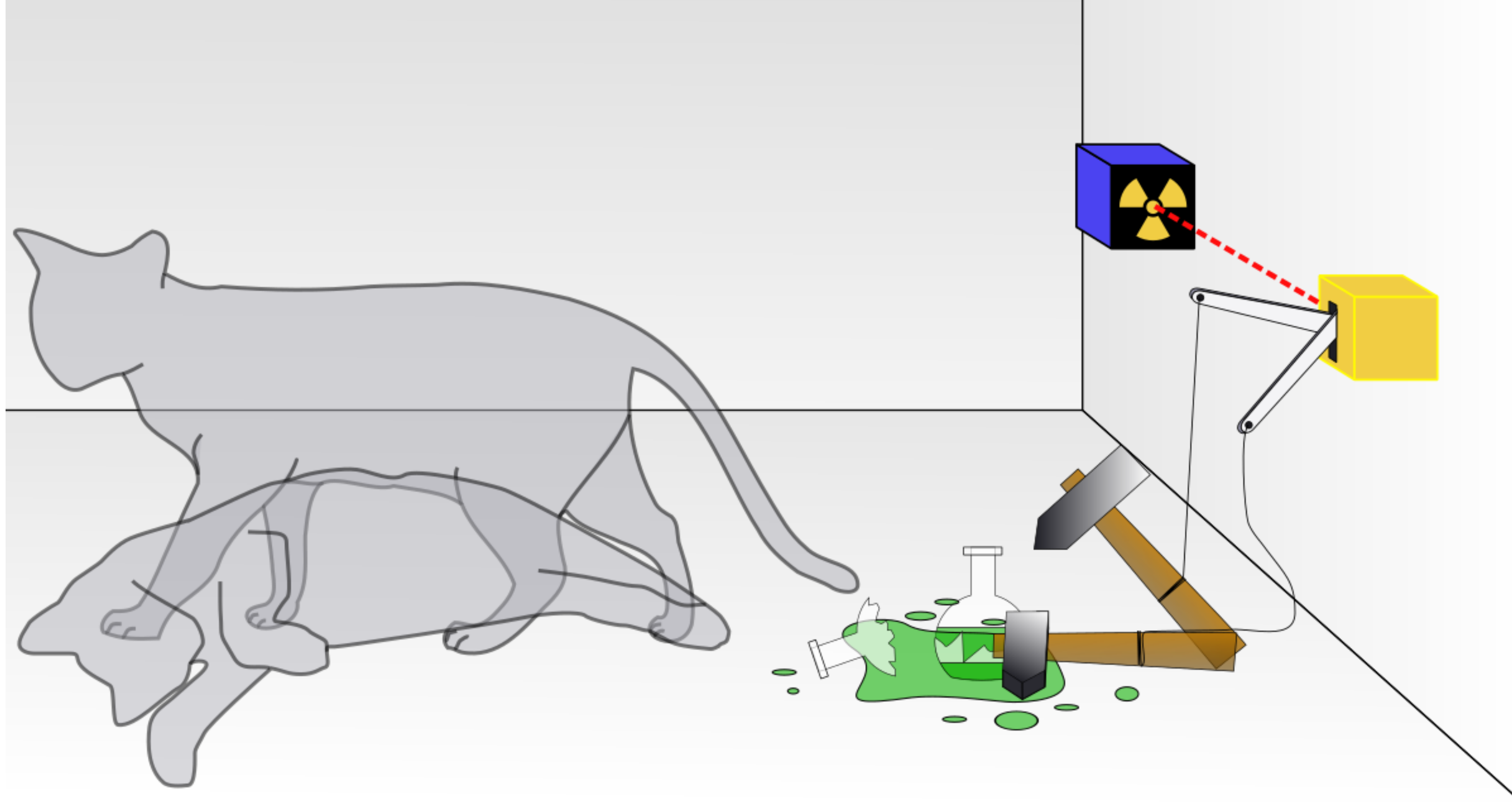




Lecture 06

Step potential and Harmonic Oscillator

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.

