Introduction to Quantum Theory

Pre- Quantum Mechanics (History of quantum mechanics)

Laws of motion formulated by Galileo, Newton, Lagrange, Hamilton, Maxwell which preceded quantum theory are referred to as Classical Mechanics.

•The essence of classical mechanics is given in Newton's laws

$$m\frac{d^2\vec{r}}{dt^2} = F$$

•For a given force if the initial position and the velocity of the particle is known all physical quantities such as position, momentum, angular momentum, energy etc. at all subsequent times can be calculated.

Other formulations provide same information as obtained from Newton's Formulation.

Failures of Classical mechanics led to the **Need of Quantum mechanics**.

- Classical mechanics describes the motion of a baseball, the spinning of a top, and the flight of an airplane.
- Quantum mechanics describes the motion of electrons and the shapes of molecules such as trans fats, as well as electrical conductivity and superconductivity.

Classical mechanics failed to describe experiments on atomic and molecular phenomena :

1. classical physics cannot describe light particles (for example, electrons)
2. a new theory is required (i.e., quantum mechanics)

Recall that classical physics:

1. allows energy to have any desired value
2. predicts a precise trajectory for particles (i.e., deterministic)

The de Broglie Hypothesis

In 1924, de Broglie suggested that if waves of wavelength λ were associated with particles of momentum $p=h/\lambda$, then it should also work the other way round…….

A particle of mass m, moving with velocity v has momentum p given by:

$$p = mv = \frac{h}{\lambda}$$

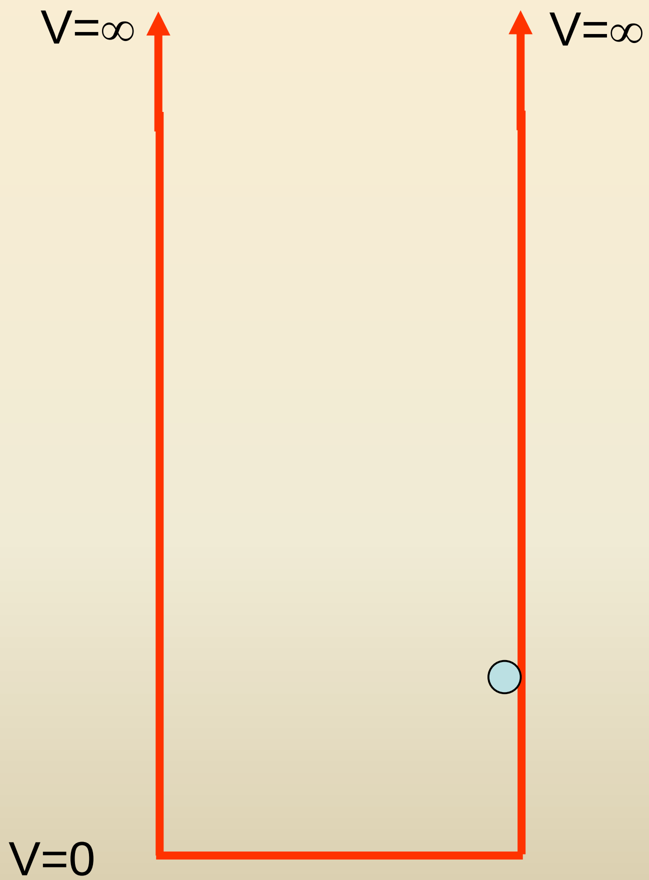
Kinetic Energy of particle

$$KE = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m}$$

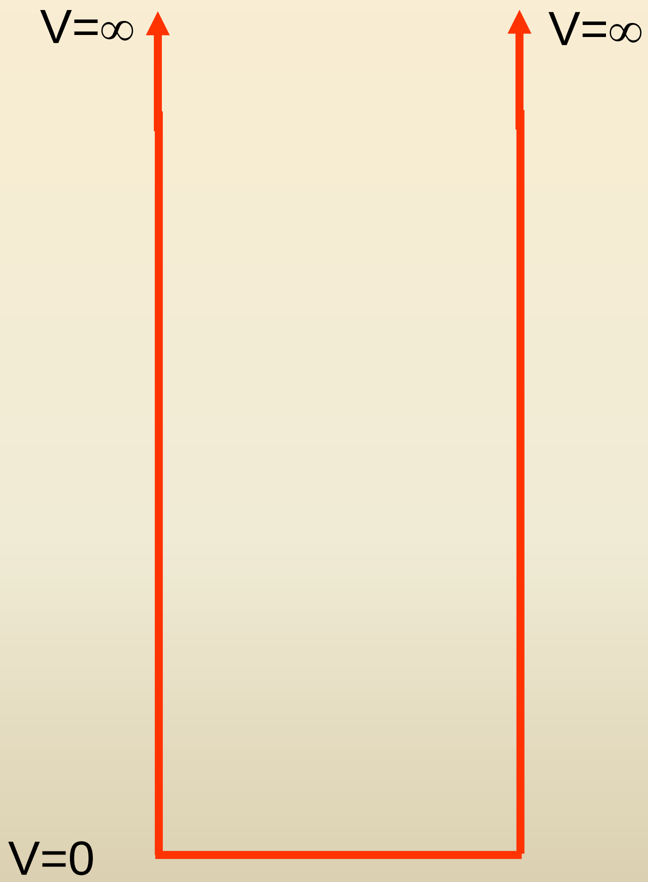
If the de Broglie hypothesis is correct, then a stream of classical particles should show evidence of wave-like characteristics……………………………………………

