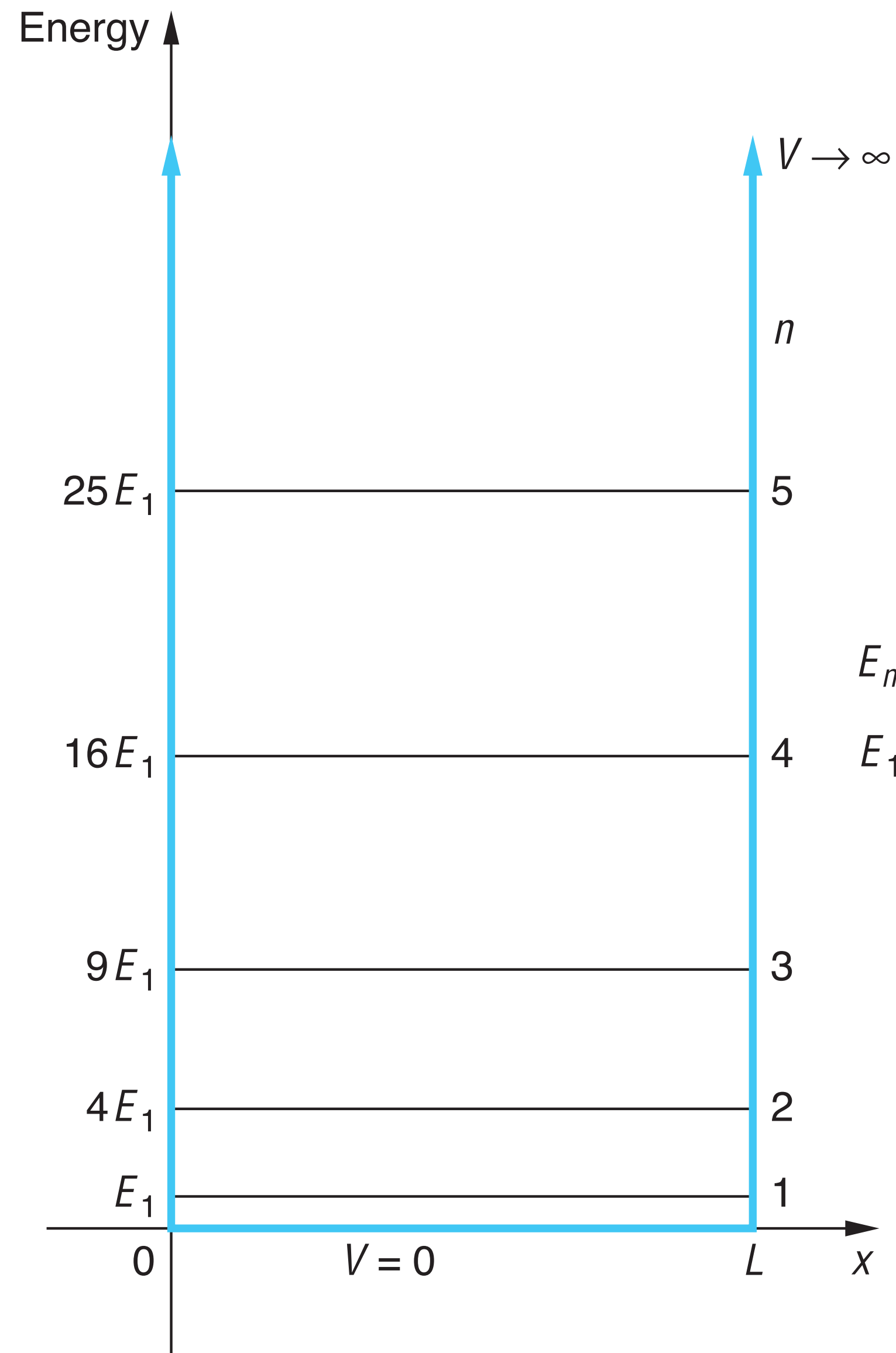
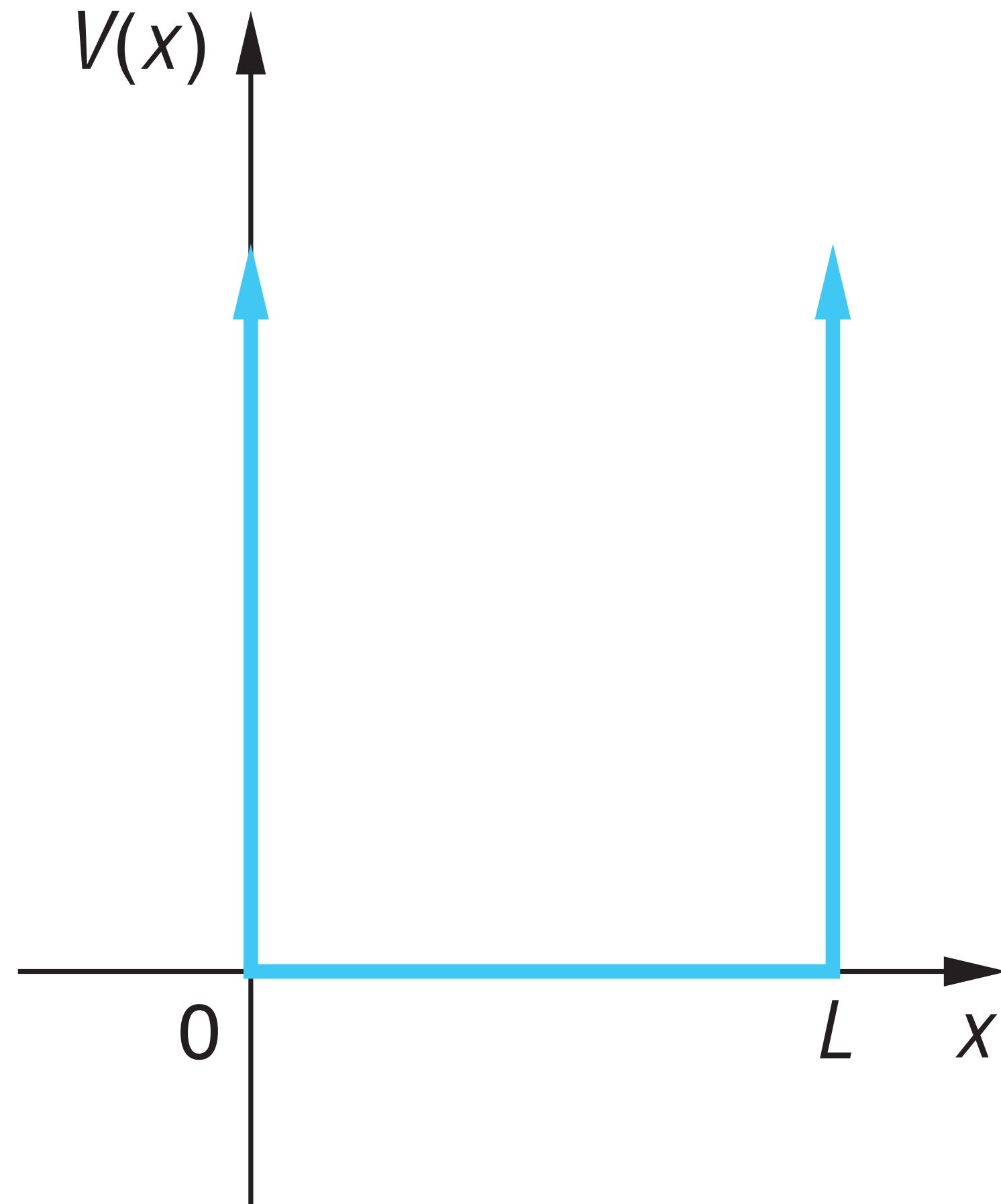