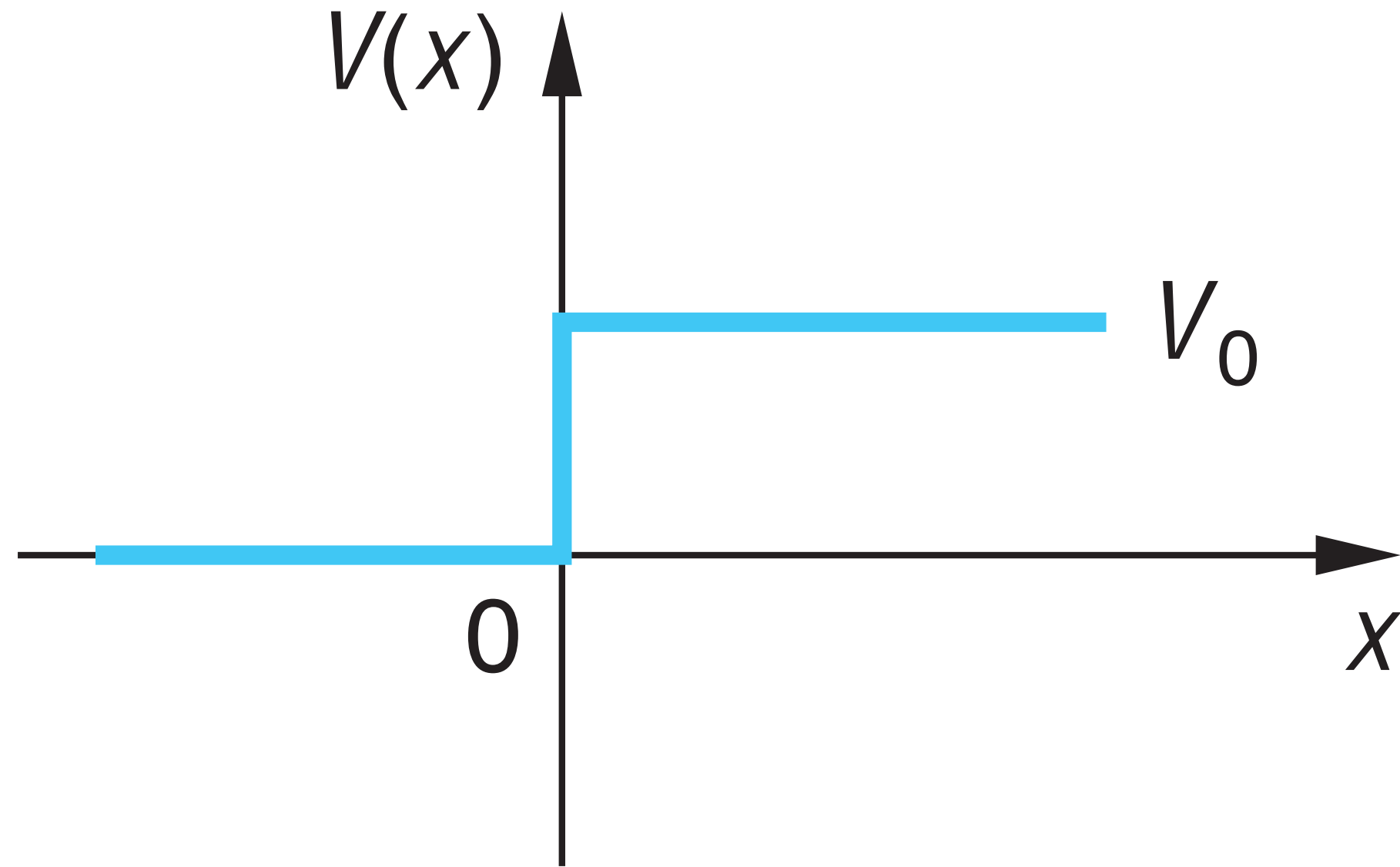
$$\hat{A}|\psi(t)\rangle = a_n|\psi_n\rangle,$$

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

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

