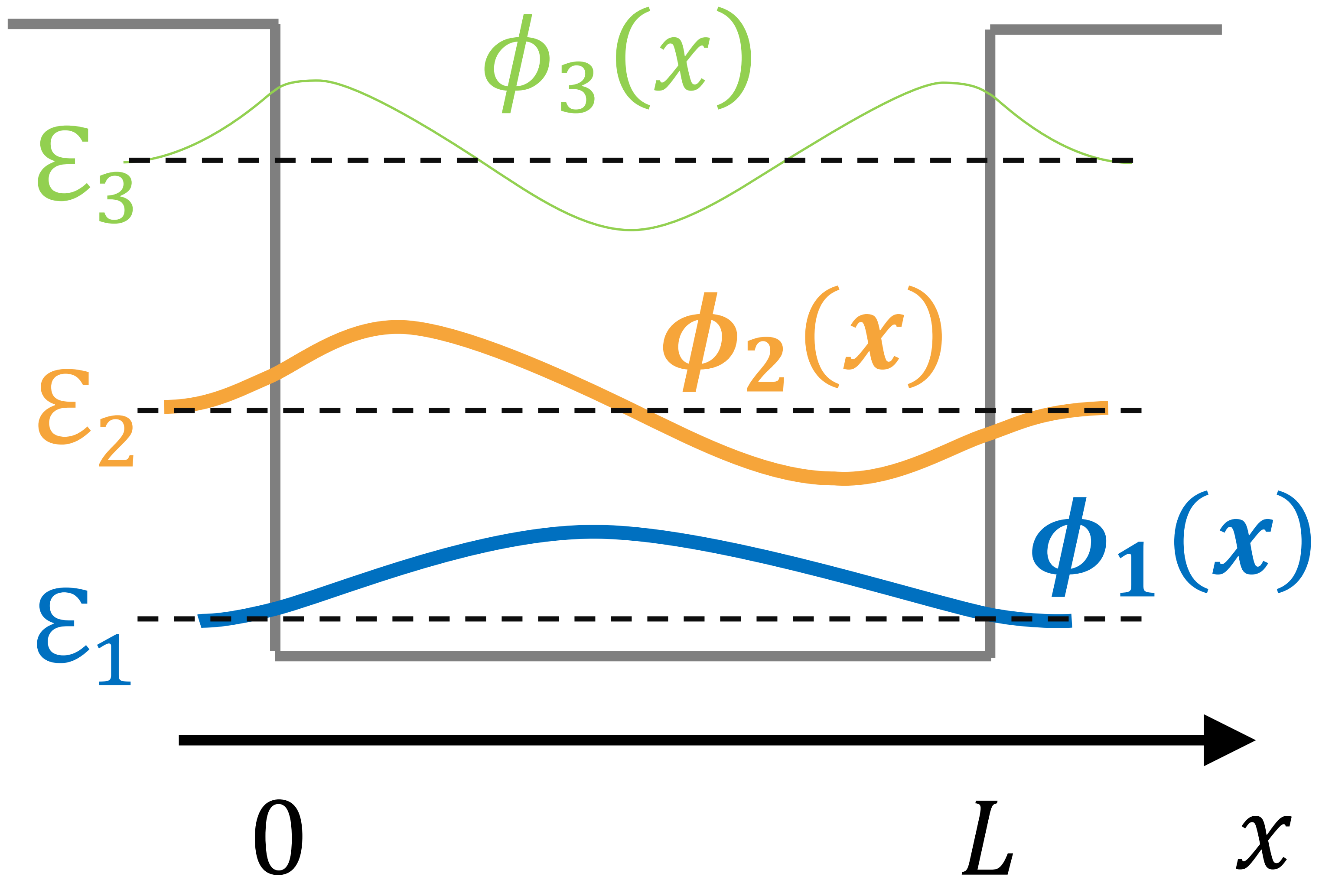


FINITE WELL: SUPERPOSITION

- Unlike infinite well (box) energies are not multiples: $\mathcal{E}_n \neq n^2 \mathcal{E}_1$
- Interference of 2 solutions results in **chaotic** probability density in time
- Example superposition:

$$\Phi(x,t) = \phi_1(x)\, e^{\frac{i\mathcal{E}_1 t}{\hbar}} + \phi_2(x)\, e^{\frac{i\mathcal{E}_2 t}{\hbar}}$$