## *Lecture 05*

# *Step Potential, Operators & expectation values*

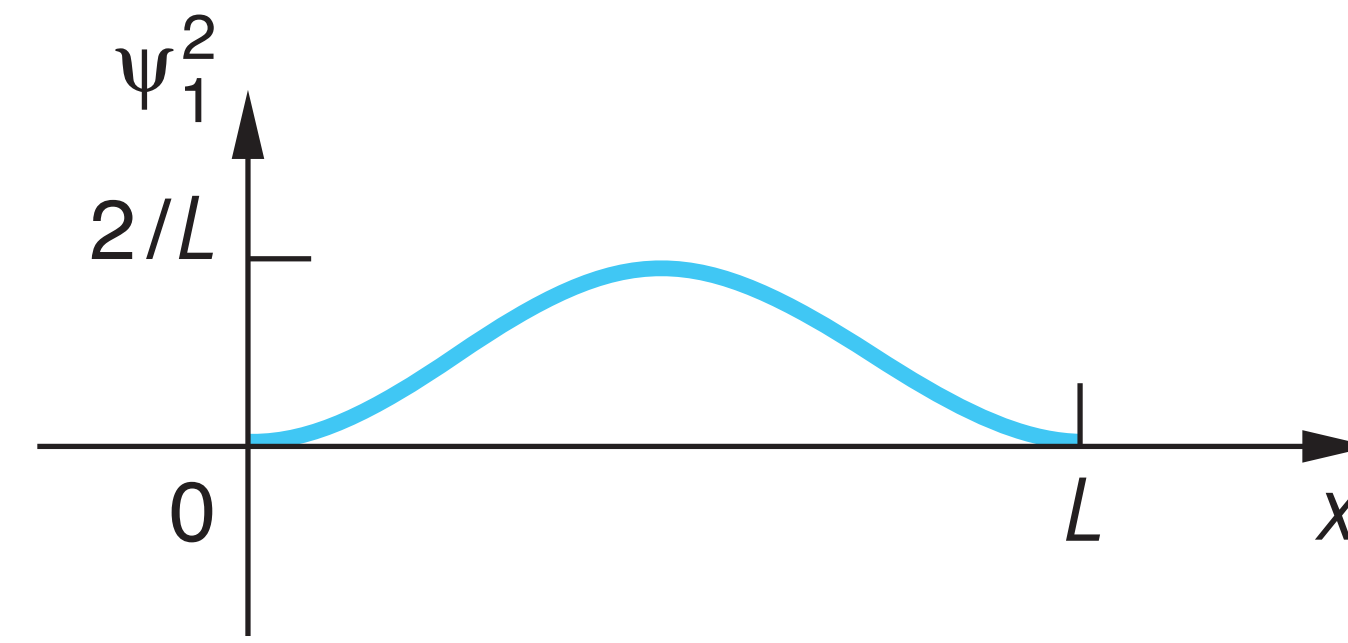
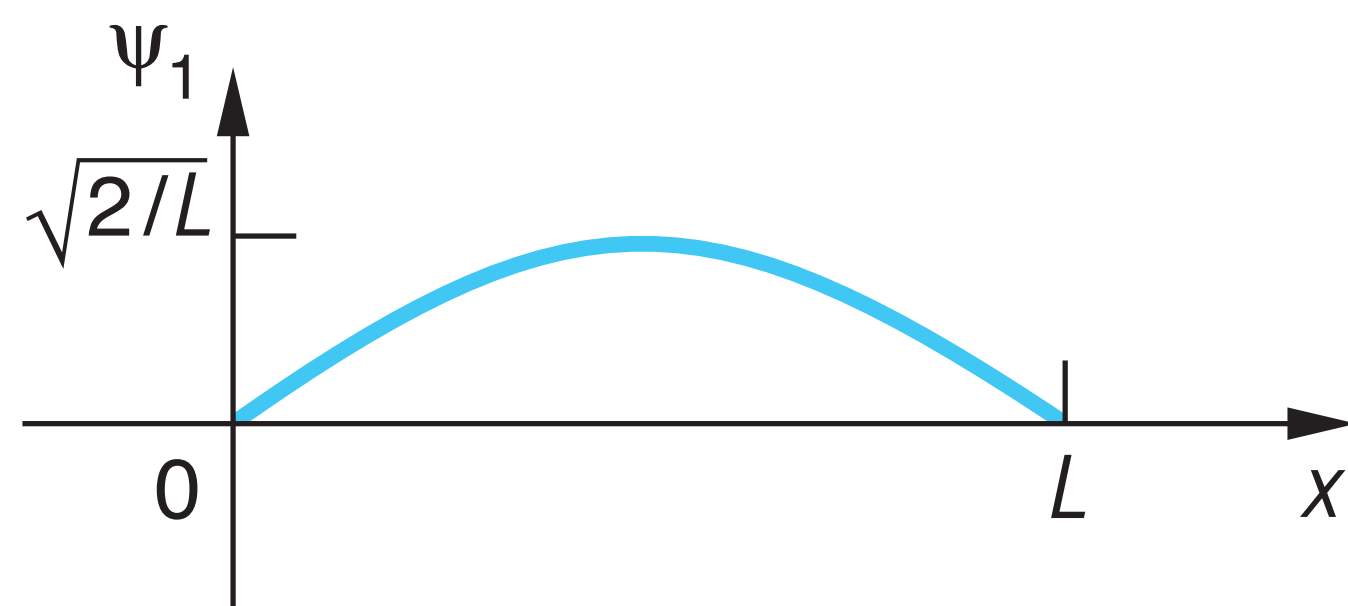
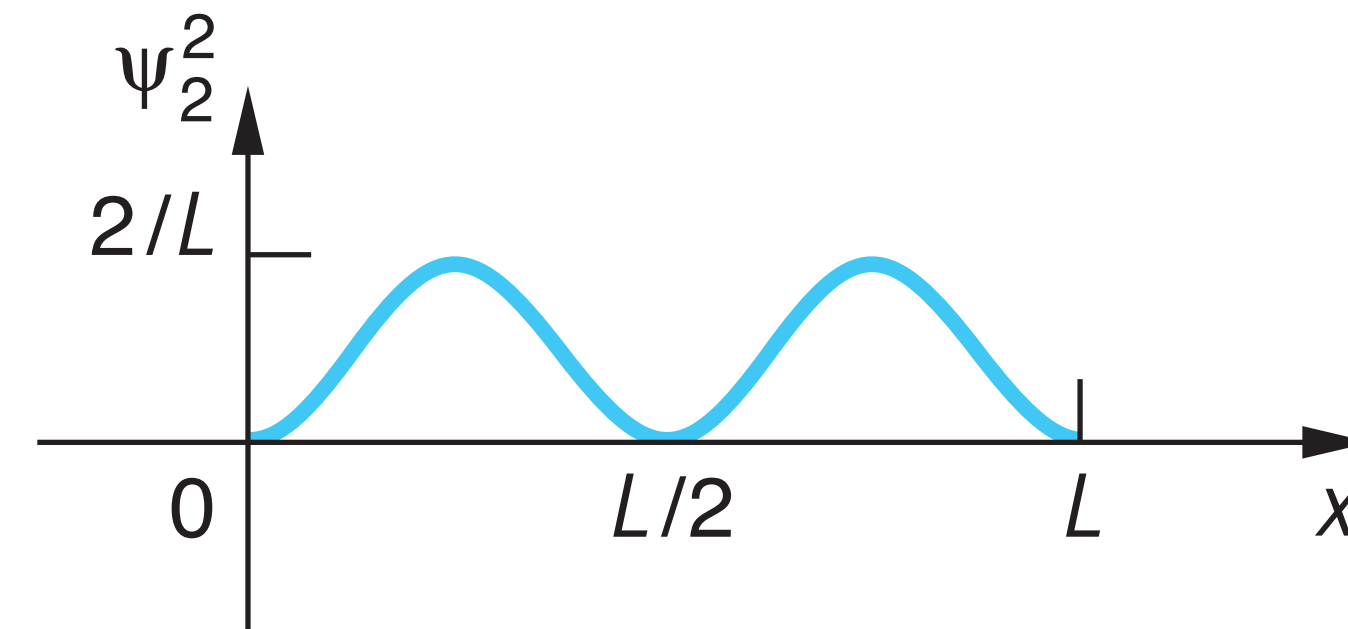