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

Step Potential



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

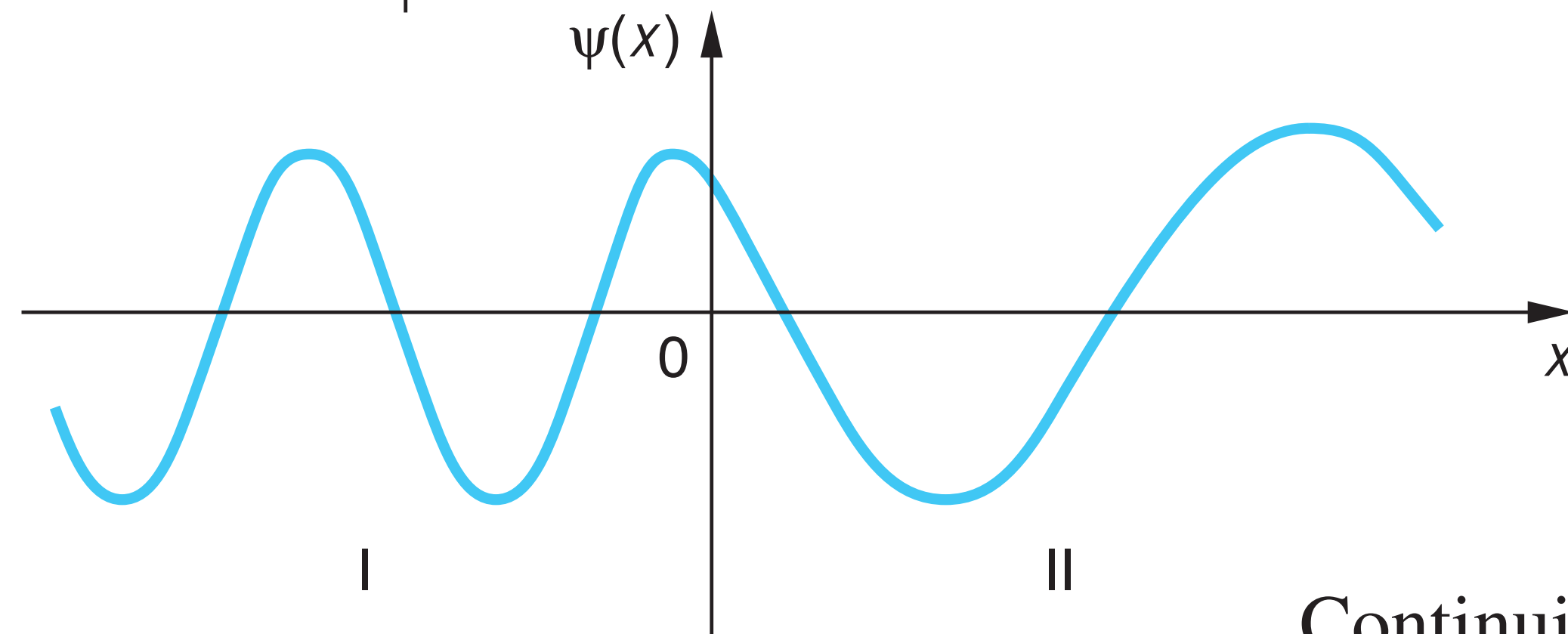
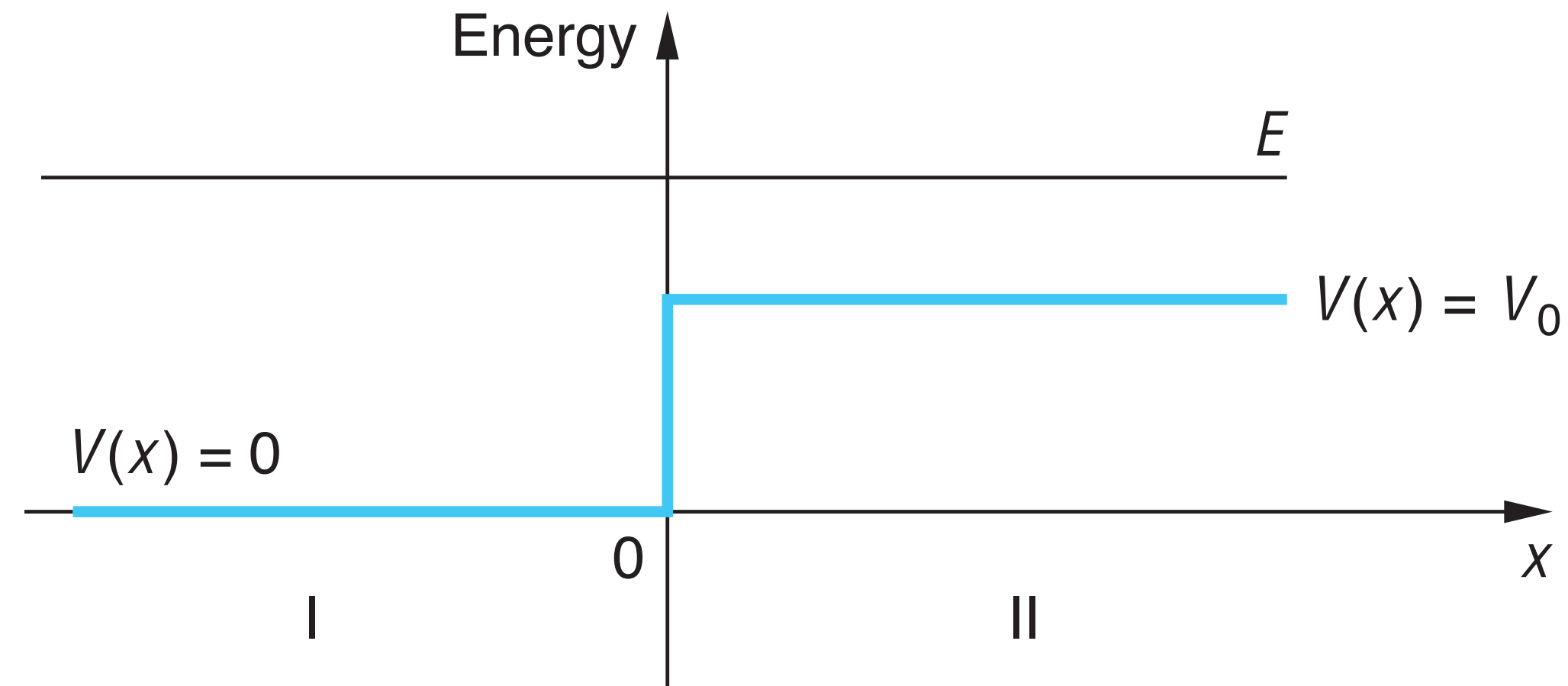
$$V(x) = V_0 \quad \text{for} \quad x > 0$$

