Ch. 8 Quantum Mechanics

References:

1. Young & Freedman, “University Physics”, 13th ed. Ch. 40

2. Halliday et al., “Principles of Physics”, 9th ed. Ch. 39

Outline

8.1 Particle in a Box
8.2 Potential Wells
8.3 Potential Barriers and Tunneling
8.4 The Harmonic Oscillator
8.5 Three-Dimensional Problems

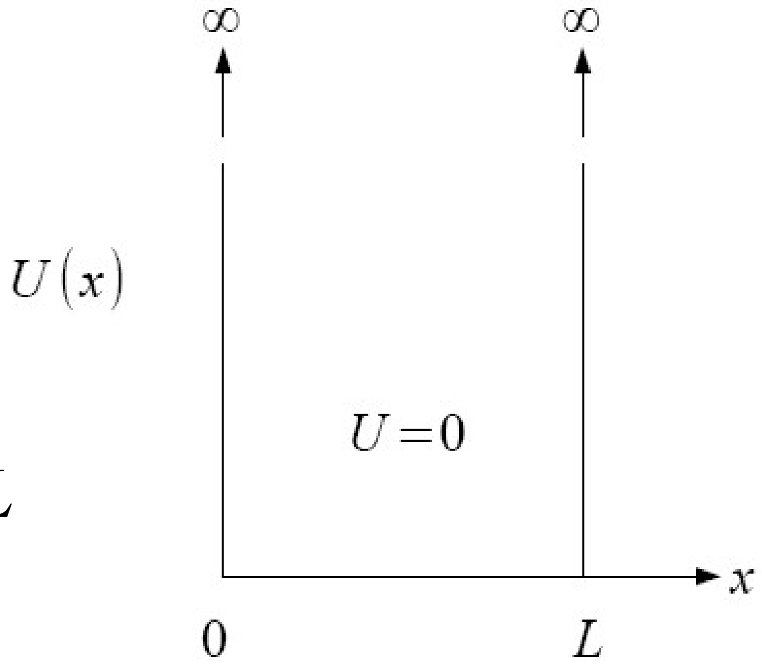
8.1 Particle in a Box

We want to solve the Schrödinger equation

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

with the potential energy

$$U(x)=\begin{cases}0 & \text{for } 0\le x\le L\\ \infty & \text{for } x<0 \text{ and } x>L\end{cases}$$



(infinite square well)

- ***Wave Function***

The particle is confined inside the box => $\psi(x)$=0 outside the box

1. $\psi(x)$ must be continuous

    => Boundary conditions $\psi(0) = \psi(L) = 0$

2. $d\psi/dx$ must also be continuous
   (except at the points where $U = \infty$)

Inside the box (U = 0): $$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}=E\,\psi(x)$$

General solution: $$\psi(x)=A\,e^{ikx}+B\,e^{-ikx} \qquad \left(k=\sqrt{2mE}/\hbar\right)$$

Impose B.C. =>

$$\psi(0)=A+B=0 \qquad \Rightarrow \quad B=-A$$

$$\psi(L)=A\,e^{ikL}+B\,e^{-ikL}=0$$

=> $$A\left(e^{ikL}-e^{-ikL}\right)=0$$

(assume E > 0)

$$2A\sin(kL)=0$$

Recall: $$e^{i\theta}=\cos\theta+i\sin\theta \quad ; \quad \sin\theta=\frac{e^{i\theta}-e^{-i\theta}}{2i}$$

In order to have non-trivial solution ($A \neq 0$):

$$\sin(kL) = 0 \quad \Rightarrow \quad kL = n\pi \quad (n = 1,2,3\ldots)$$

$$\Rightarrow \quad k = \frac{n\pi}{L} \quad \text{and} \quad \lambda = \frac{2\pi}{k} = \frac{2L}{n}$$

Wave function inside the box:

$$\psi_n(x) = A e^{ikx} - A e^{-ikx}$$
$$= C \sin(kx) = C \sin\left(\frac{n\pi x}{L}\right) \qquad (C \equiv 2iA)$$

Note: If $E < 0$, k becomes imaginary ($k = i\alpha$)

$$\psi = A e^{-\alpha x} - A e^{+\alpha x}$$

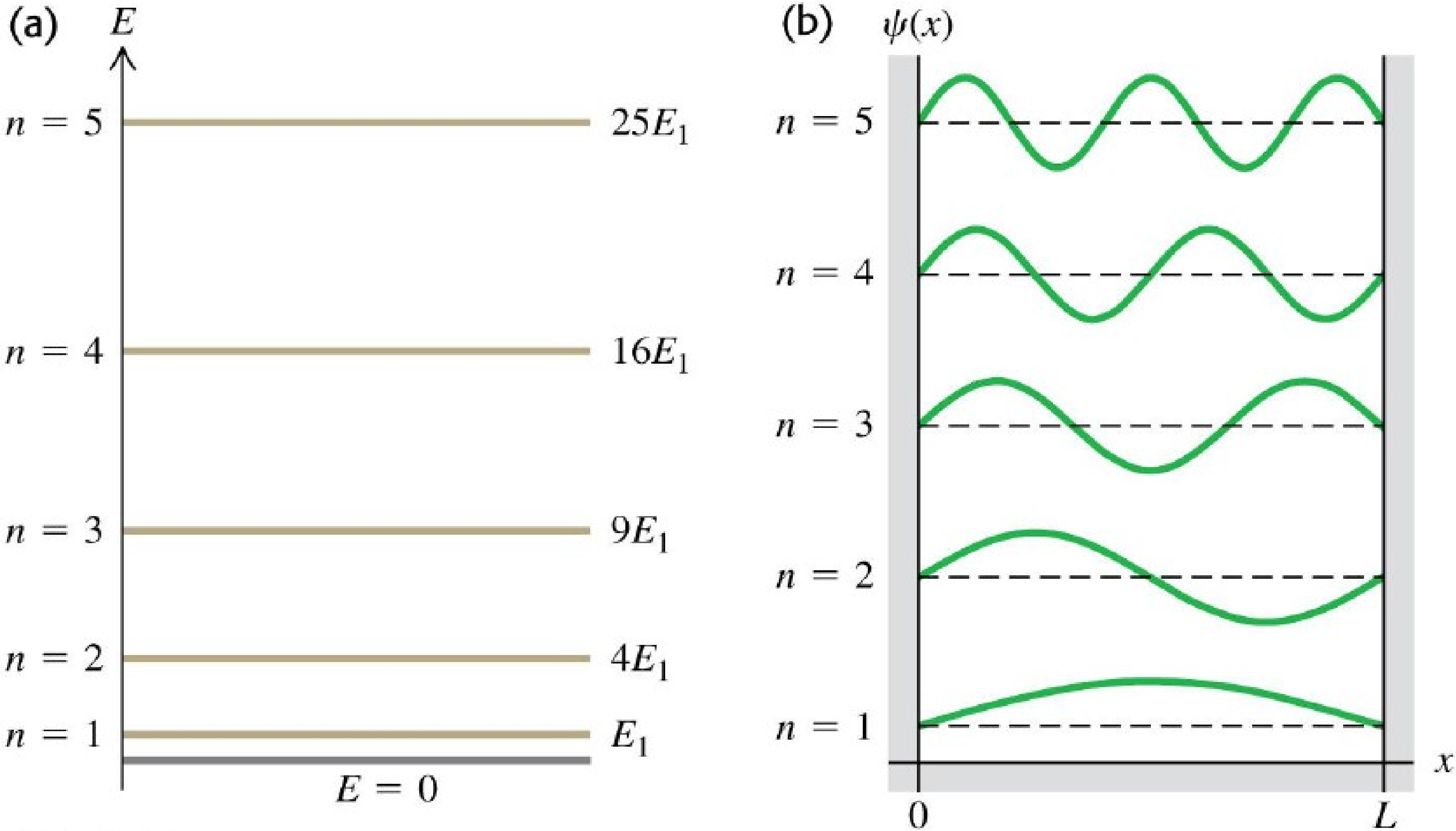
B.C.: $\psi(L) = 0 \quad \Rightarrow \quad A = 0$

- ***Energy Levels***

The possible energy levels are given by $E=\frac{p^2}{2m}=\frac{(\hbar k)^2}{2m}$

$$k=\frac{n\pi}{L} \quad \Rightarrow \quad E_n=\frac{n^2\pi^2\hbar^2}{2mL^2} \quad (n=1,2,3\ldots)$$

Note: Zero energy (n = 0) is not allowed because the wave function would be zero.