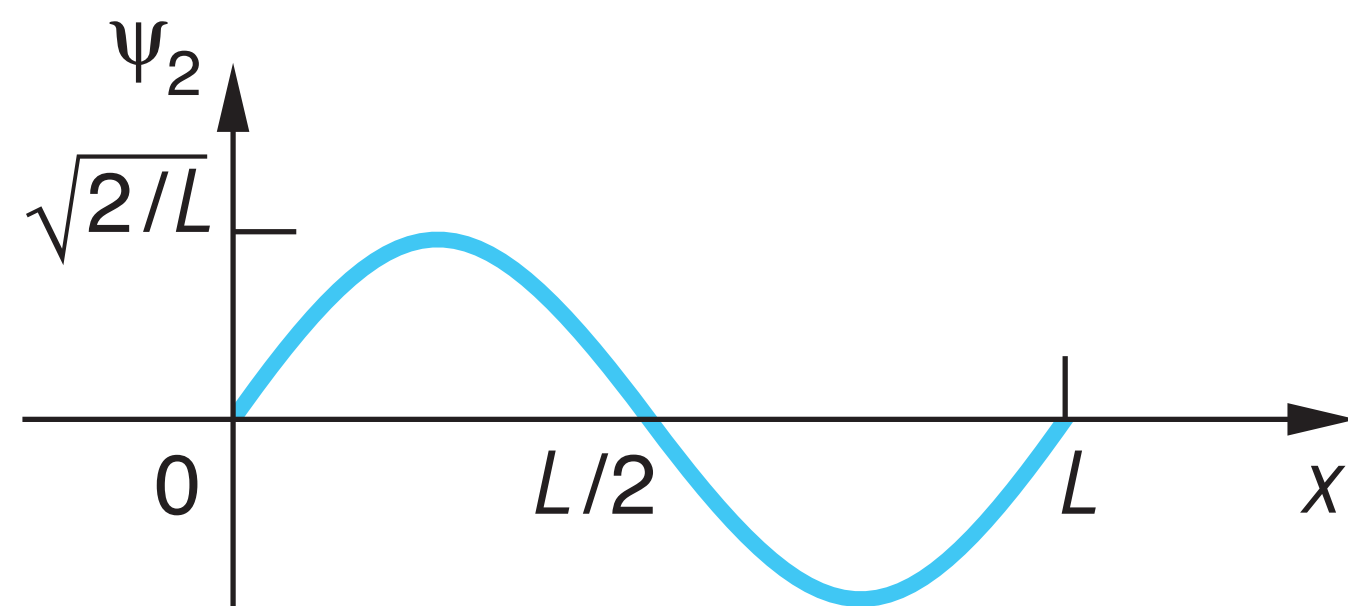
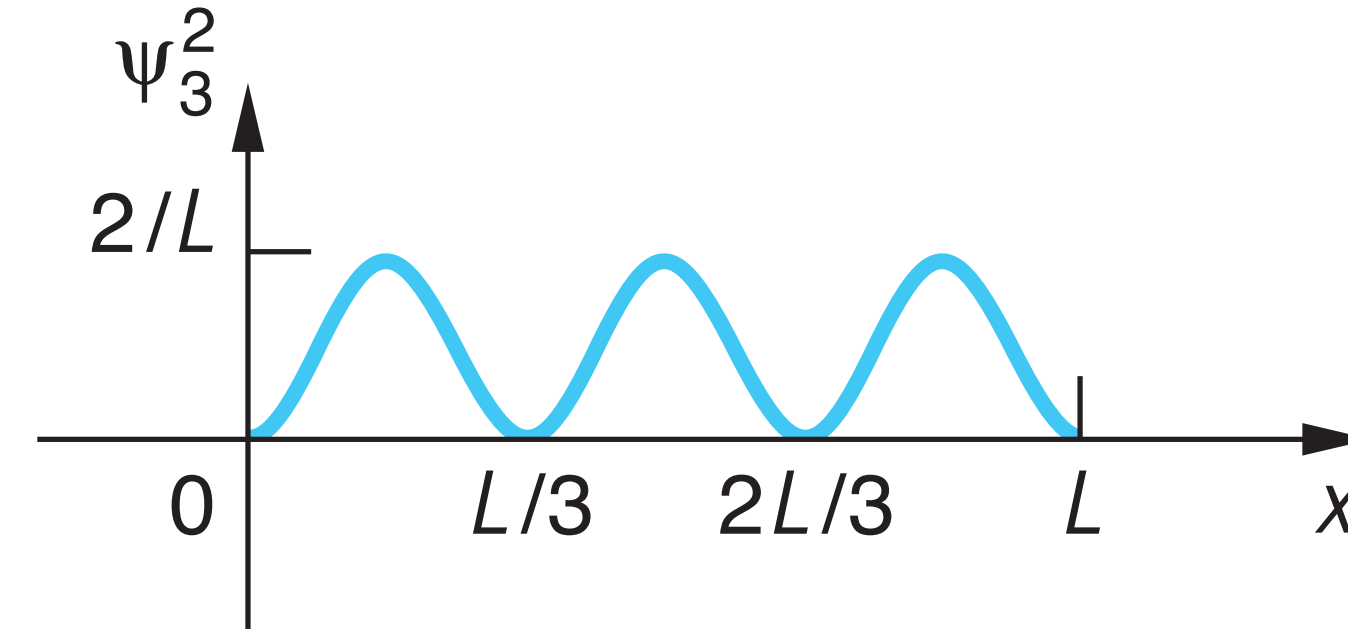
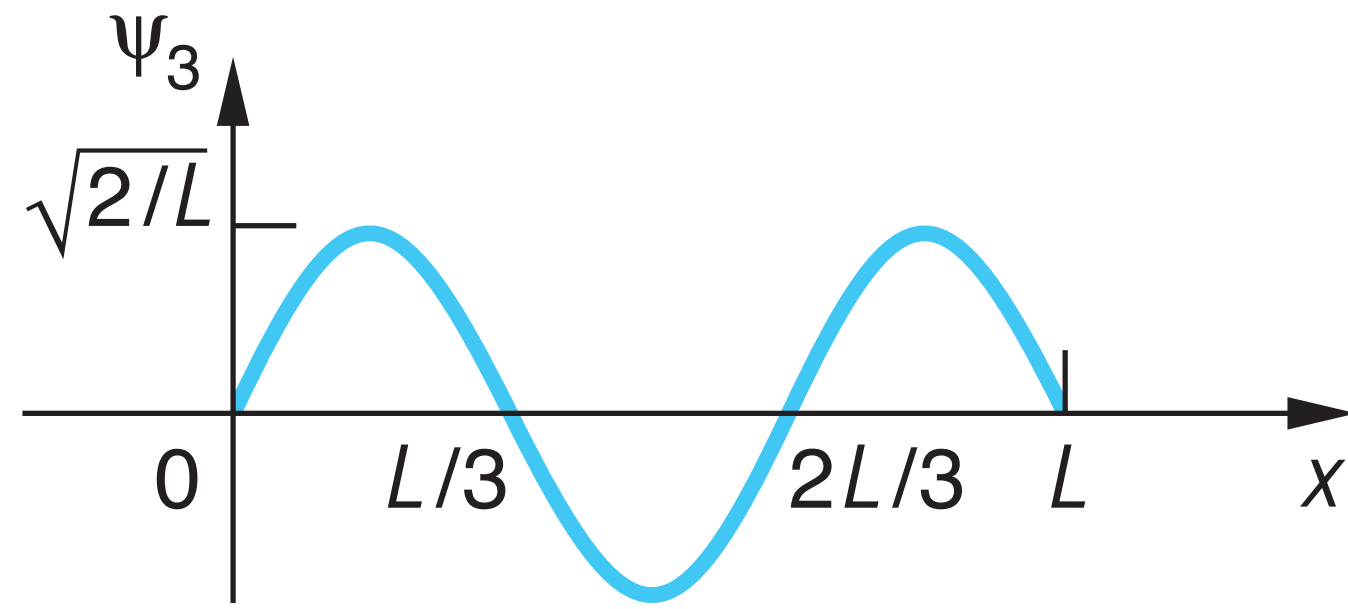
# Infinite potential well