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

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

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

Step Potential



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

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

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

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

$$A + B = C$$

Continuity of $d\psi/dx$ at $x = 0$ gives

$$k_1A - k_1B = k_2C$$

Step Potential



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

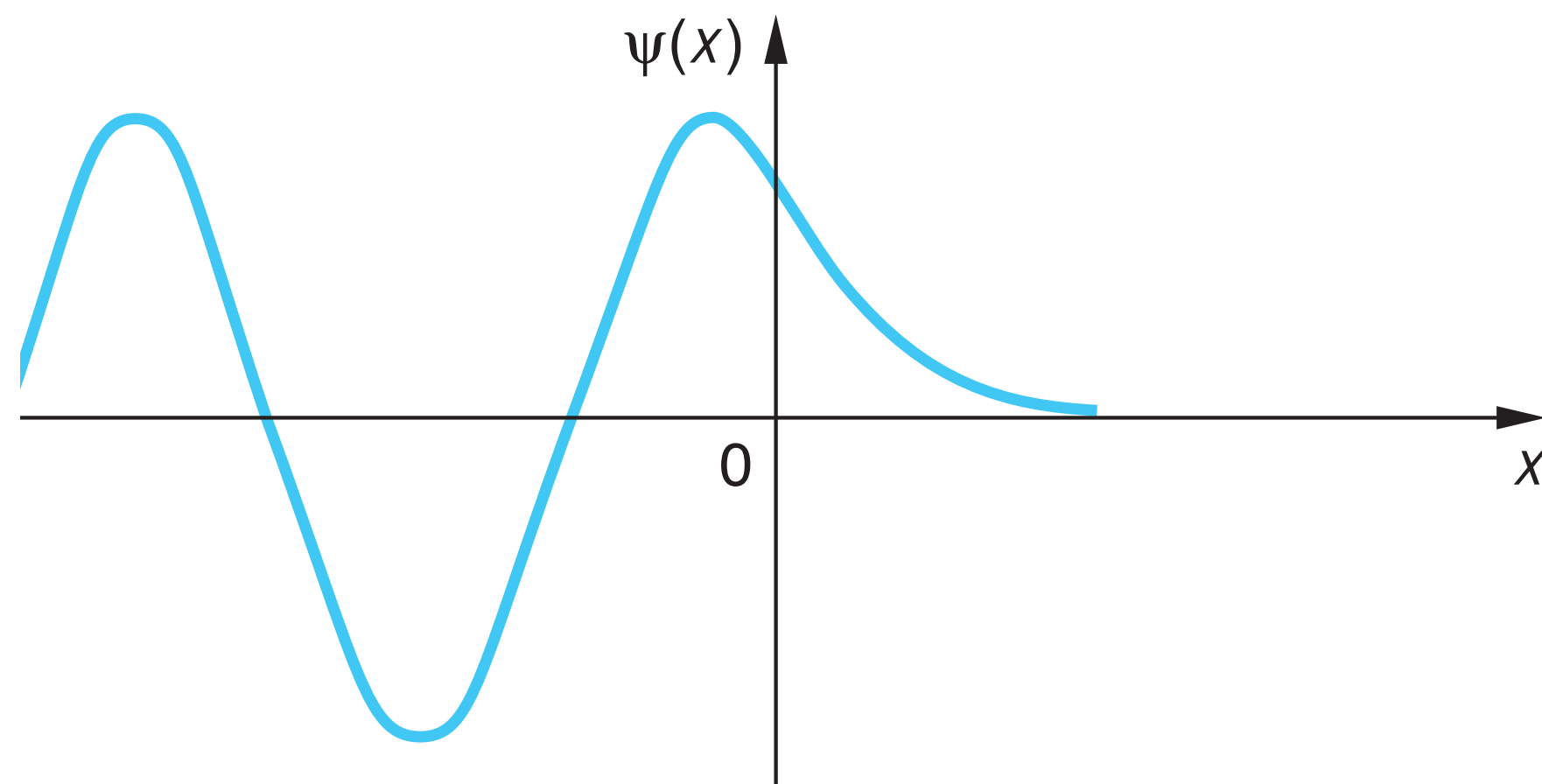
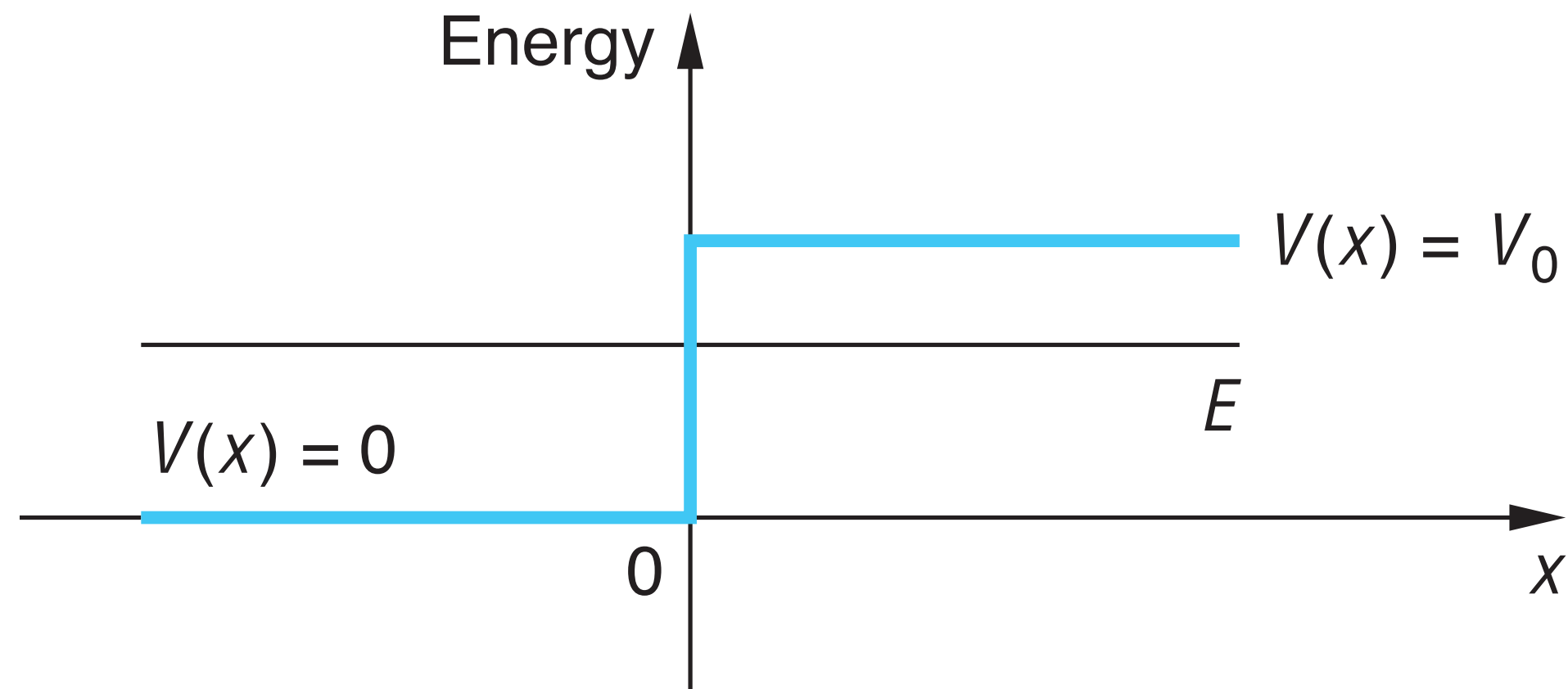
$$C = \frac{2k_1}{k_1 + k_2} A = \frac{2E^{1/2}}{E^{1/2} + (E - V_0)^{1/2}} A$$