(a)
E
n = 5
25E1
n = 4
16E1
n = 3
9E1
n = 2
4E1
n = 1
E1
E = 0
(b)
ψ(x)
n = 5
n = 4
n = 3
n = 2
n = 1
x
0
L

- ***Probability and Normalization***

The particle must be somewhere in space:

=> $$\int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = 1$$ (Normalization condition)

Wave function: $$\psi_n(x) = \begin{cases} C \sin\left(\dfrac{n\pi x}{L}\right) & \text{for } 0 \le x \le L \\ 0 & \text{for } x < 0 \text{ and } x > L \end{cases}$$

=> $$C^2 \int_0^L \sin^2(n\pi x / L) \, dx = 1$$

Note: $$\int_0^L \sin^2(n\pi x/L)\,dx = \frac{1}{2}\int_0^L [1-\cos(2n\pi x/L)]\,dx$$
$$= \frac{L}{2}$$

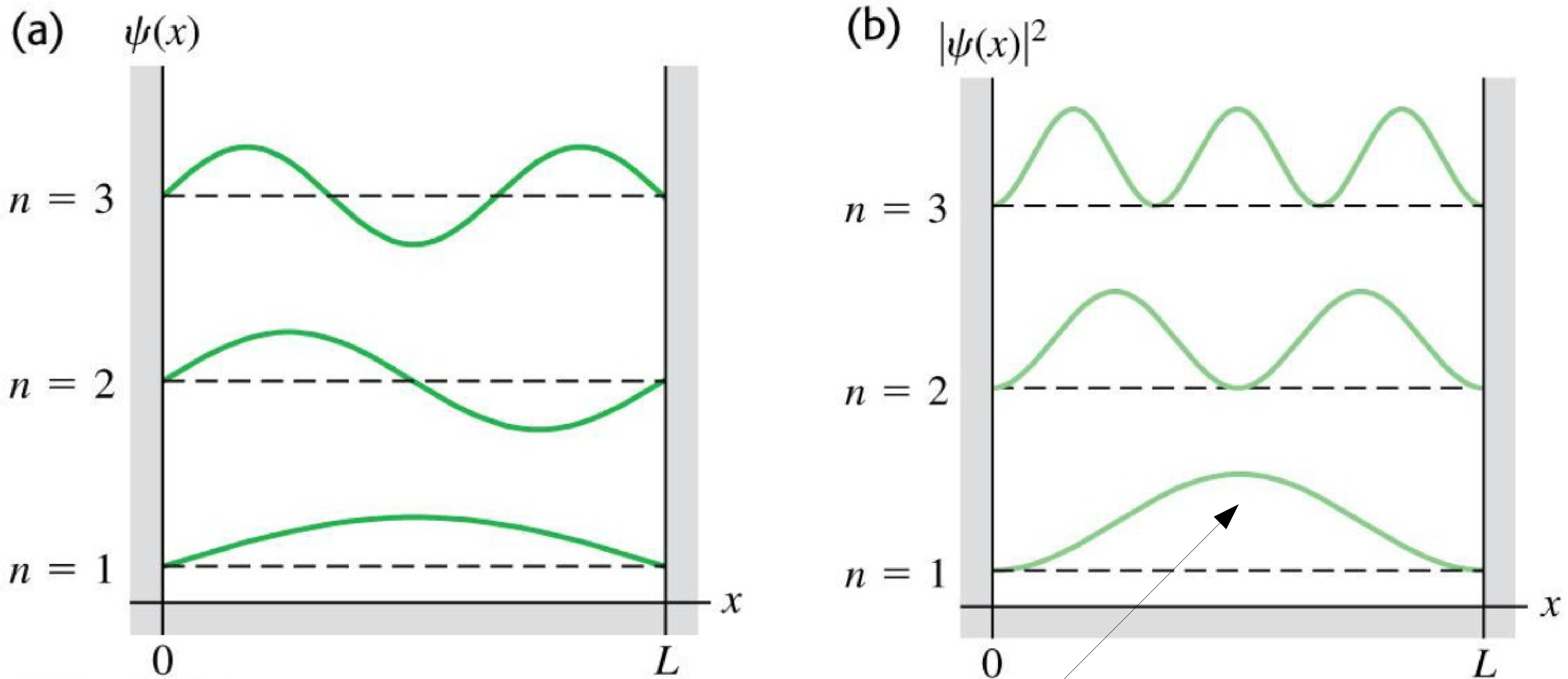
=> $C^2(L/2)=1$ $\qquad (C=\sqrt{2/L})$

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

(Normalized wave functions)

Recall:

$$|\psi(x)|^2 dx =$$ Probability of finding the particle in a small interval dx around the point x

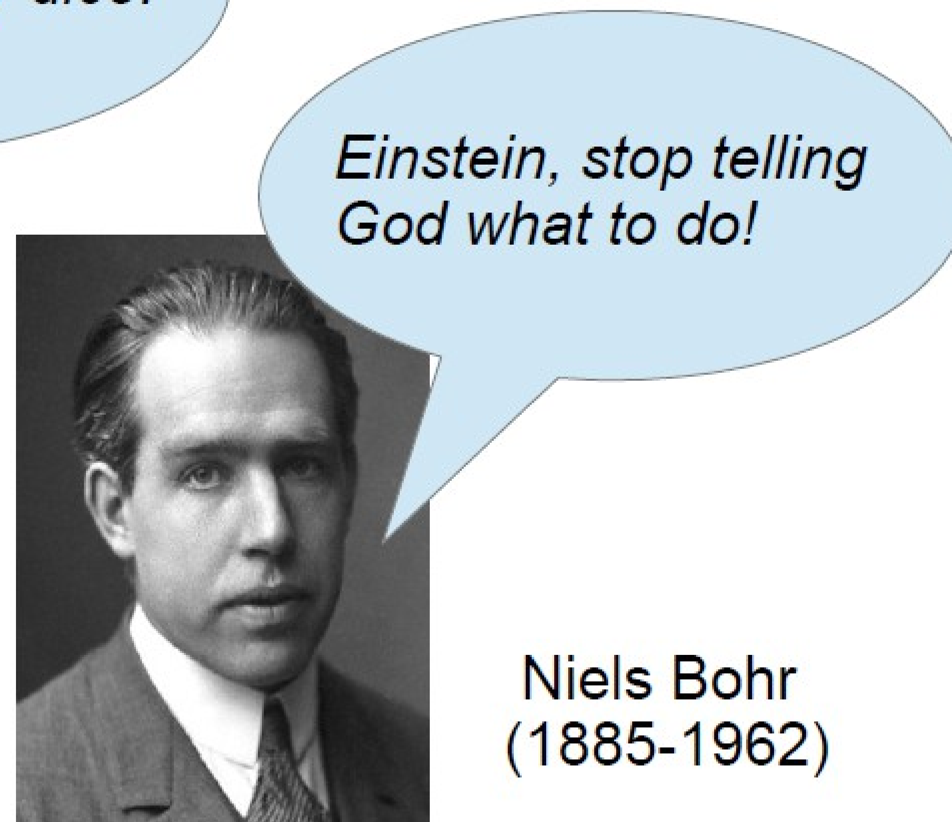


Max = Highest probability to find the particle there

- ***Indeterminacy***

In quantum physics, we cannot predict the outcome with certainty!