# Infinite potential well

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



# Finite Potential Well



$$\psi_{II}(x) = C\sin k'x + D\cos k'x$$

$$\psi_I(x) = Ae^{kx}$$

$$\psi_{III}(x) = Fe^{-kx}$$

$$k^2 = -\frac{2mE}{\hbar^2} \quad k'^2 = \frac{2m}{\hbar^2}(V_0 + E)$$

$$k^2 + k'^2 = \frac{2mV_0}{\hbar^2}$$

$$k'L = z$$

$$z_0 = \frac{L}{\hbar} \sqrt{2mV_0}$$

$$z^2 + (kL)^2 = z_0^2$$

$$kL = \sqrt{z_0^2 - z^2}$$

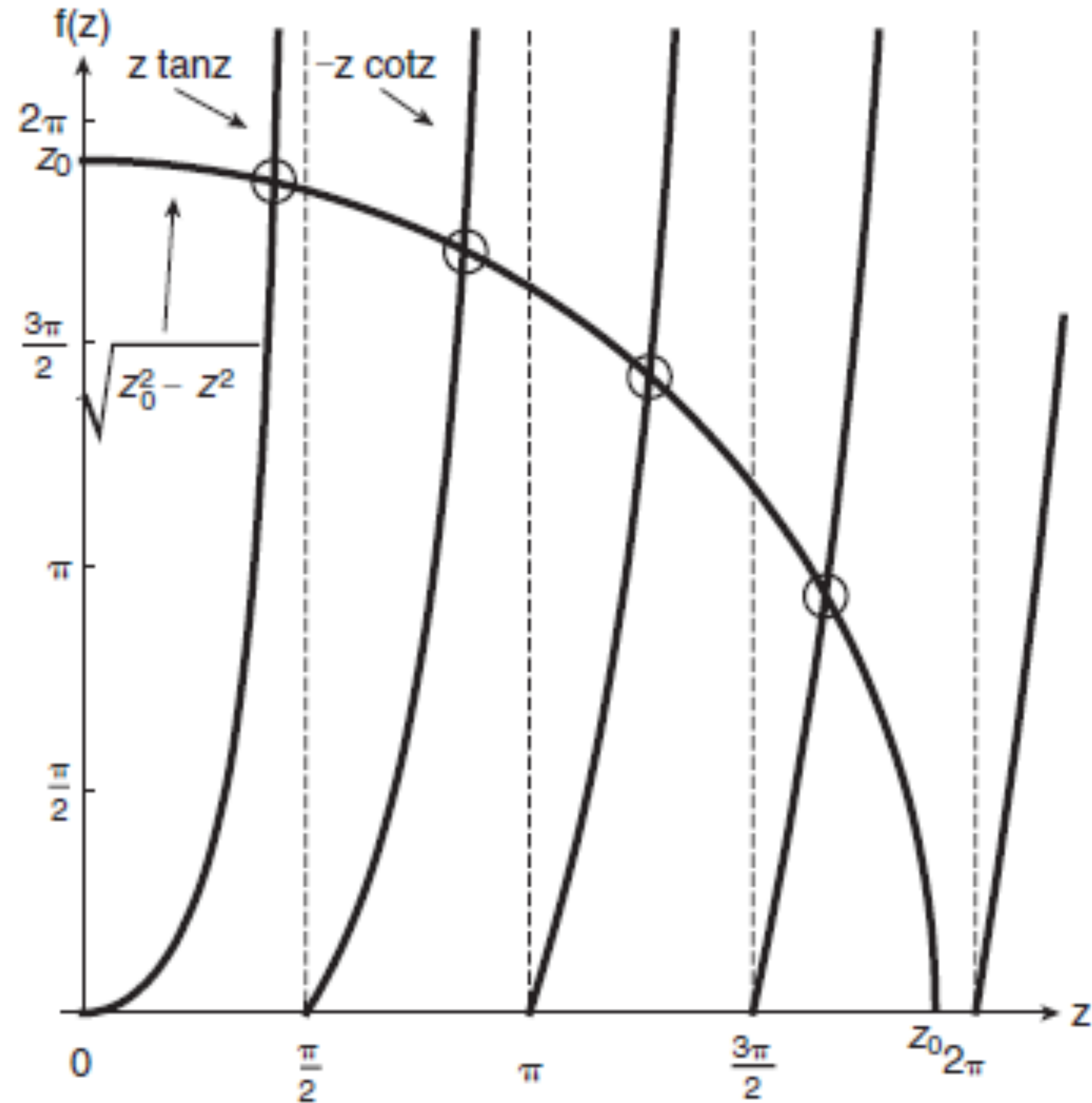
$$k = k' \tan k'L$$

$$kL = k'L \tan k'L$$

$$z \tan z = \sqrt{z_0^2 - z^2}$$

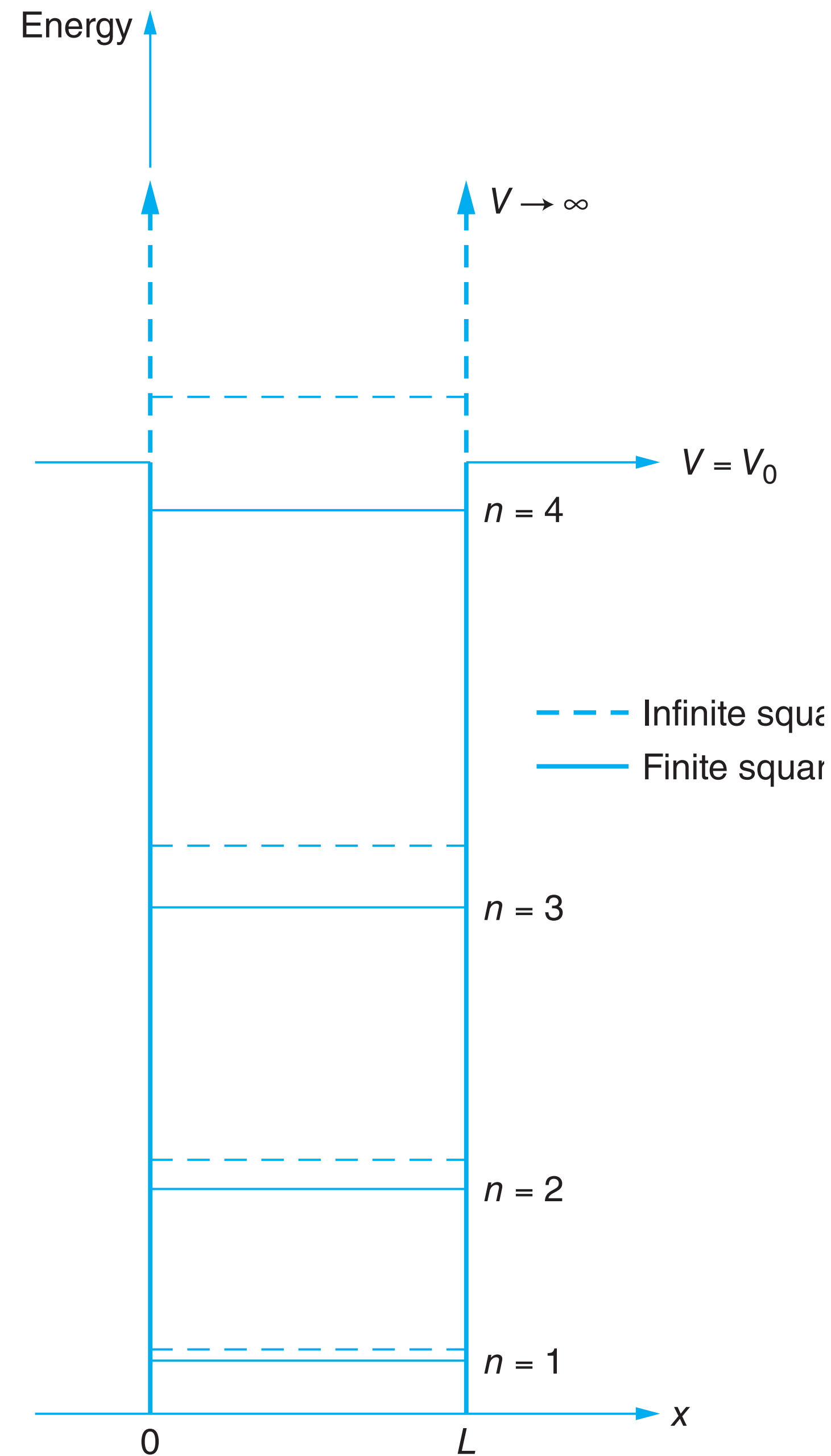
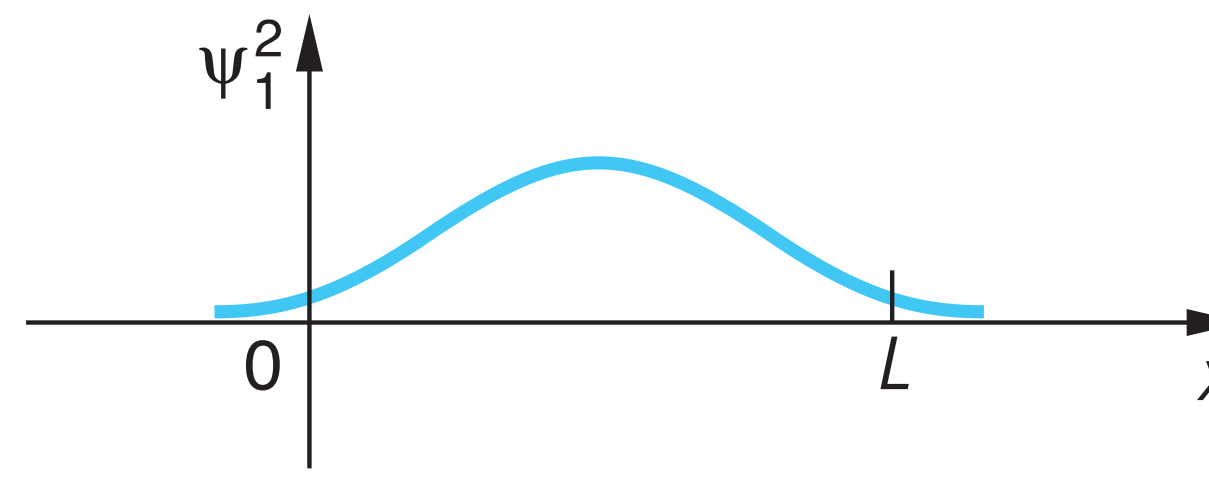
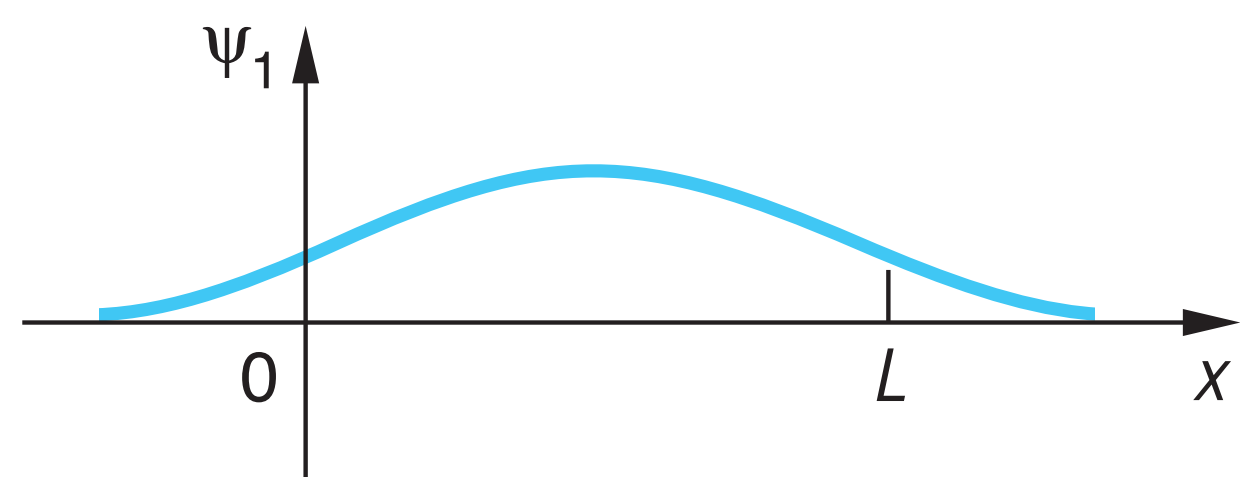
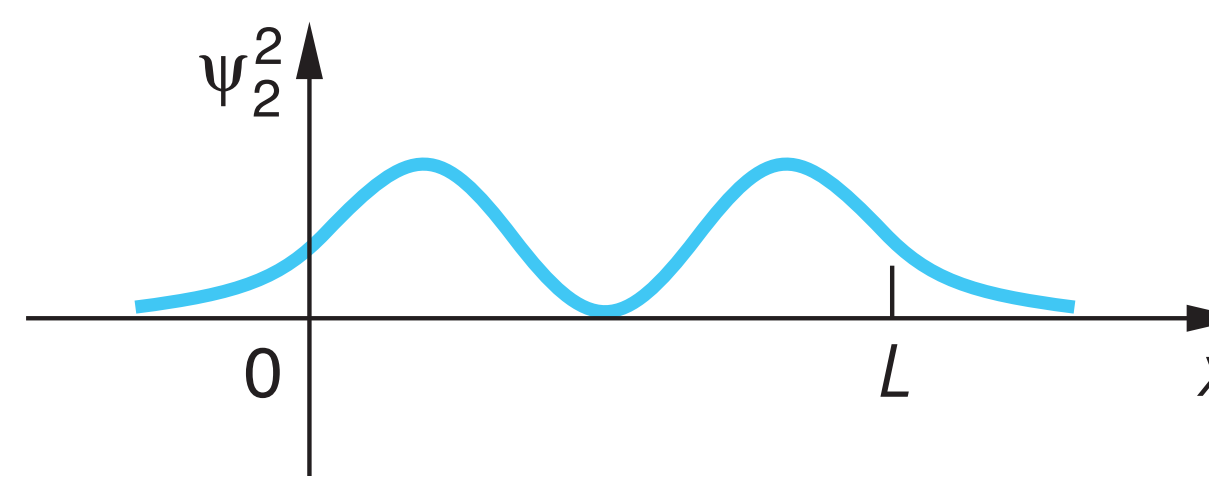
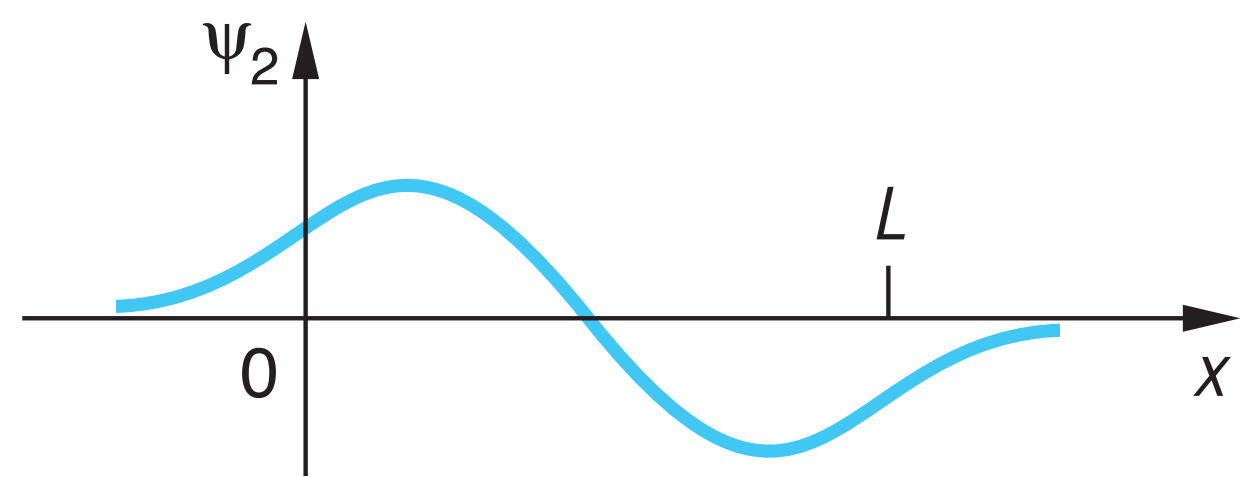
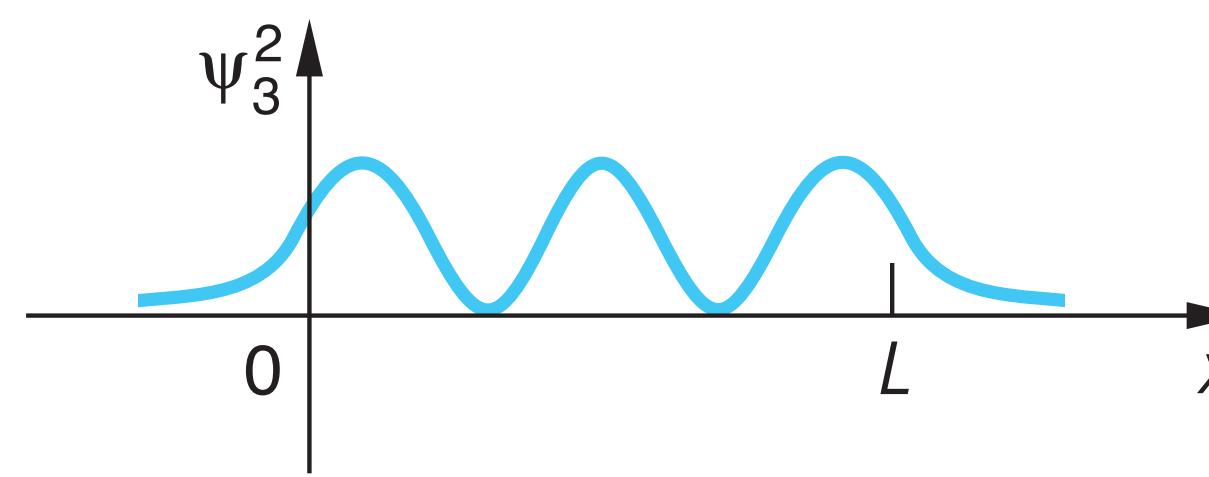
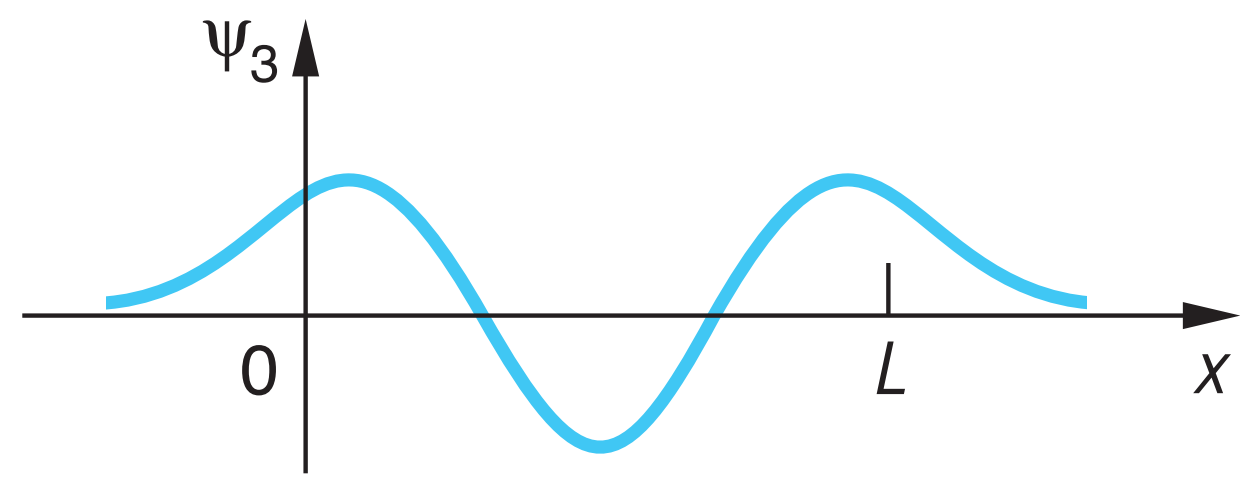