$$T + R = 1$$

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

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

Step Potential



$$E < V_0.$$

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

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

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

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

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



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



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

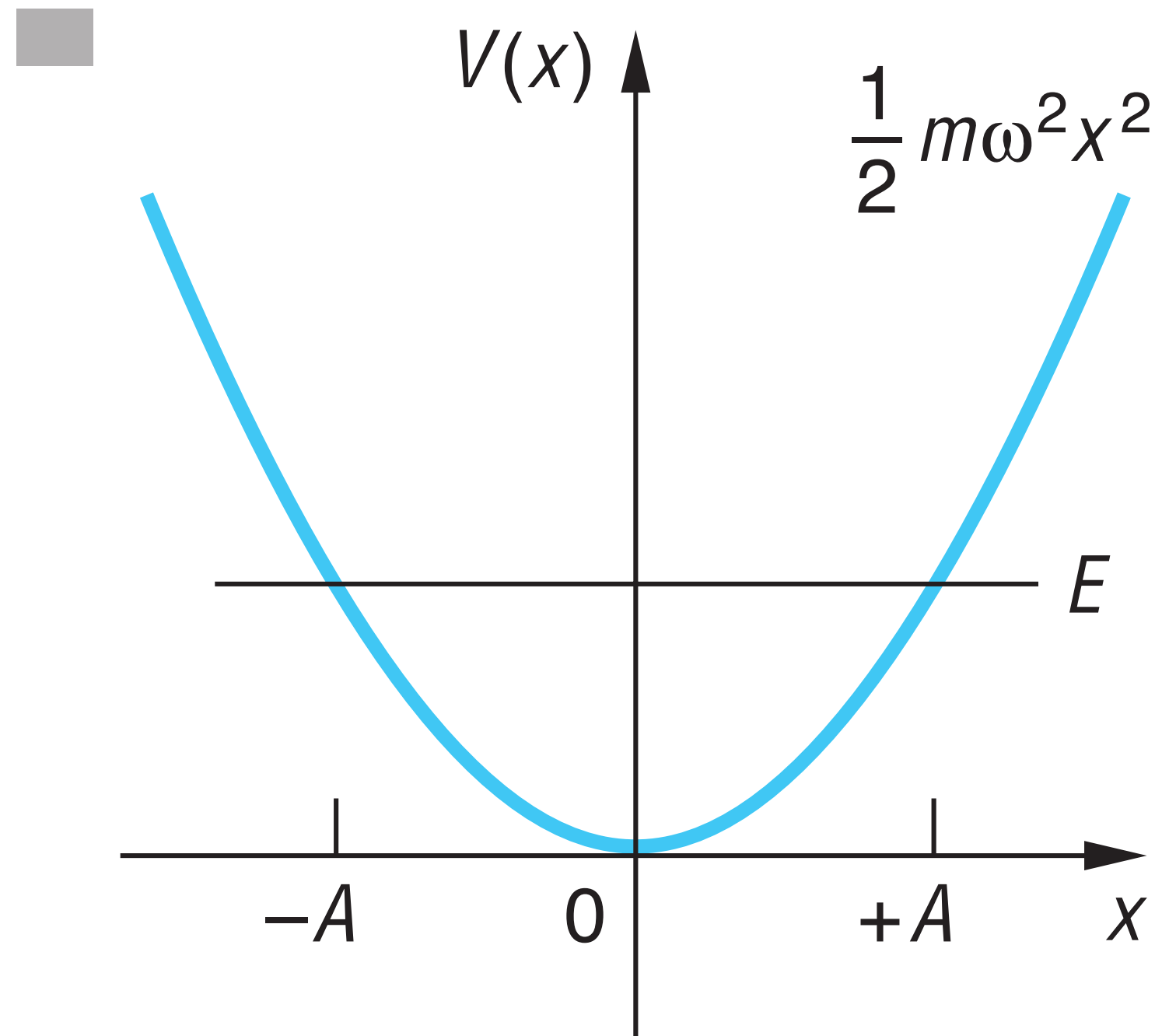
$$\begin{aligned}\frac{\hbar}{i} \frac{\partial}{\partial X} \left(\frac{\hbar}{i} \frac{\partial}{\partial X} \right) \psi &= -\hbar^2 \frac{\partial^2 \psi}{\partial X^2} = -\hbar^2 \left(-\frac{\pi^2}{L^2} \sqrt{\frac{2}{L}} \sin \frac{\pi X}{L} \right) \\ &= +\frac{\hbar^2 \pi^2}{L^2} \psi\end{aligned}$$

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

Harmonic Oscillator



So far in our previous lectures we have studied the experiments that lead to the development of New theory of Physics, now called quantum mechanics. We discussed wave particle duality of radiation and matter. Further we postulated wave equation that described dynamics of particle under the influence of various time independent potential. Today we shall focus on a time independent potential that is not only of theoretical interest but provides deep insight of many quantum systems.



Revising Classical Harmonic oscillator

$$V(x) = \frac{1}{2} Kx^2 = \frac{1}{2} m\omega^2 x^2$$

$$\frac{1}{2} mv^2 + \frac{1}{2} m\omega^2 x^2 = E$$

Harmonic Oscillator



$$P_c(x) dx \propto \frac{dx}{v} = \frac{dx}{\sqrt{(2/m) \left(E - \frac{1}{2} m \omega^2 x^2 \right)}}$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi(x) = E \psi(x)$$

$$|\psi(-x)|^2 = |\psi(x)|^2 \quad \therefore \psi(-x) = +\psi(x), \quad \therefore \psi(-x) = -\psi(x).$$