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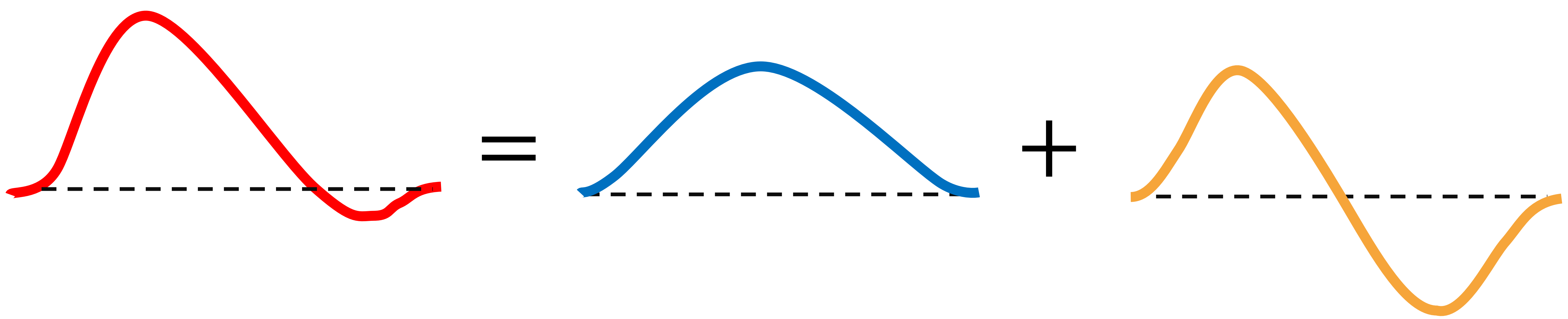
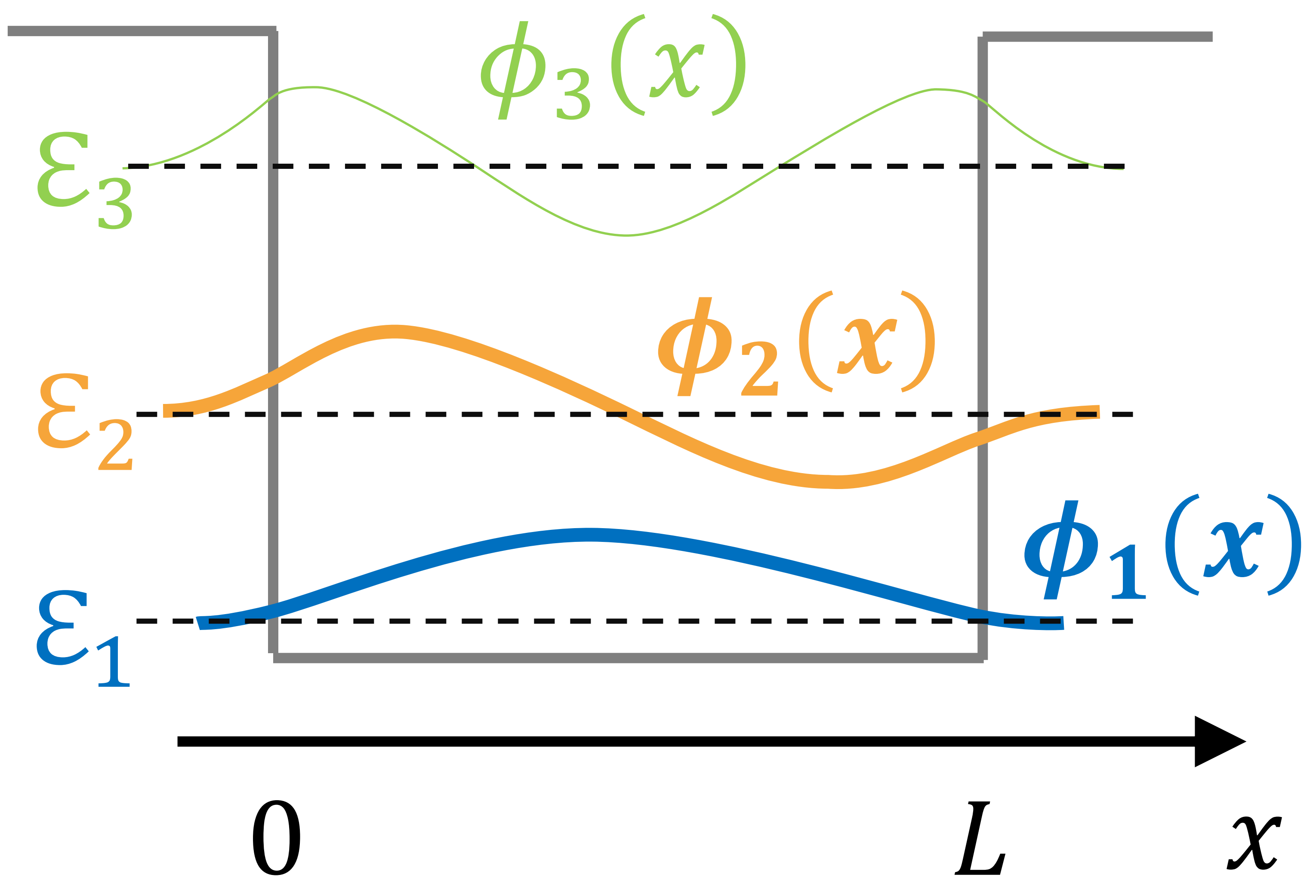
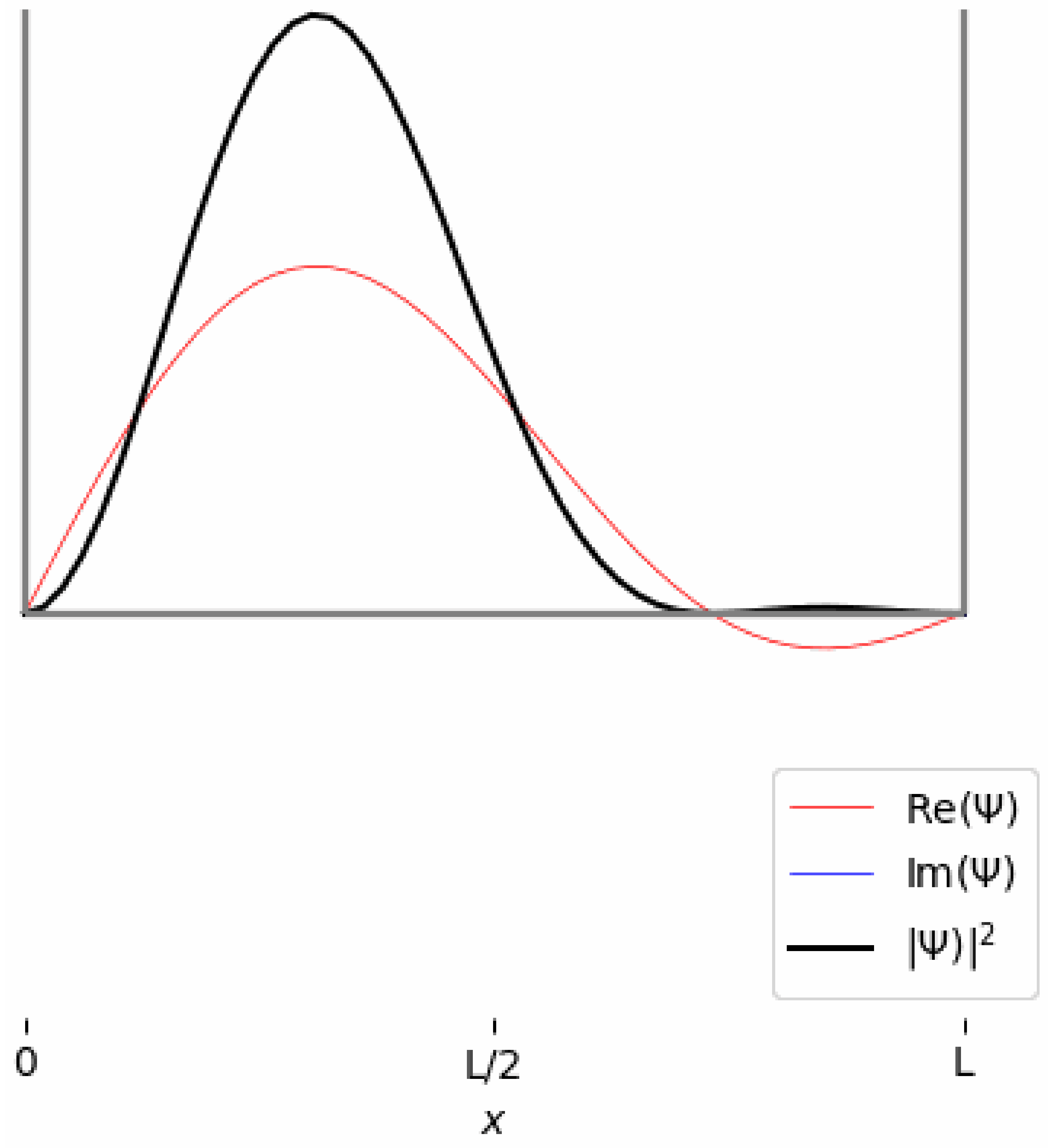