# Finite Potential Well

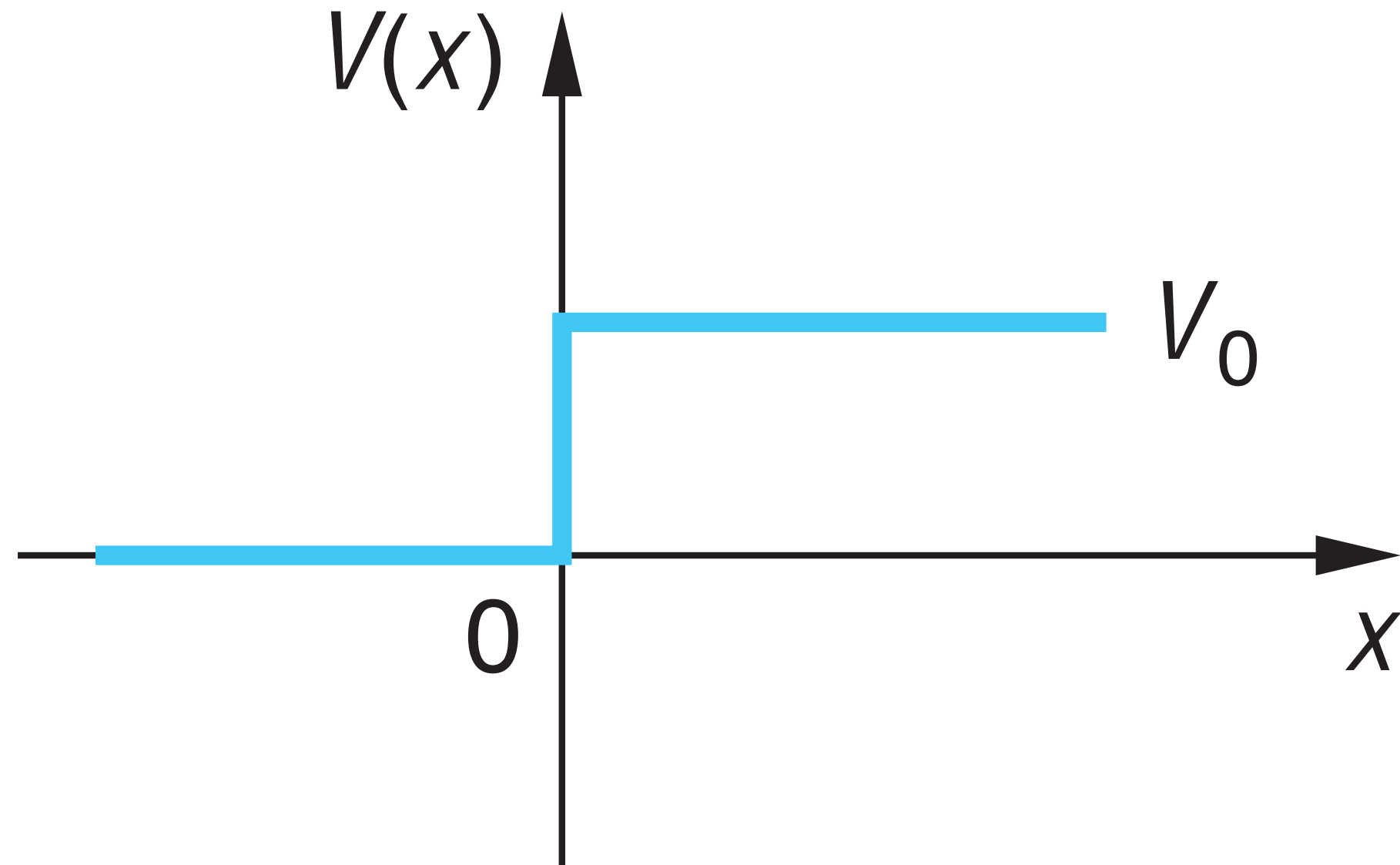


Graphical solution of the transcendental equations for the allowed energies of a finite square well ( $z_0 = 6$ ).

# Finite Potential Well



# Step Potential



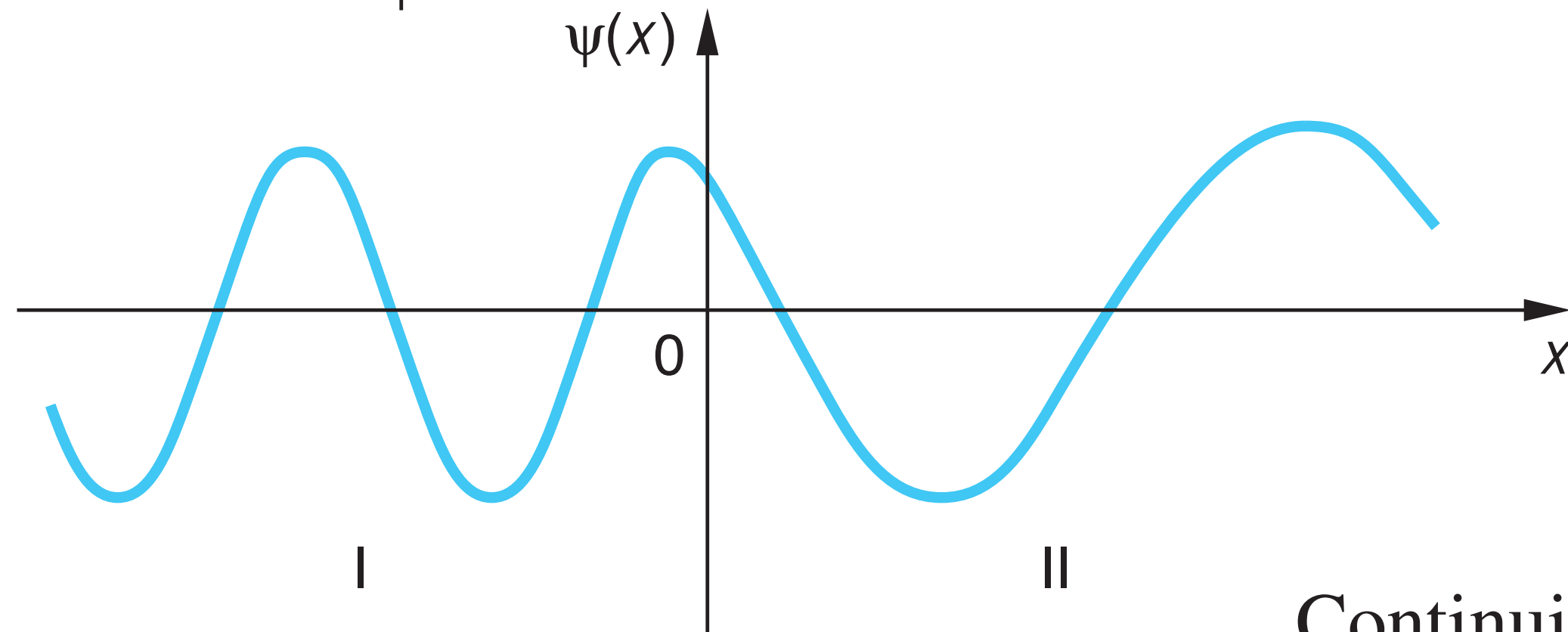
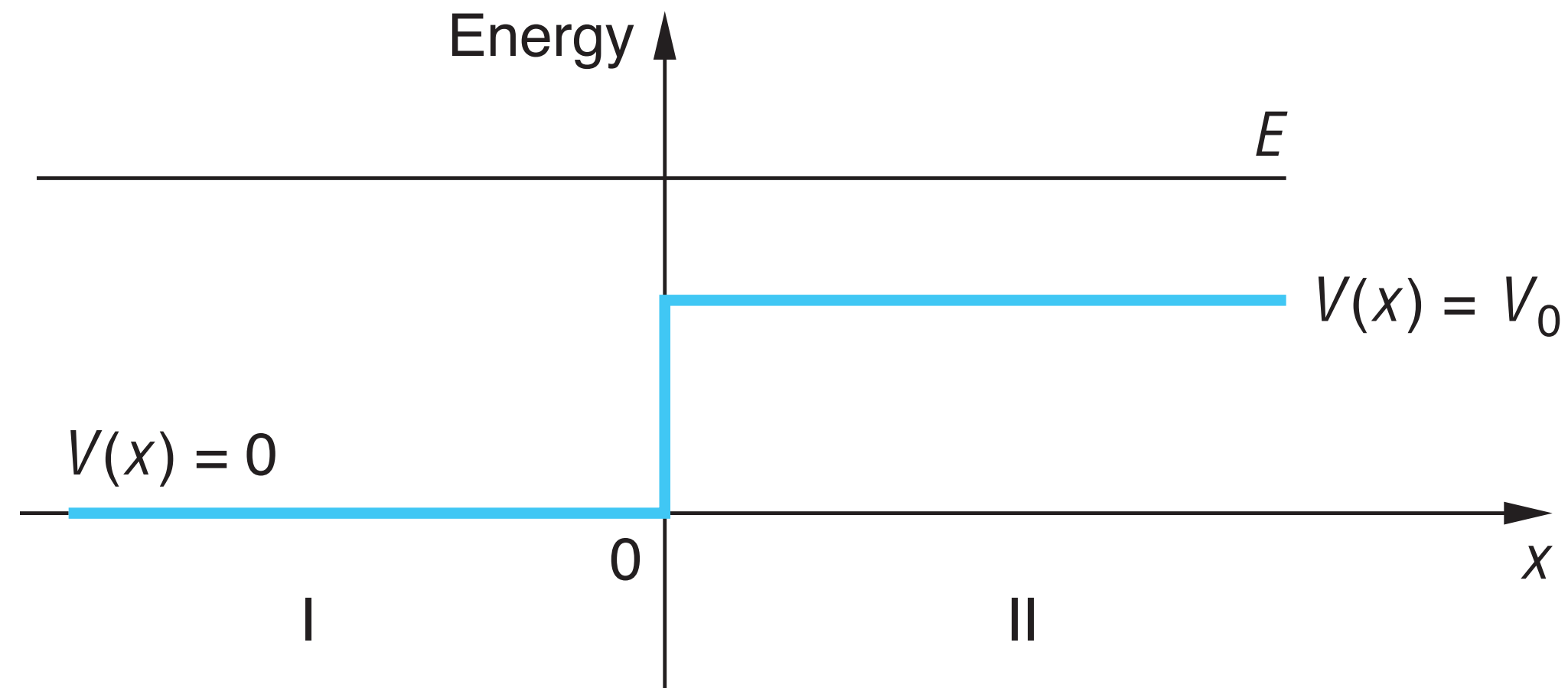
$$V(x) = 0 \quad \text{for} \quad x < 0$$
$$V(x) = V_0 \quad \text{for} \quad x > 0$$