$$\psi''(x) = -k^2 \psi(x)$$

$$k^2 = \frac{2m}{\hbar^2} [E - V(x)]$$

$$\psi''(x) = +\alpha^2 \psi(x)$$

$$\alpha^2 = \frac{2m}{\hbar^2} [V(x) - E]$$

Harmonic Oscillator



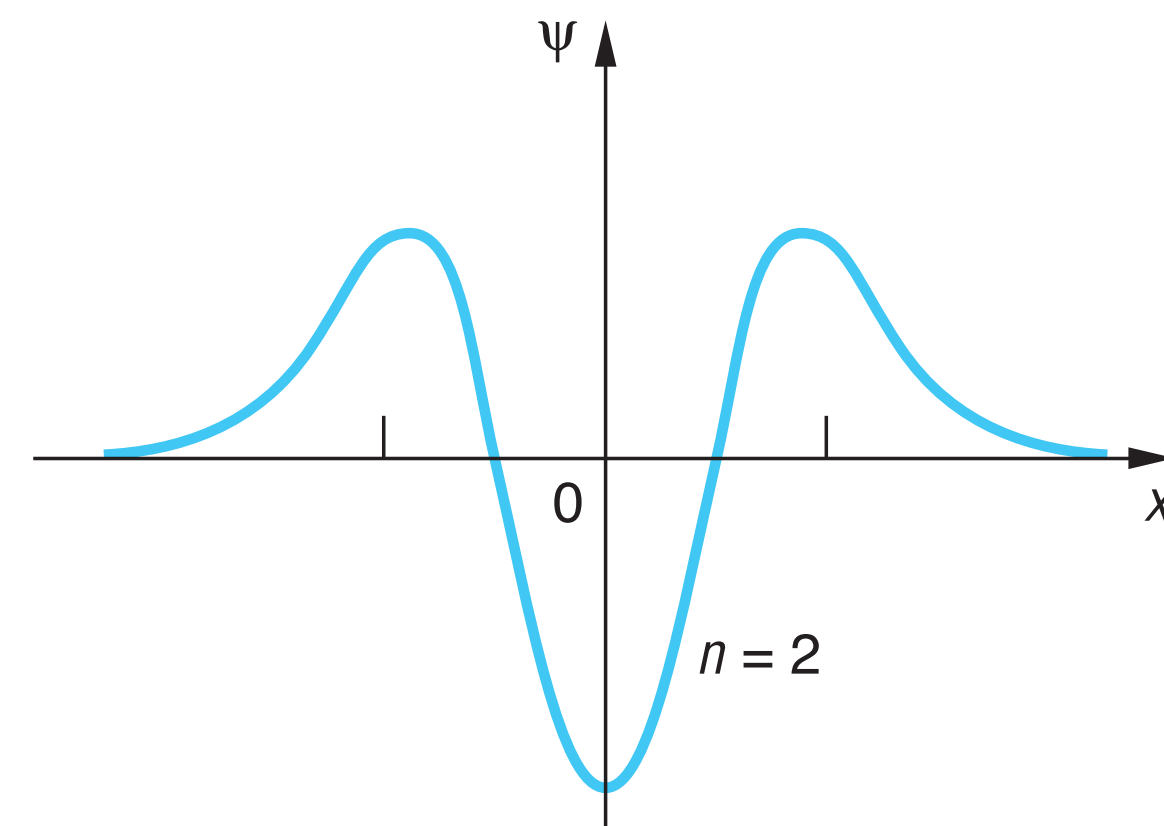
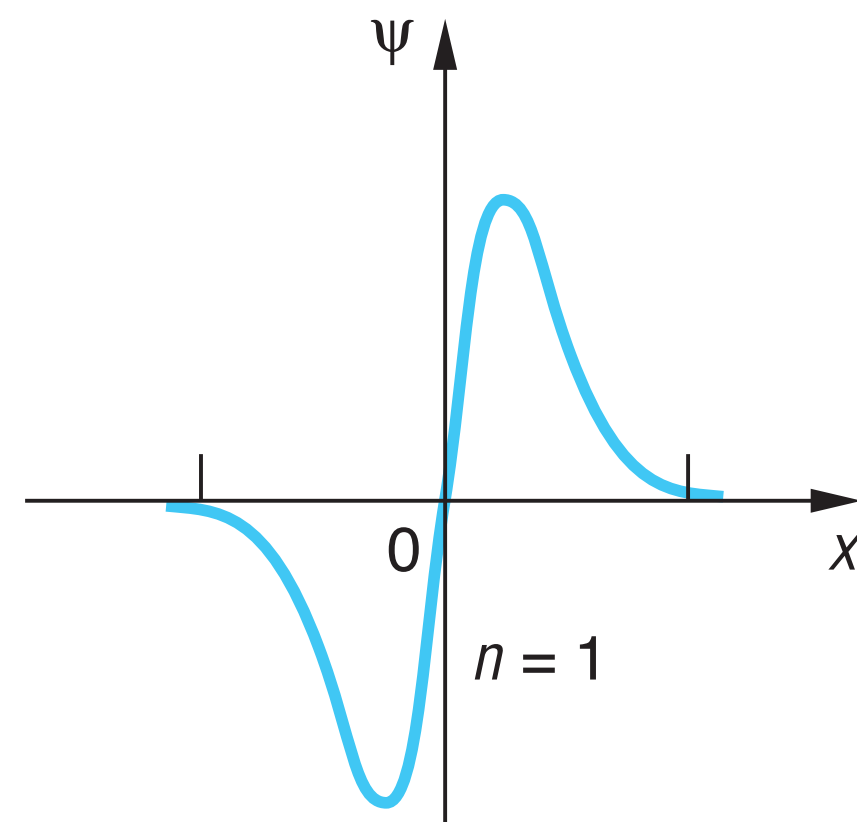
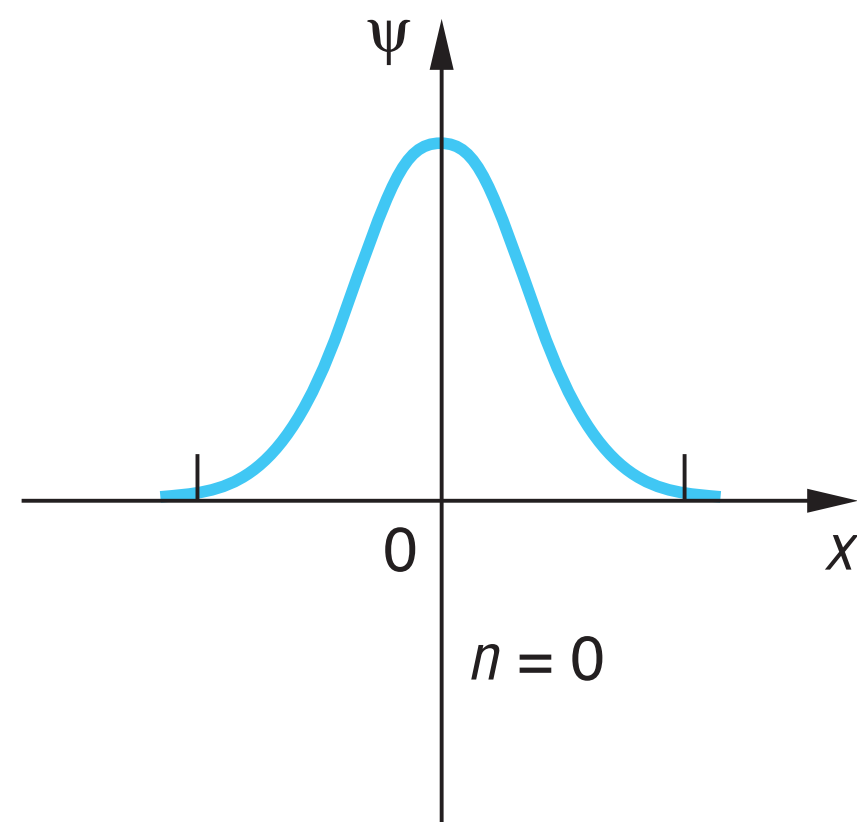
$$E_n = \left(n + \frac{1}{2} \right) \hbar \omega \quad n = 0, 1, 2, \dots$$