Albert Einstein
(1879-1955)



Niels Bohr
(1885-1962)

- ***Time Dependence***

Recall: The time-dependent wave function for a stationary state:

$$\Psi(x,t)=\psi(x)e^{-iEt/\hbar}$$

=> For a particle in a box

$$\Psi_n(x,t)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-iE_nt/\hbar} \qquad (n=1,2,3\ldots)$$

Note: The probability density does not depend on time

$$|\Psi_n(x,t)|^2=|\psi_n(x)|^2$$

- ***Expectation Values***

For a normalized wave function $\Psi(x, t)$, we define

$$<x> = \int_{-\infty}^{\infty} x |\Psi|^2 dx$$

(Expectation value of the position of a particle)

In general, we define the expectation value of any function $F(x)$:

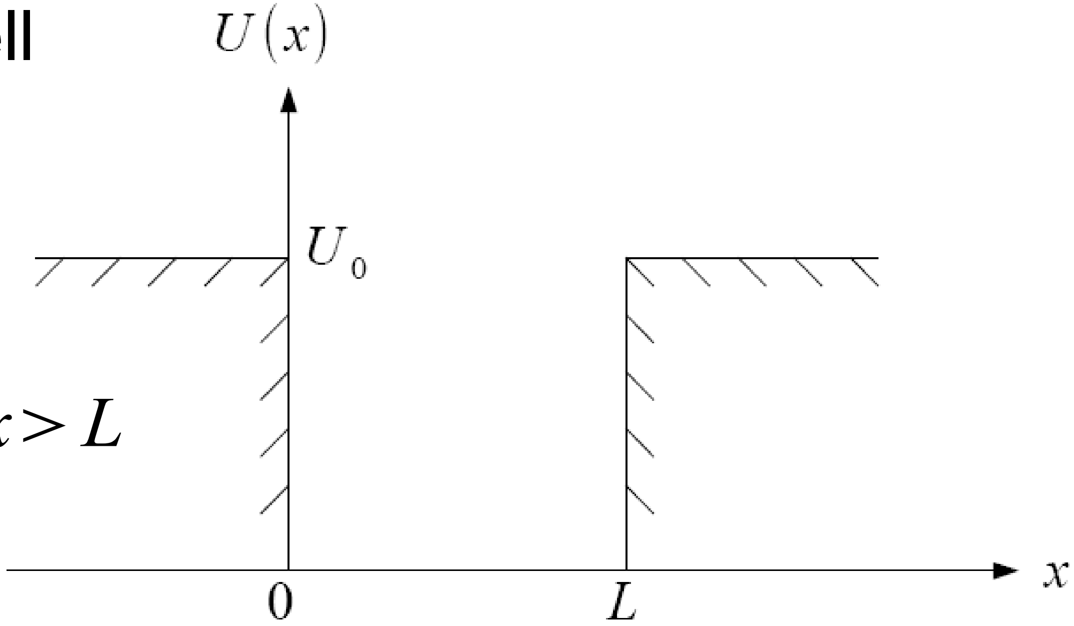
$$<F(x)> = \int_{-\infty}^{\infty} F(x) |\Psi|^2 dx$$

8.2 Potential Wells

A potential well is a potential-energy function $U(x)$ that has a minimum.

Example: Finite square well

$$U(x)=\begin{cases} 0 & \text{for } 0\leq x\leq L \\ U_0 & \text{for } x<0 \text{ and } x>L \end{cases}$$



• ***Bound States of a Square-Well Potential***

Inside the well: $U(x)$ = 0

=> $$\frac{d^2\psi}{dx^2} = -k^2\psi \qquad \left(k = \sqrt{2mE}/\hbar\right)$$

$$\psi(x) = A\cos kx + B\sin kx \qquad \text{for } 0 \le x \le L$$

Outside the well: $U(x)$ = U_0

$$\frac{d^2\psi}{dx^2} = \alpha^2\psi \qquad \left(\alpha = \sqrt{2m\left(U_0 - E\right)}/\hbar\right)$$

$$\psi(x) = Ce^{\alpha x} + De^{-\alpha x}$$

Note:

1. the wave function should be finite everywhere

=> $$\psi(x)=\begin{cases} C e^{\alpha x} & \text{for } x<0 \\ A\cos kx + B\sin kx & \text{for } 0\le x\le L \\ D e^{-\alpha x} & \text{for } x>L \end{cases}$$

2. ψ and $d\psi/dx$ should be continuous

At $x = 0$ =>

$$C = A \quad \text{(Eq.1)}$$
$$\alpha C = k B \quad \text{(Eq.2)}$$

At $x = L$ =>

$$A\cos kL + B\sin kL = D e^{-\alpha L} \quad \text{(Eq.3)}$$
$$-k A\sin kL + k B\cos kL = -\alpha D e^{-\alpha L} \quad \text{(Eq.4)}$$

(Eq.1) & (Eq.2) => $$B = \frac{\alpha}{k} C = \frac{\alpha}{k} A$$

With (Eq.3) & (Eq.4) => $$A\left[2\alpha k + \left(\alpha^2 - k^2\right)\tan kL\right] = 0$$

We must have $A \neq 0$.
(otherwise $A = B = C = D = 0$ => $\psi = 0$ for all x)

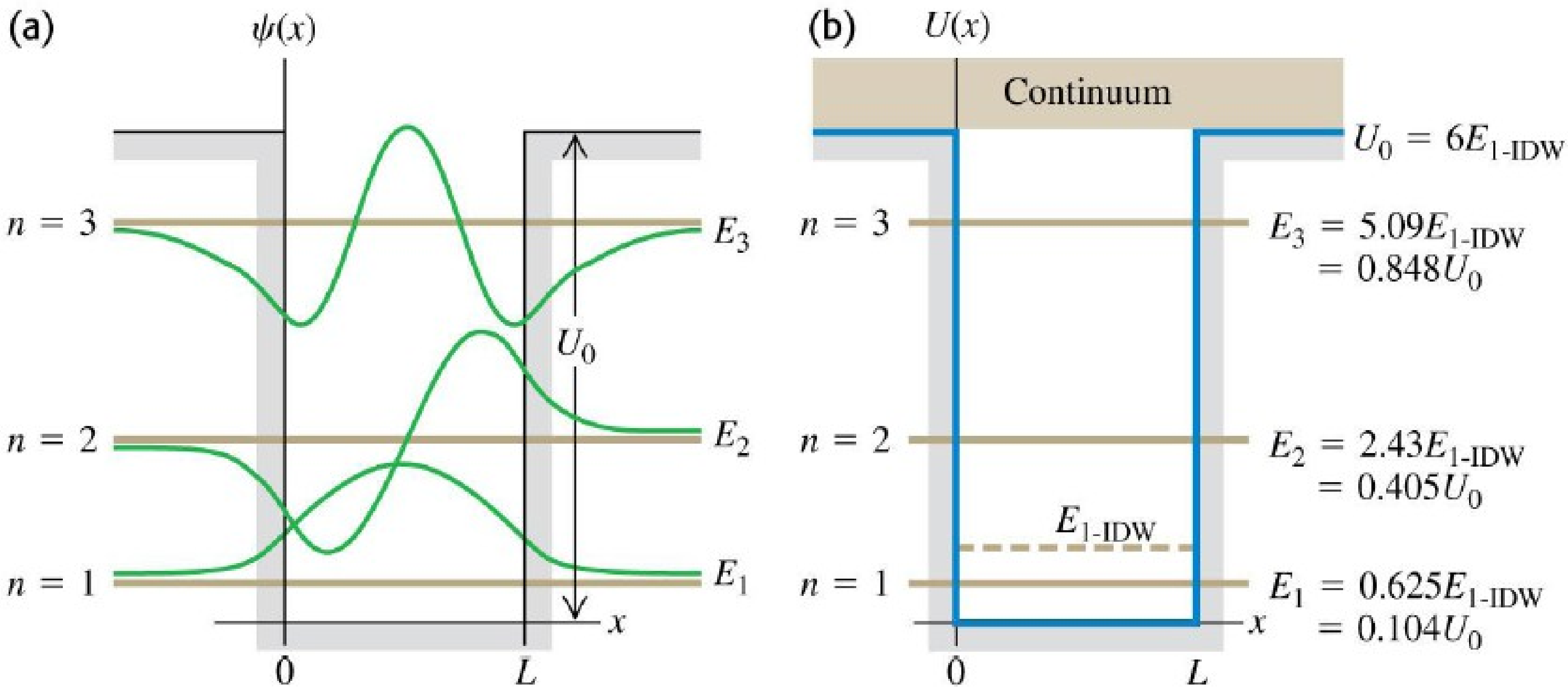
The allowed energies (E) are determined by:

$$2\alpha k + \left(\alpha^2 - k^2\right)\tan kL = 0$$

where $\alpha = \sqrt{2m\left(U_0 - E\right)}/\hbar$, $k = \sqrt{2mE}/\hbar$

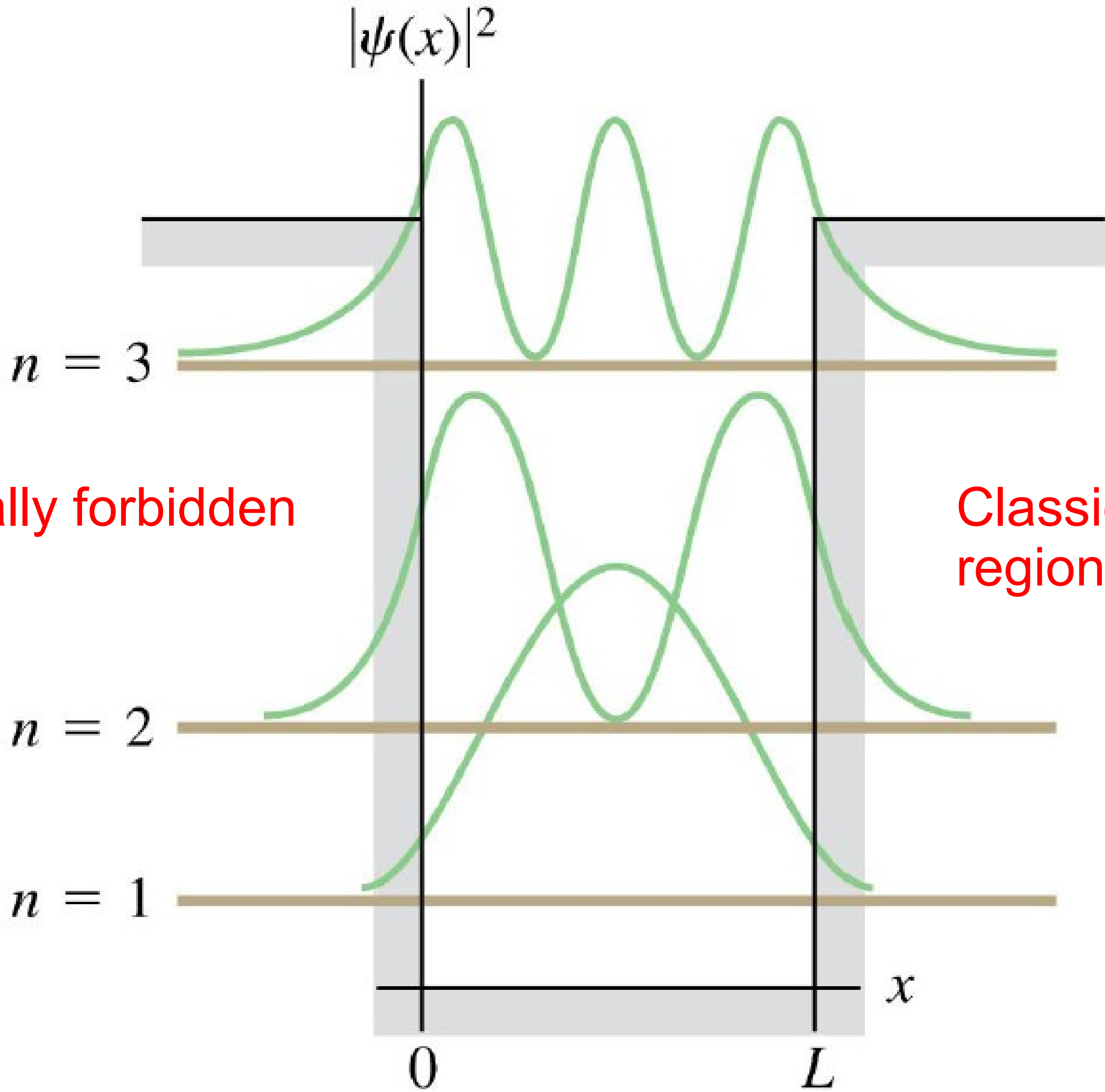
Note: This equation can be solved numerically.
(we will not discuss the details)

Example: A finite square well with $U_0 = 6\,E_{1\text{-IDW}}$.
(There are 3 bound states)



Ground-state energy for the infinity deep well: $E_{1-\mathrm{IDW}} = \dfrac{\pi^2 \hbar^2}{2 m L^2}$

Probability distribution function

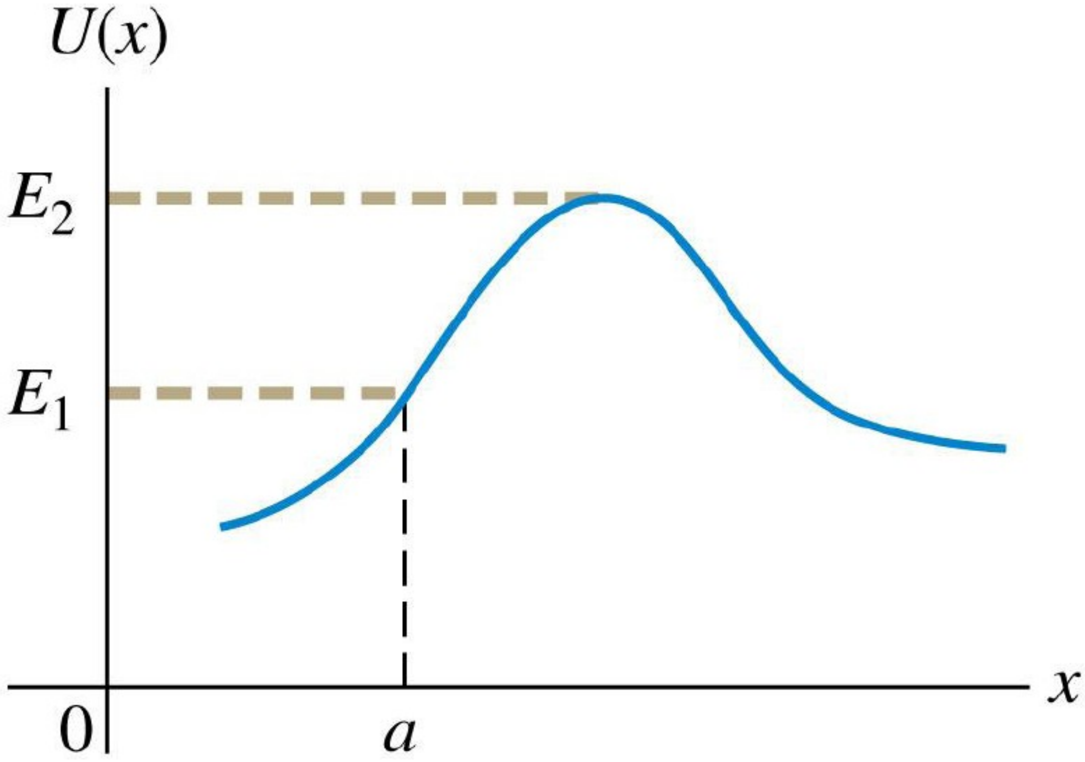


Classically forbidden region

Classically forbidden region

8.3 Potential Barriers and Tunneling

A potential barrier is a potential-energy function $U(x)$ that has a maximum.