$$(x < 0) \quad \frac{d^2\psi(x)}{dx^2} = -k_1^2\psi(x)$$

$$(x > 0) \quad \frac{d^2\psi(x)}{dx^2} = -k_2^2\psi(x)$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

# Step Potential



$$(x < 0) \quad \psi_{\text{I}}(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$(x > 0) \quad \psi_{\text{II}}(x) = Ce^{ik_2x} + De^{-ik_2x}$$

$$\psi_{\text{I}}(0) = \psi_{\text{II}}(0) \text{ and } \frac{d\psi}{dx}(0) = \frac{d\psi_{\text{II}}(0)}{dx}.$$

$$\psi_{\text{I}}(0) = A + B = \psi_{\text{II}}(0) = C$$

$$A + B = C$$

Continuity of  $\frac{d\psi}{dx}$  at  $x = 0$  gives

$$k_1A - k_1B = k_2C$$



# Step Potential

$$B = \frac{k_1 - k_2}{k_1 + k_2} A = \frac{E^{1/2} - (E - V_0)^{1/2}}{E^{1/2} + (E - V_0)^{1/2}} A$$

$$C = \frac{2k_1}{k_1 + k_2} A = \frac{2E^{1/2}}{E^{1/2} + (E - V_0)^{1/2}} A$$

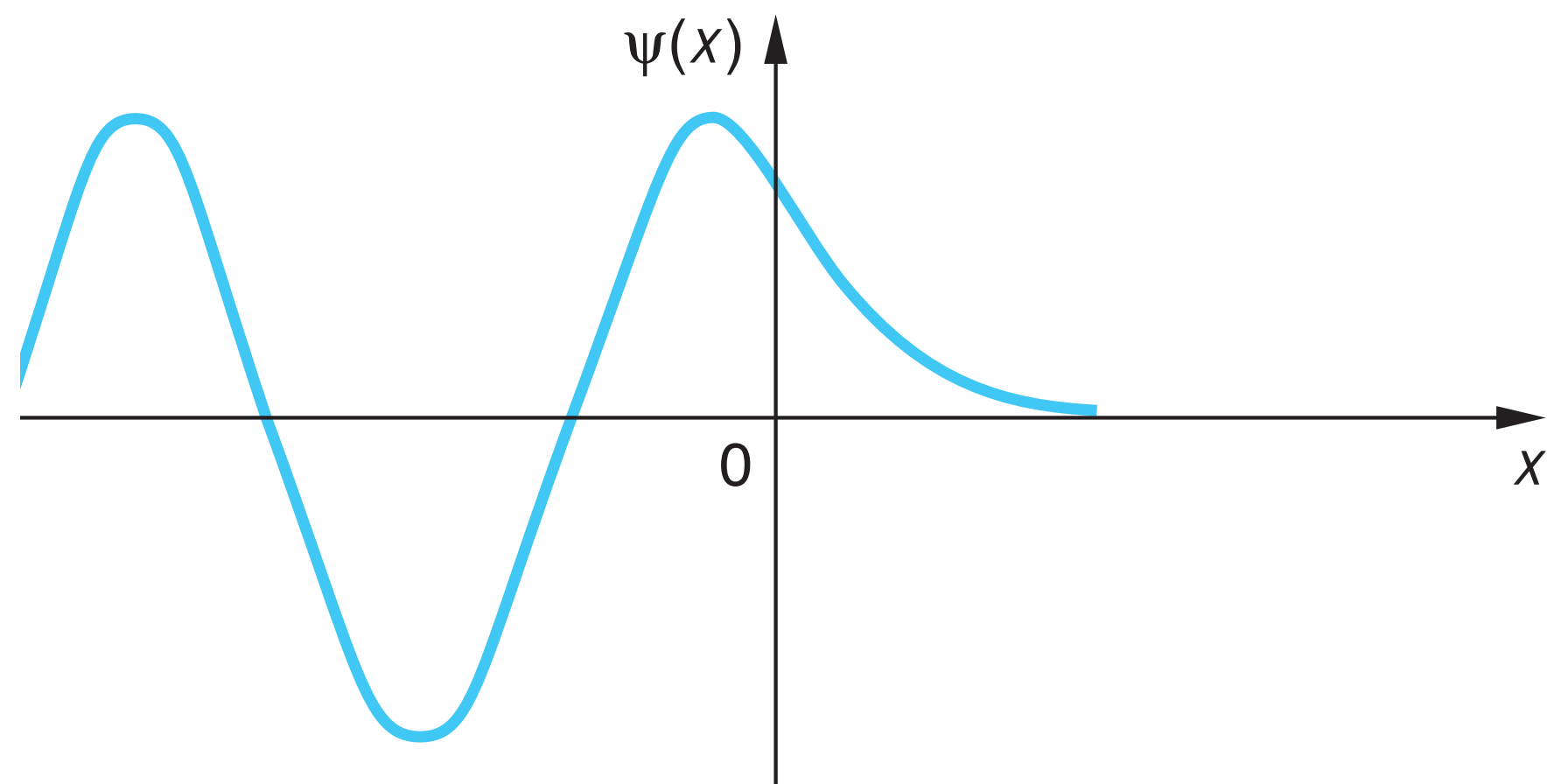
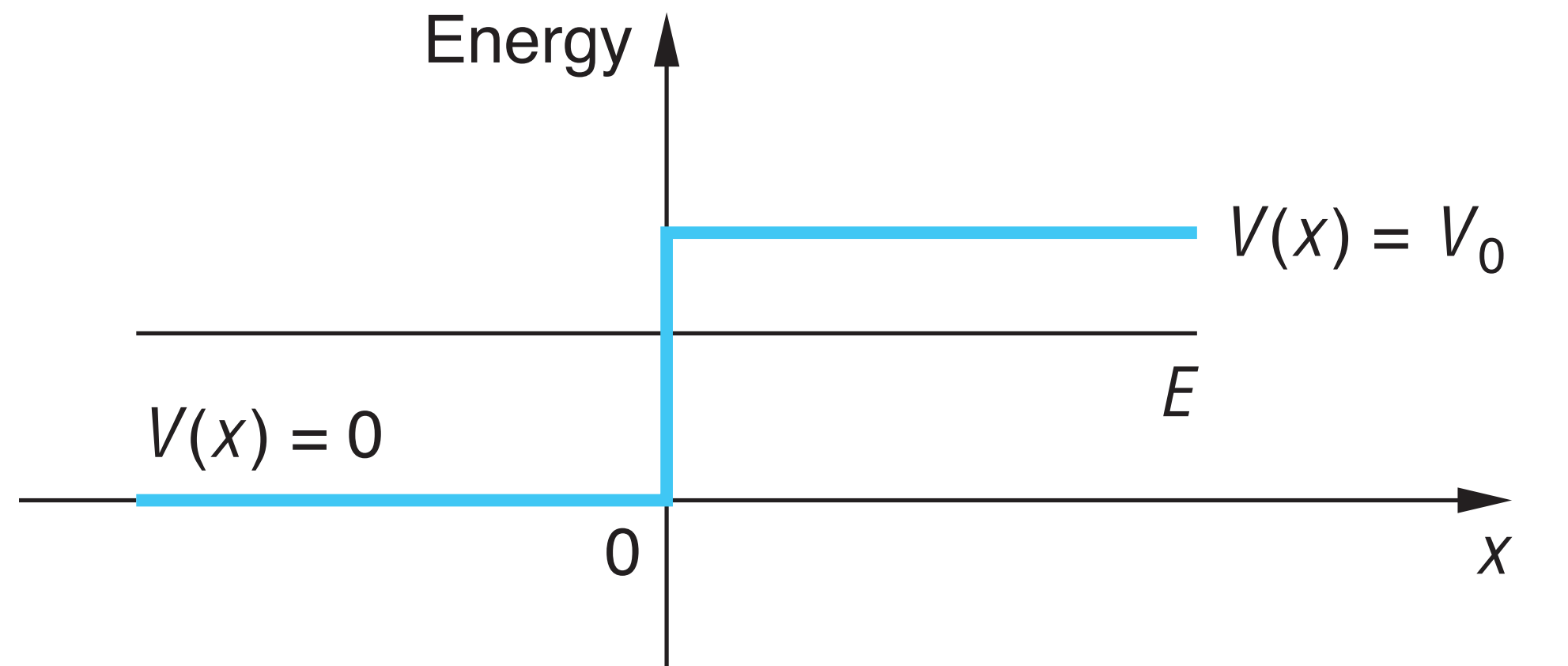
$$R = \frac{|B|^2}{|A|^2} = \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2$$