INFINITE WELL VERSUS FINITE WELL: SUPERPOSITION

- For an **infinite well** energies were multiples $E_n = n^2 E_1$
- **Interference** gives probability density **periodic in time**:

$$\Psi(x,t) = \psi_1(x)\, \boldsymbol{e}^{\frac{iE_1 t}{\hbar}} + \psi_2(x)\, \boldsymbol{e}^{\frac{i4E_1 t}{\hbar}}$$



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- Finite well **interference** of 2 solutions results in **chaotic** probability density in time:

$$\Phi(x,t) = \phi_1(x)\, \boldsymbol{e}^{\frac{\boldsymbol{i\mathcal{E}_1t}}{\hbar}} + \phi_2(x)\, \boldsymbol{e}^{\frac{\boldsymbol{i\mathcal{E}_2t}}{\hbar}}$$

SUMMARY FINITE WELL

- For energies lower than the potential outside the well:
  - Discrete energies **lower** than those of the infinite well
  - Wave functions penetrate the walls
  - **Nonzero probability outside** well
  - **Superposition** of solutions leads to **chaotic** wave function (and probability densities) in time

- For energies higher than the outside potential
  - **Continuous spectrum**
  - Solutions are left and right traveling waves
  - Wave numbers inside the well are larger (larger frequency)