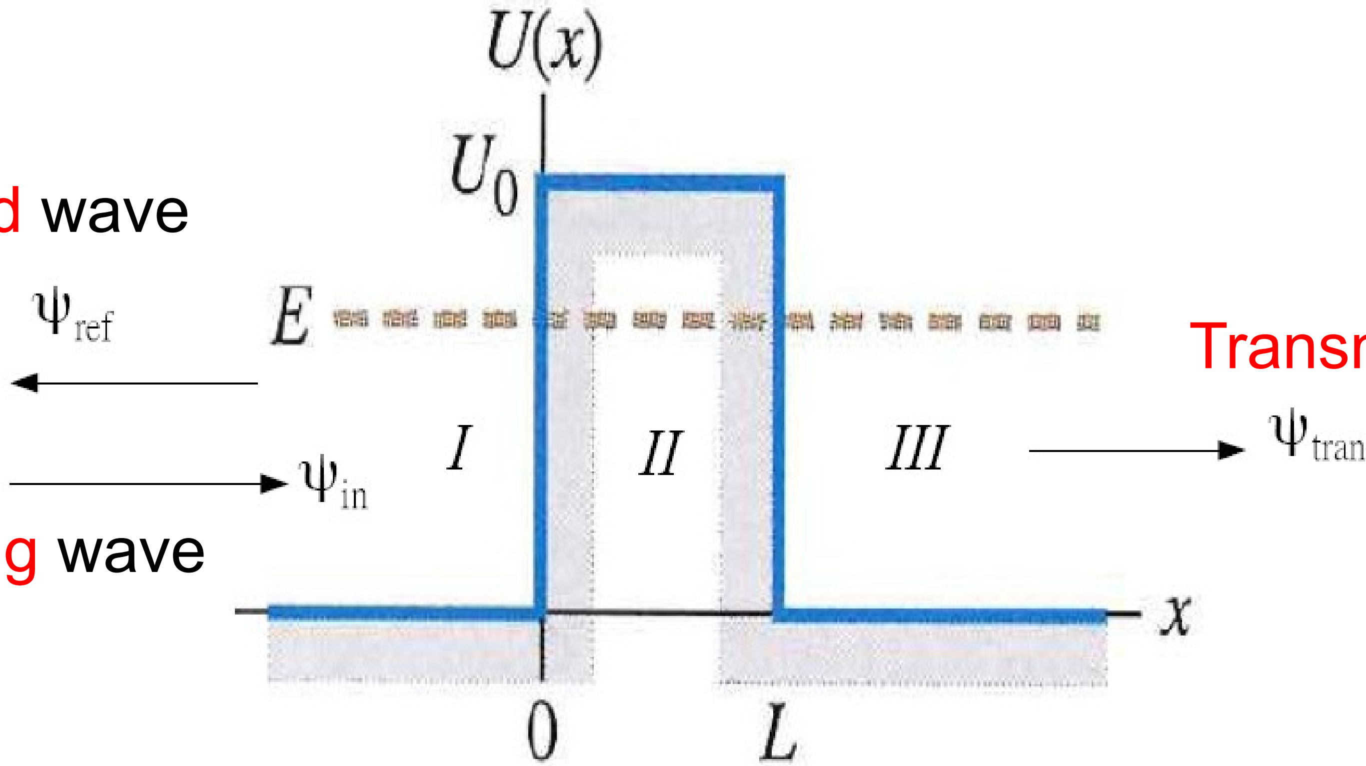


Quantum mechanics
=> tunneling is possible

- ***Tunneling Through a Rectangular Barrier***

Reflected wave

Transmitted wave



Incoming wave

In regions I and III : $\dfrac{d^2\psi}{dx^2} = -k^2\psi$ $\quad \left(k = \sqrt{2mE}/\hbar\right)$

In region II: $\dfrac{d^2\psi}{dx^2} = \alpha^2\psi$ $\quad \left(\alpha = \sqrt{2m\left(U_0 - E\right)}/\hbar\right)$

In region *I*: $$\psi_{\mathrm{I}} = A e^{ikx} + B e^{-ikx}$$
$$= \psi_{\mathrm{in}} + \psi_{\mathrm{ref}}$$

Note: $\psi_{\mathrm{in}} e^{-i\omega t} = A e^{i(kx - \omega t)}$

corresponds an incoming wave (particle) traveling from left to right

In region *II*: $$\psi_{\mathrm{II}} = C e^{\alpha x} + D e^{-\alpha x}$$

In region *III*: There can only be a transmitted wave

$$\psi_{\mathrm{III}} = F e^{ikx}$$

Boundary conditions: ψ and $d\psi/dx$ continuous at x=0 and L

At x = 0: $\psi_{I}=\psi_{II}$, $\dfrac{d\psi_{I}}{dx}=\dfrac{d\psi_{II}}{dx}$

At x = L: $\psi_{II}=\psi_{III}$, $\dfrac{d\psi_{II}}{dx}=\dfrac{d\psi_{III}}{dx}$

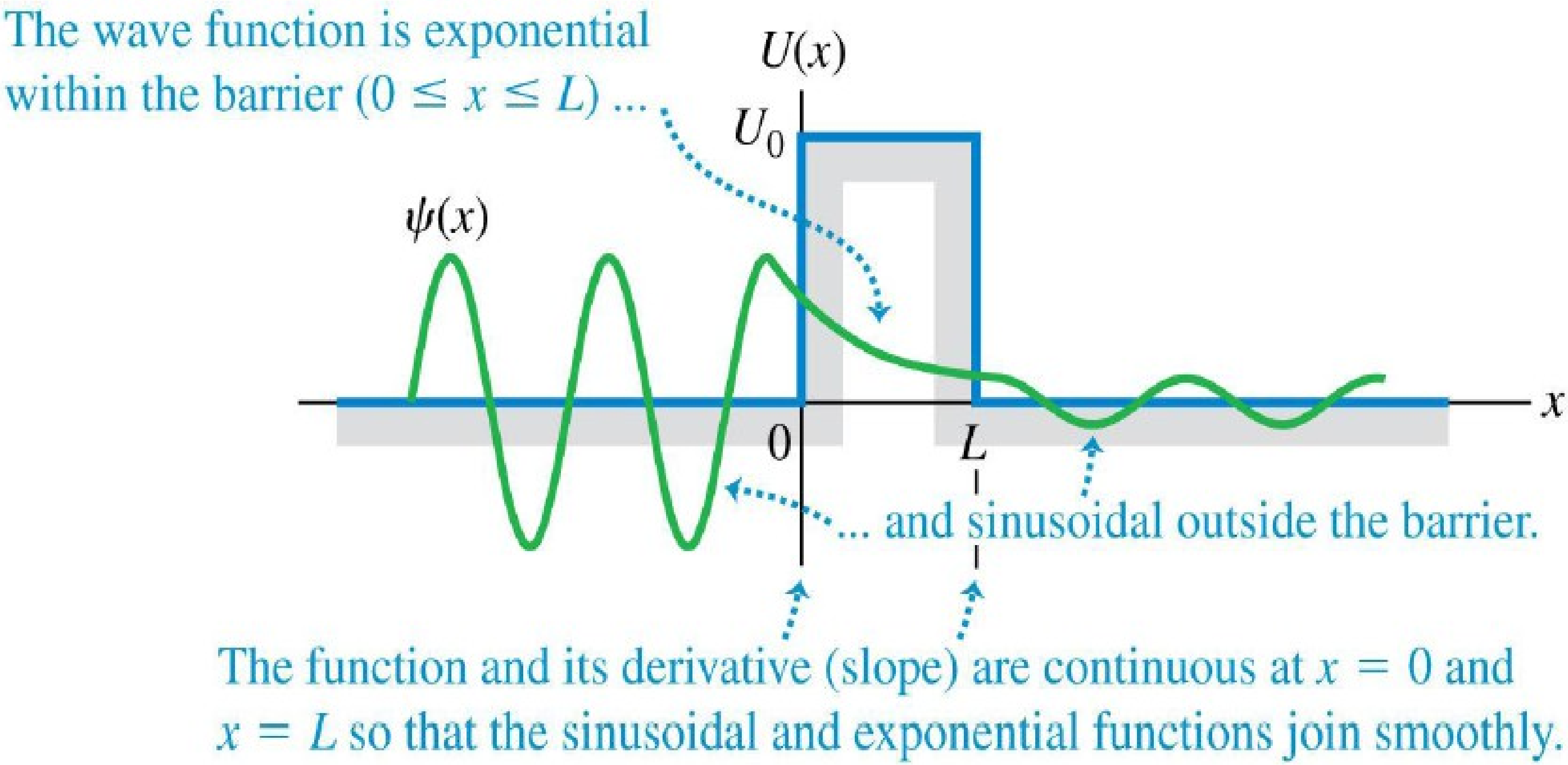
The wave amplitudes are determined by these conditions.