$$T = \frac{k_2 |C|^2}{k_1 |A|^2} = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

$$T + R = 1$$



# Step Potential



$$E < V_0.$$

$$\psi_{II}(x) = Ce^{ik_2x} = Ce^{-\alpha x}$$

$$\alpha = \sqrt{2m(V_0 - E)}/\hbar$$

$$\psi_{II} \rightarrow 0 \text{ as } x \rightarrow \infty$$

$$|B|^2 = |A|^2, R = 1, \text{ and } T = 0.$$

$$|\psi_{II}|^2 = |C|^2 e^{-2\alpha x}$$



# Operators and expectation values



$$\dot{x}/dt = \partial H/\partial p \text{ and } dp/dt = -\partial H/\partial x,$$

To every physically measurable quantity  $A$ , called an observable or dynamical variable, there corresponds a linear Hermitian operator  $\hat{A}$  whose eigenvectors form a complete basis.

$$\hat{A}|\psi(t)\rangle = a_n|\psi_n\rangle,$$

$$f(\vec{r}, \vec{p}) \longrightarrow F(\hat{\vec{R}}, \hat{\vec{P}}) = f(\hat{\vec{R}}, -i\hbar\vec{\nabla}),$$

$$H = \frac{1}{2m}\vec{p}^2 + V(\vec{r}, t)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\hat{\vec{R}}, t),$$

# Operators and expectation values



| Symbol | Physical quantity  | Operator                                      |
|--------|--|---|
| $f(x)$ | Any function of $x$ —the position $x$ , the potential energy $V(x)$ , etc. | $f(x)$  |
| $p_x$  | $x$ component of momentum  | $\frac{\hbar}{i} \frac{\partial}{\partial x}$ |
| $p_y$  | $y$ component of momentum  | $\frac{\hbar}{i} \frac{\partial}{\partial y}$ |
| $p_z$  | $z$ component of momentum  | $\frac{\hbar}{i} \frac{\partial}{\partial z}$ |



# Operators and expectation values



| Symbol | Physical quantity                 | Operator  |
|--------|-----------------------------------|---|
| $E$    | Hamiltonian (time independent)    | $\frac{p_{\text{op}}^2}{2m} + V(x)$                   |
| $E$    | Hamiltonian (time dependent)      | $i\hbar \frac{\partial}{\partial t}$                  |
| $E_k$  | Kinetic energy                    | $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$ |
| $L_z$  | $z$ component of angular momentum | $-i\hbar \frac{\partial}{\partial \phi}$              |

# Operators and expectation values

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x, t) x \Psi(x, t) dx$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^*(x) x \psi(x) dx$$

$$\langle p \rangle = \int_{-\infty}^{+\infty} \Psi^* \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi dx$$

$$\langle p^2 \rangle = \int_{-\infty}^{+\infty} \Psi^* \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi dx$$



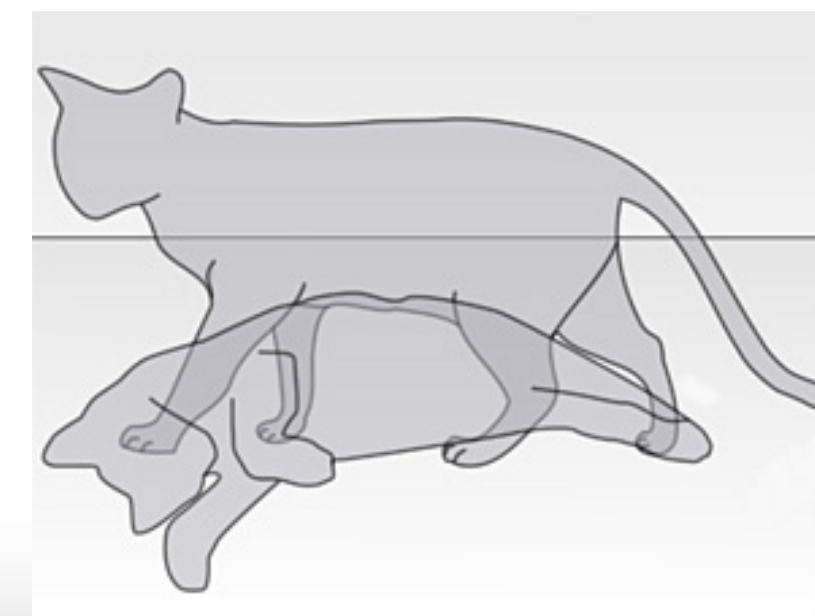
# Expectation values of $p$ and $p^2$ for ground state of Infinite well



$$\begin{aligned}\langle p \rangle &= \int_0^L \left( \sqrt{\frac{2}{L}} \sin \frac{nX}{L} \right) \left( \frac{\hbar}{i} \frac{\partial}{\partial X} \right) \left( \sqrt{\frac{2}{L}} \sin \frac{nX}{L} \right) dx \\ &= \frac{\hbar}{i} \frac{2}{L} \frac{\pi}{L} \int_0^L \sin \frac{\pi X}{L} \cos \frac{\pi X}{L} dx = 0\end{aligned}$$

$$\begin{aligned}\frac{\hbar}{i} \frac{\partial}{\partial X} \left( \frac{\hbar}{i} \frac{\partial}{\partial X} \right) \psi &= -\hbar^2 \frac{\partial^2 \psi}{\partial X^2} = -\hbar^2 \left( -\frac{\pi^2}{L^2} \sqrt{\frac{2}{L}} \sin \frac{\pi X}{L} \right) \\ &= +\frac{\hbar^2 \pi^2}{L^2} \psi\end{aligned}$$

$$\langle p^2 \rangle = \frac{\hbar^2 \pi^2}{L^2} \int_0^L \psi^* \psi dx = \frac{\hbar^2 \pi^2}{L^2}$$



# Curiosity Kills the Cat

*Lecture 05*  
*Concluded*