$$\psi_n(x) = C_n e^{-m\omega x^2/2\hbar} H_n(x)$$

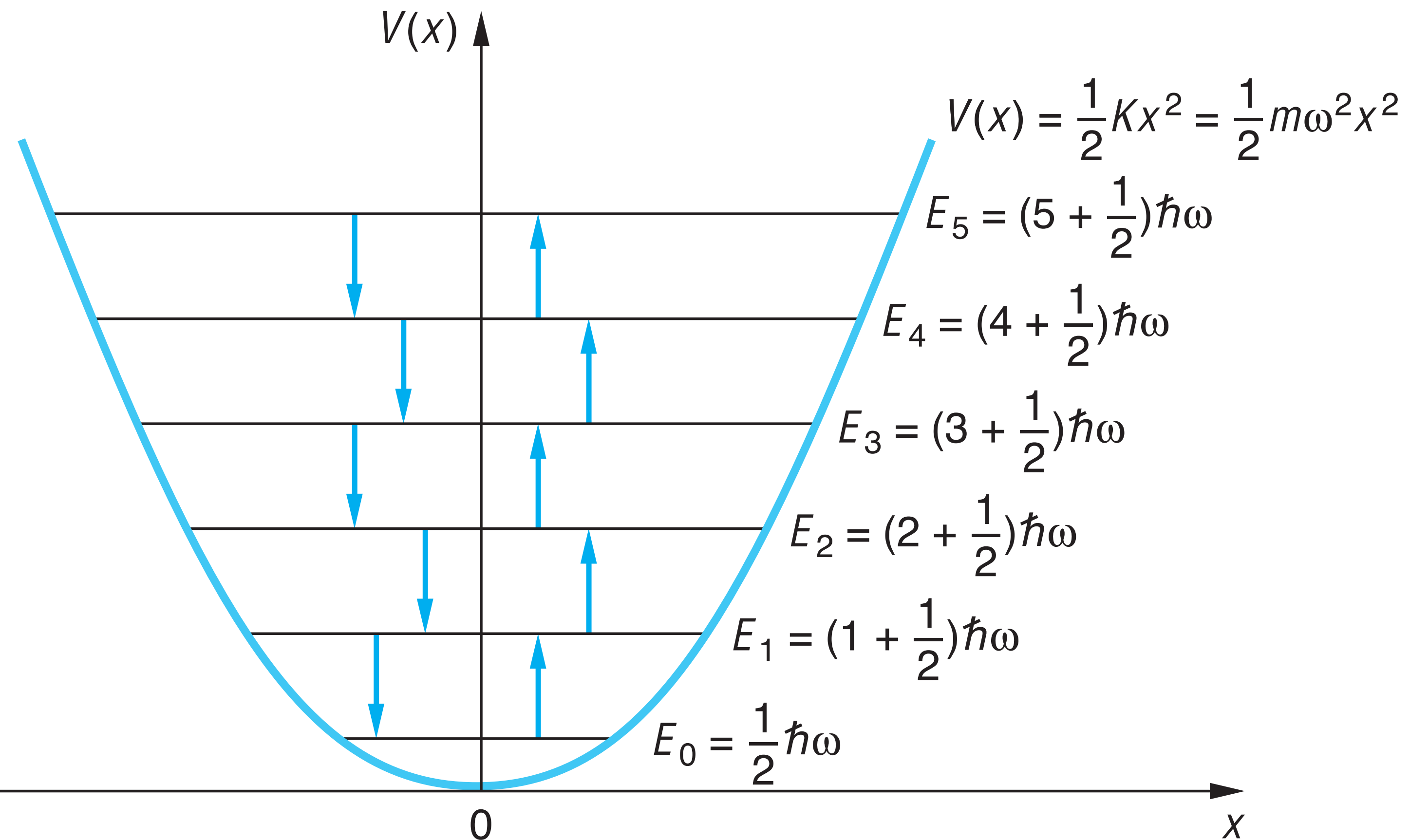
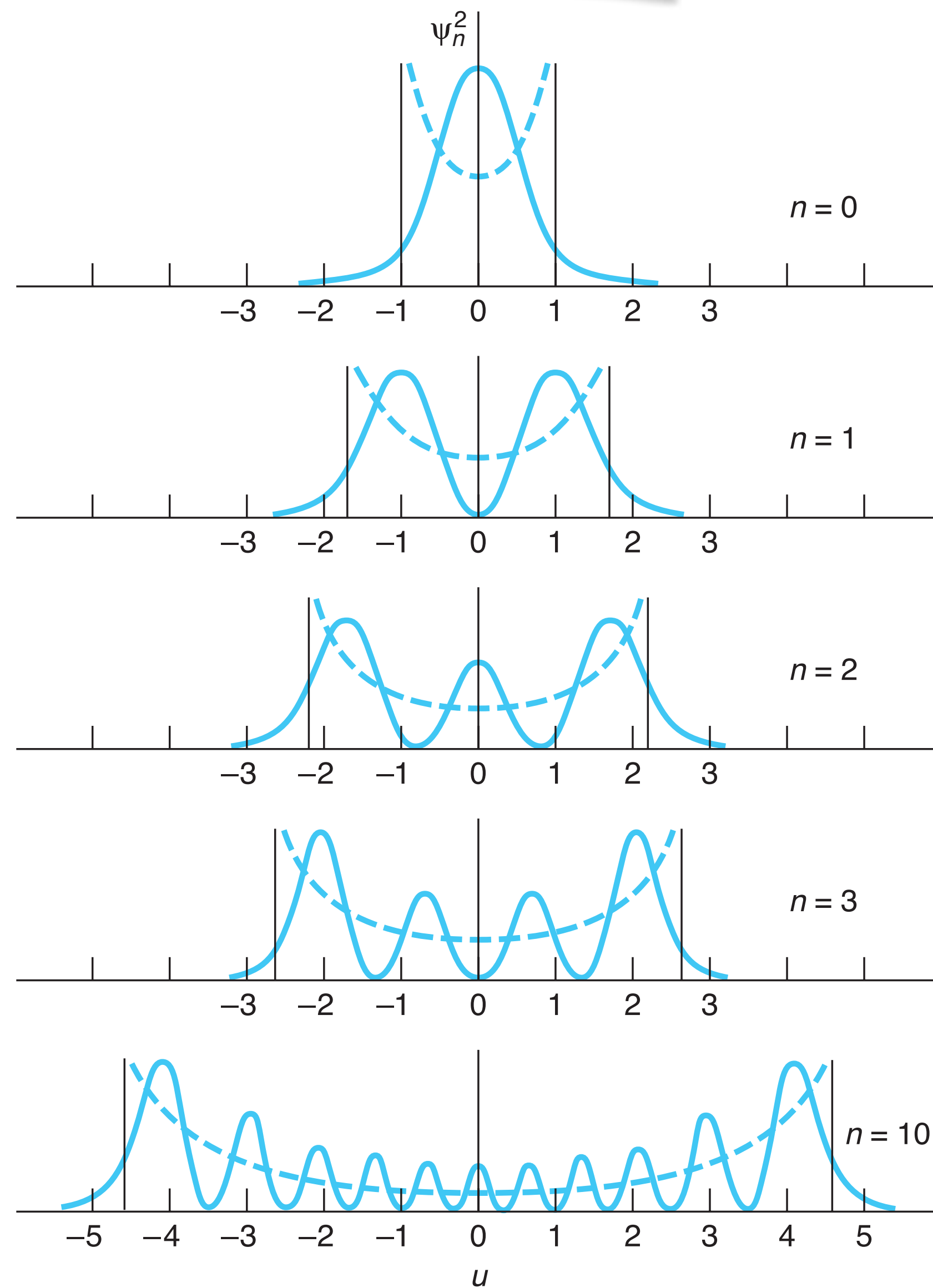
$$\psi_0(x) = A_0 e^{-m\omega x^2/2\hbar}$$