Main conclusion:

The probability T that the particle gets through the barrier is given approximately by (when T << 1)

$$T=G e^{-2\alpha L}$$

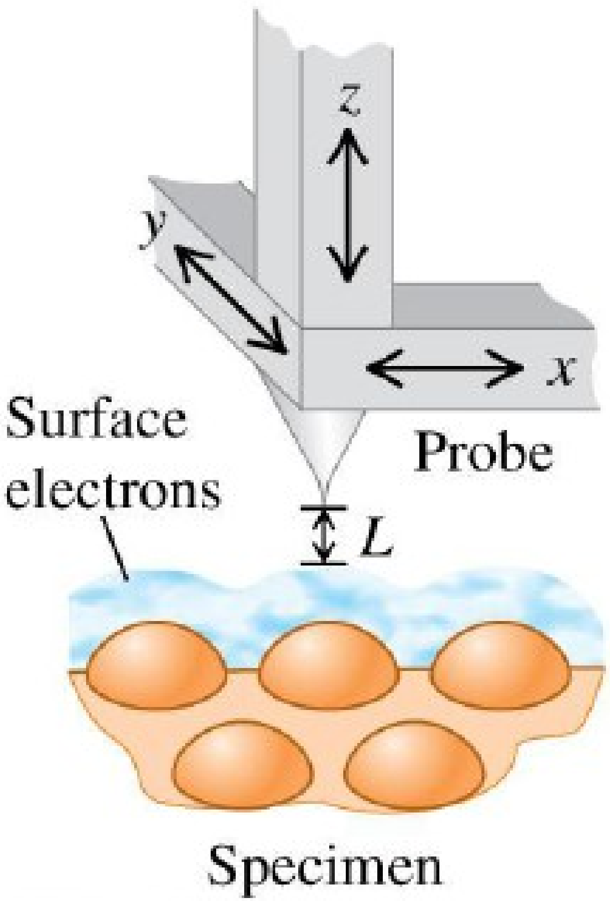
where $G=16\dfrac{E}{U_0}\left(1-\dfrac{E}{U_0}\right)$; $\alpha=\sqrt{2m(U_0-E)}/\hbar$

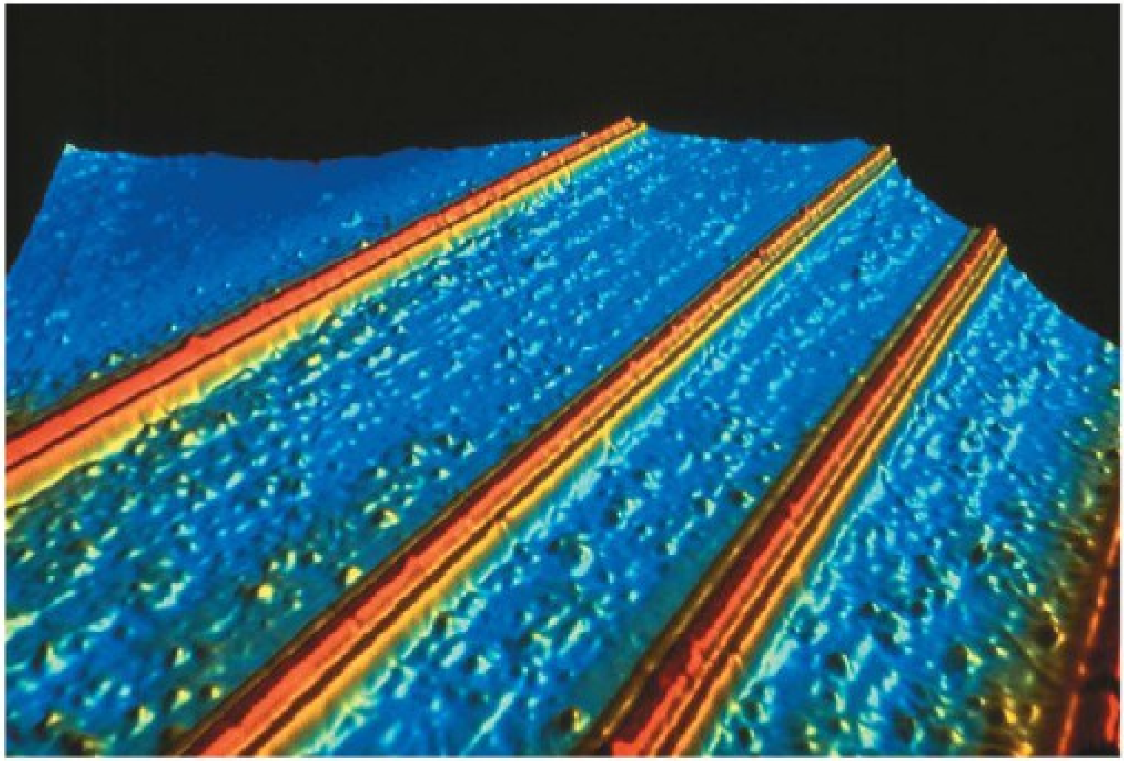


The wave function is exponential within the barrier ($0 \leq x \leq L$) ...
$U(x)$
U_0
$\psi(x)$
x
0
L
... and sinusoidal outside the barrier.
The function and its derivative (slope) are continuous at $x = 0$ and $x = L$ so that the sinusoidal and exponential functions join smoothly.

• *Applications of Tunneling*

Scanning tunneling microscope:



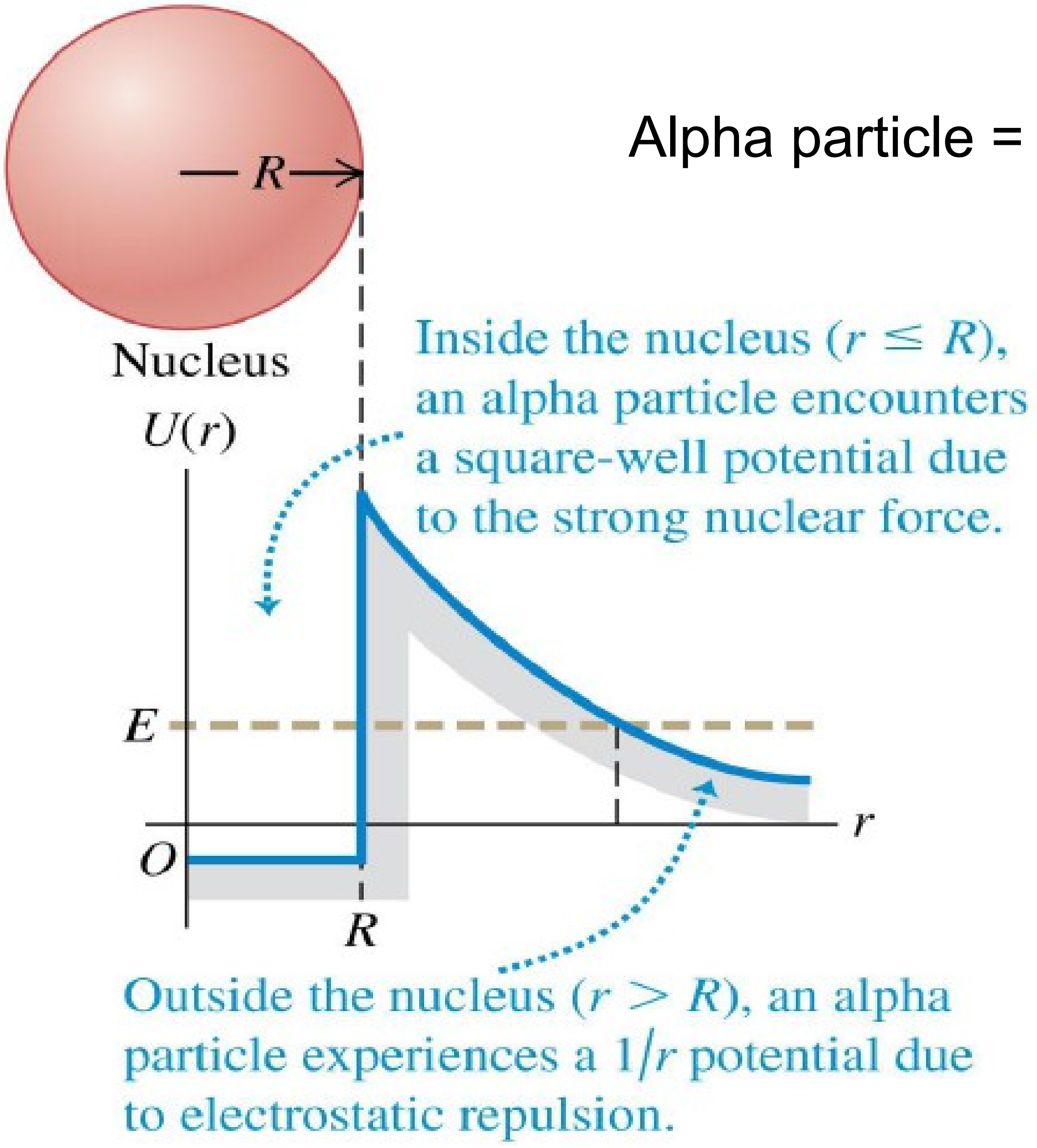


This colored STM image shows "quantum wire": thin strip, just 10 atoms wide, of a conductive rare-earth silicide atop a silicon surface.

L ~ 1 nm

Alpha decay:

Alpha particle = helium nucleus



8.4 The Harmonic Oscillator

In Newtonian mechanics

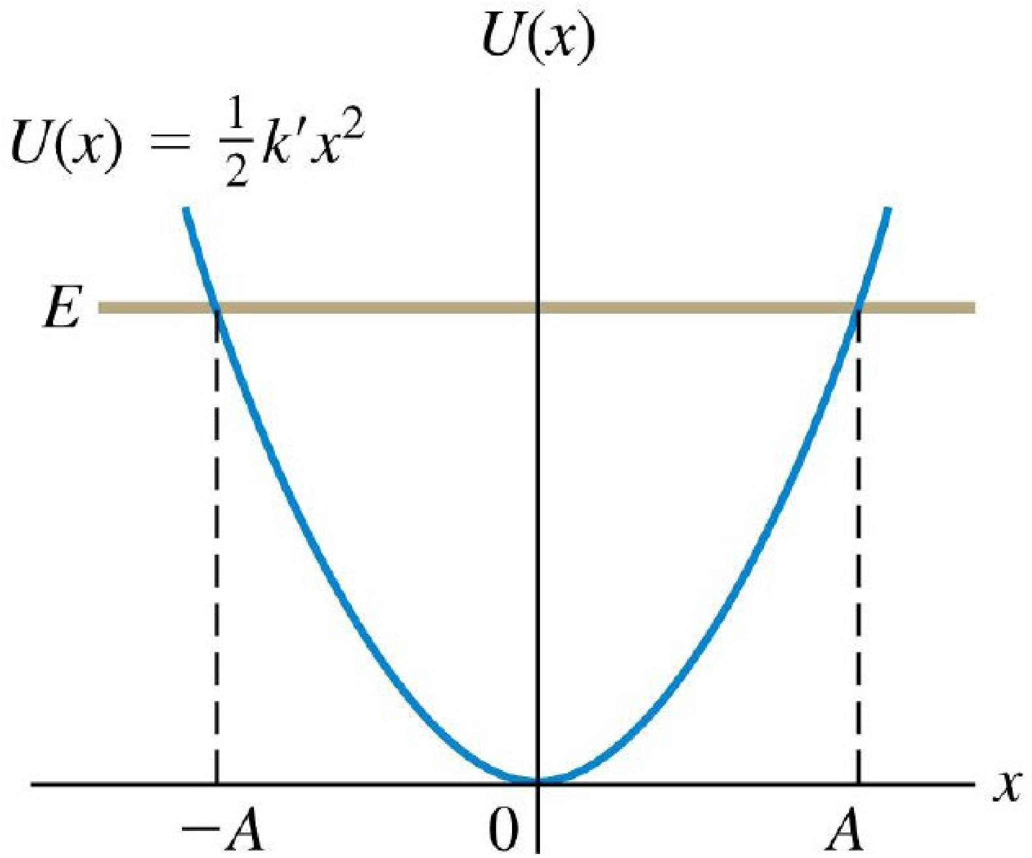
$$m\frac{d^2x}{dt^2} = F = -k'x$$

General solution:

$$x(t) = A\cos(\omega t + \phi)$$

Oscillation frequency:

$$\omega = \sqrt{\frac{k'}{m}}$$



- ***Quantum Harmonic Oscillator***

(We will only give a qualitative discussion)

Schrödinger equation: $$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}\left(E-\frac{1}{2}k'x^2\right)\psi(x)=0$$

Define new variables: $$y=\sqrt{\frac{m\omega}{\hbar}}x \quad , \quad \epsilon=\frac{2E}{\hbar\omega}$$

=> $$\frac{d^2\psi}{dy^2}+(\epsilon-y^2)\psi=0$$ (Eq.1)

Boundary conditions:

$$\psi\rightarrow 0 \quad \text{as} \quad |y|\rightarrow\infty$$

We state (without proof) that the mathematical properties of (Eq.1) and the boundary conditions require that:

$$\epsilon = 2n+1 \qquad (n=0,1,2,\ldots)$$

$$\epsilon = \frac{2E}{\hbar\omega}$$ =>

$$\boxed{E_n = \left(n+\frac{1}{2}\right)\hbar\omega \qquad (n=0,1,2,\ldots)}$$

Energy levels of harmonic oscillator

Ground state energy (n = 0):

$$E_0 = \frac{1}{2}\hbar\omega$$

(also called zero-point energy)

Note: (Eq.1) can be solved exactly. Each wave function ψ_n is related to the so-called Hermite polynomial $H_n(y)$.

Example: The ground state wave function is

$$\psi(x) = C\, e^{-x^2/2b^2} \qquad \left(b = \sqrt{\hbar / m\omega}\right)$$

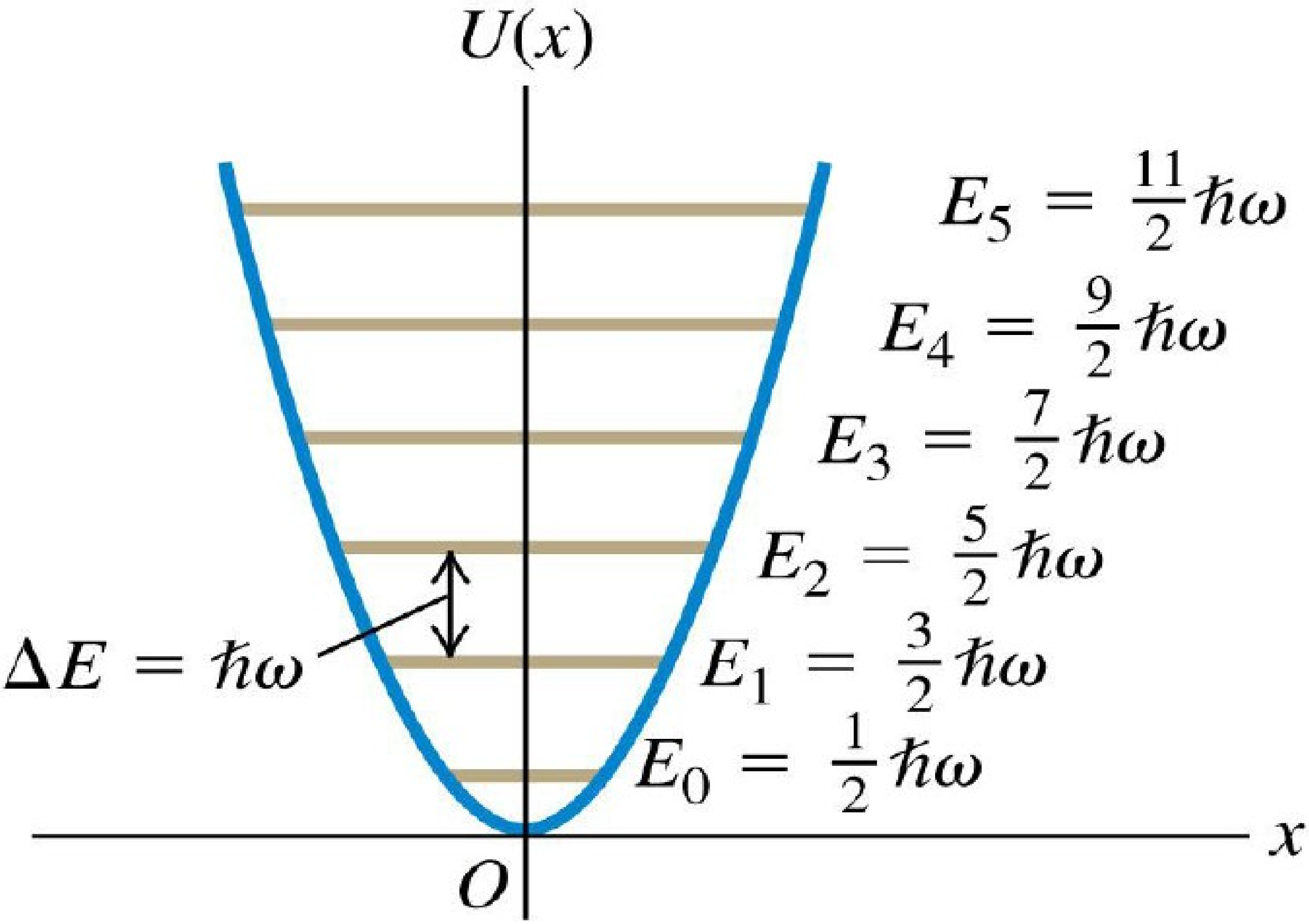
The normalization constant C is determined by

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

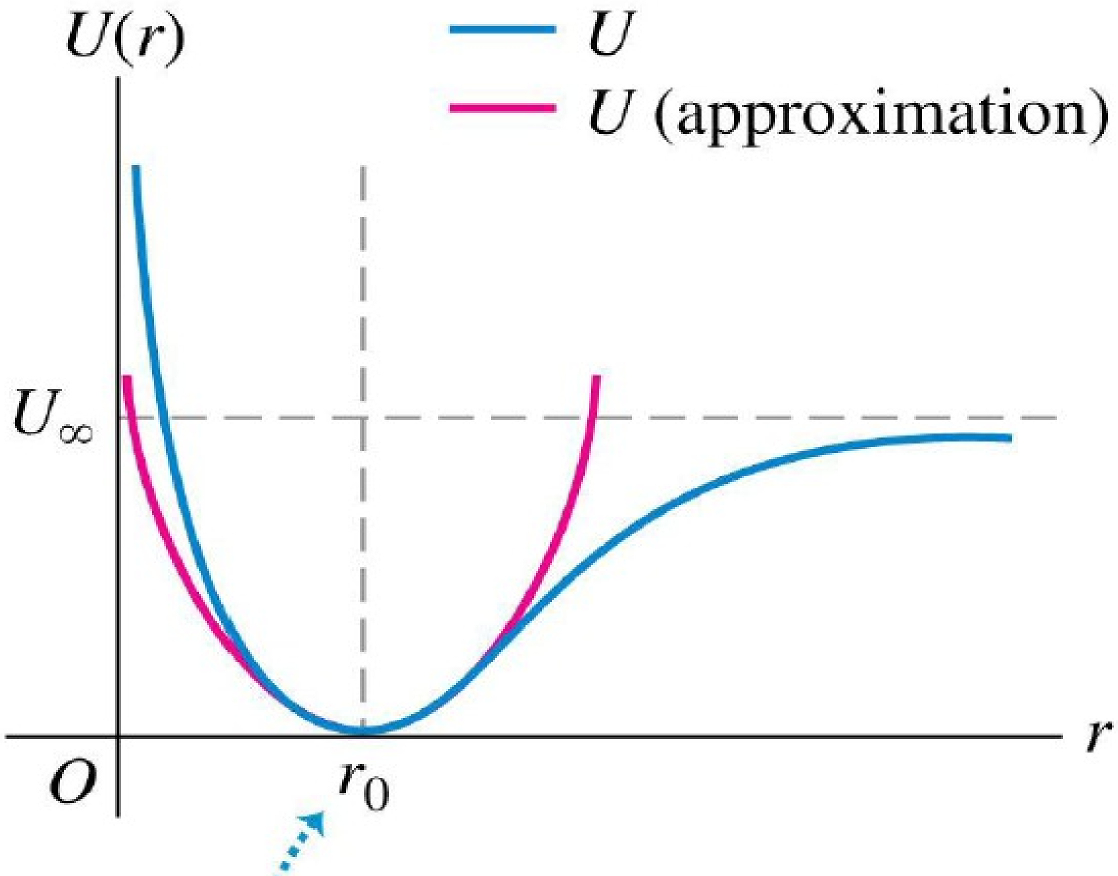
Note: Gaussian integral $\displaystyle\int_{-\infty}^{\infty} e^{-a^2 x^2}\, dx = \frac{\sqrt{\pi}}{a}$

Note: The spacing between any two adjacent energy levels is

$$\Delta E = \hbar \omega$$



Example: The potential energy function describing the interaction of two atoms in a diatomic molecule



When r is near r_0, the potential-energy curve is approximately parabolic (as shown by the red curve) and the system behaves approximately like a harmonic oscillator.

8.5 Three-Dimensional Problems

(Optional)

One-dimensional Schrödinger equation:

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

For a free particle (U = 0) $\psi = A e^{ikx}$

Note: $$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}=-\frac{\hbar^2}{2m}(A)(ik)^2 e^{ikx}=\frac{\hbar^2 k^2}{2m}\psi=\frac{p_x^2}{2m}\psi$$

K.E.

Schrödinger equation =>

$$K\psi+U\psi=E\psi$$

In three dimensions: $K = \frac{p_x^2 + p_y^2 + p_z^2}{2m}$

3D Schrödinger equation:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + U\psi = E\psi$$

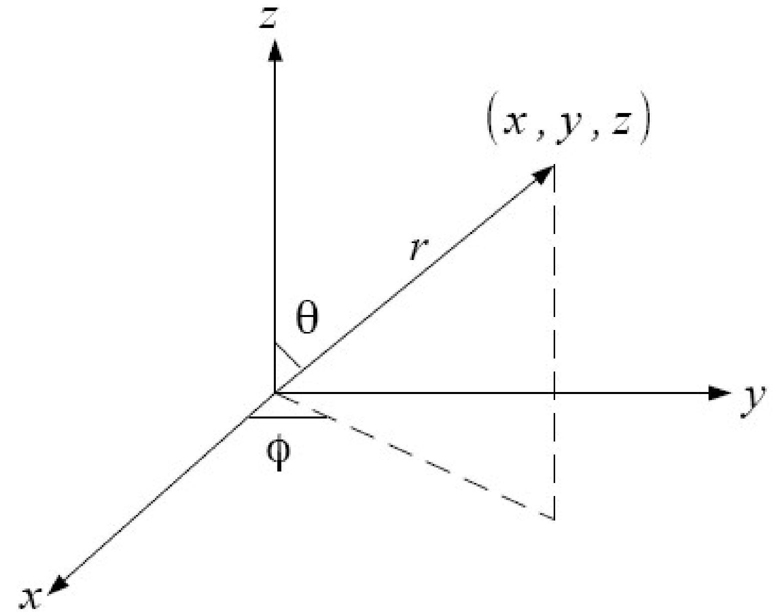
where U and ψ are functions of (x,y,z).

Define: $$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

(Laplacian operator) in Cartesian coordinates

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = E\psi$$

In many practical problems, it is convenient to use spherical coordinates (r, θ, ϕ):



$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$

=> Schrödinger equation in spherical coordinates:

$$-\frac{\hbar^2}{2m}\left\{\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi)+\frac{1}{r^2\sin\theta}\left[\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{\sin\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]\right\}+U\psi=E\psi$$

(No need to memorize!)