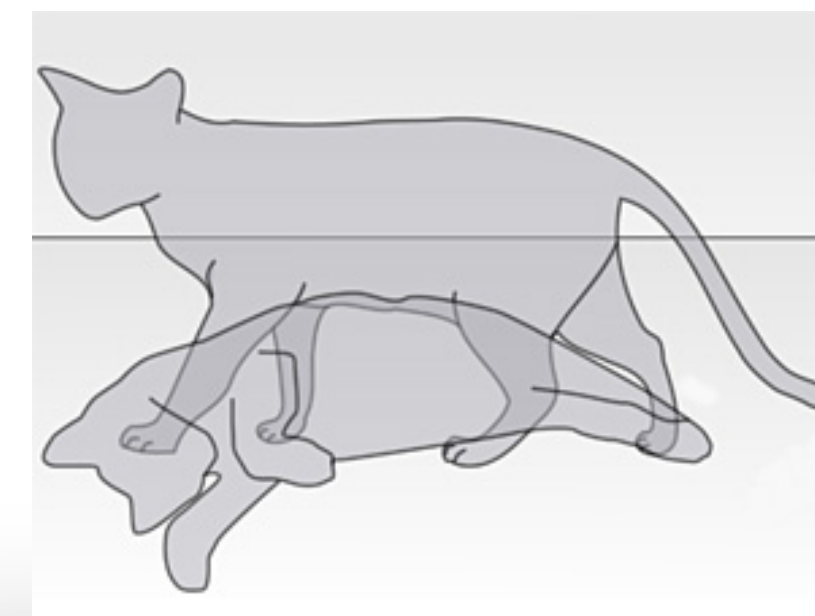
$$\psi_1(x) = A_1 \sqrt{\frac{m\omega}{\hbar}} e^{-m\omega x^2/2\hbar}$$

$$\psi_2(x) = A_2 \left(1 - \frac{2m\omega x^2}{\hbar} \right) e^{-m\omega x^2/2\hbar}$$



Harmonic Oscillator





Curiosity Kills the Cat

Lecture 05
Concluded