Standing de Broglie waves

Eg electron in a “box” (infinite potential well)

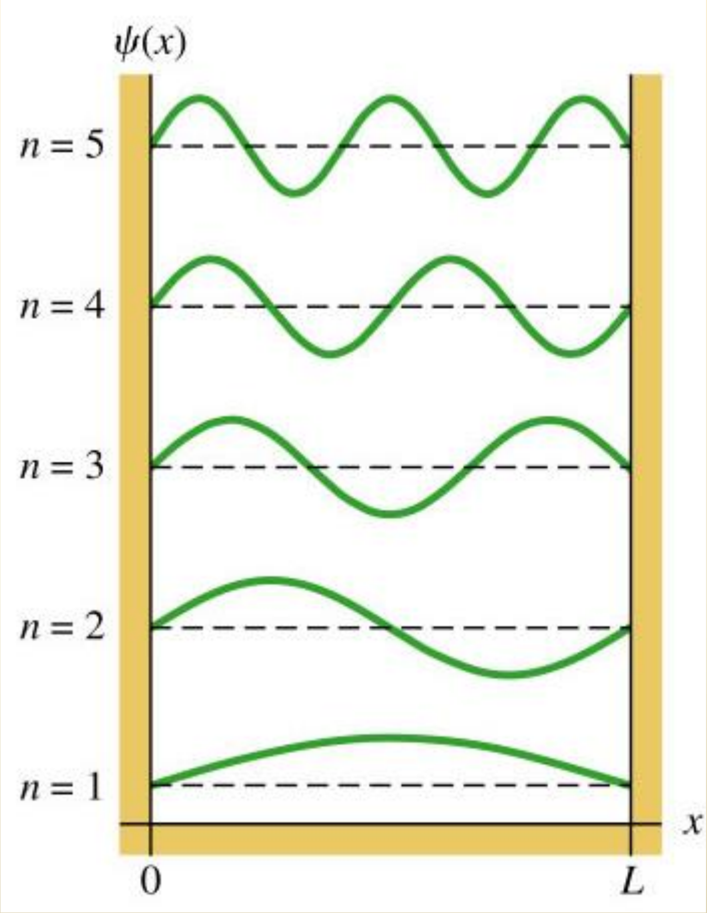


Electron “rattles” to and fro



Standing wave formed

Wavelengths of confined states



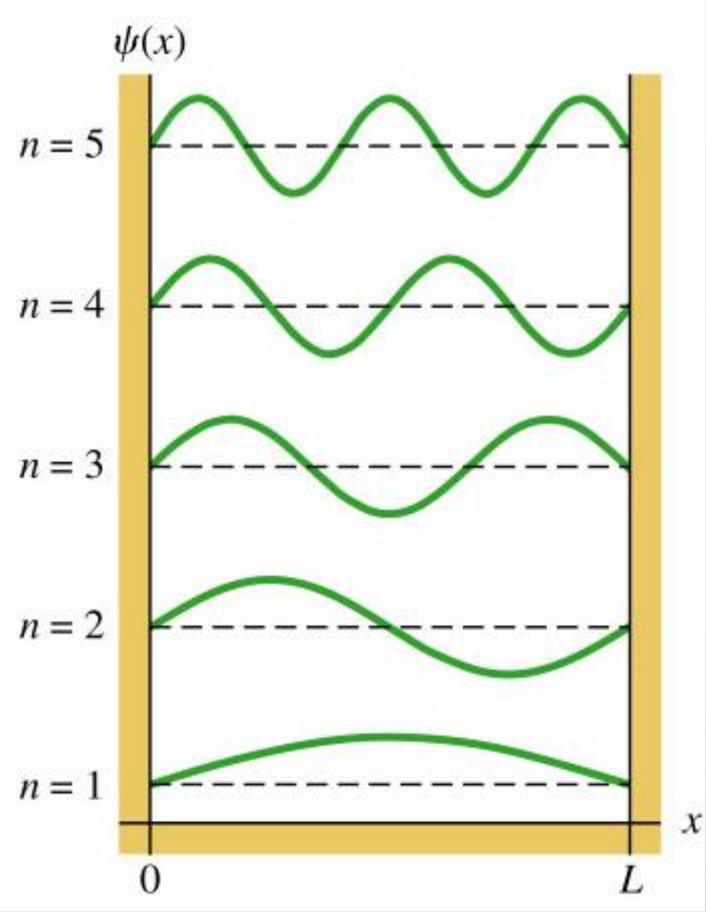
In general, k =nπ/L, n= number of antinodes in standing wave

$$\lambda = \frac{2L}{3}\,;\, k = \frac{3\pi}{L}$$

$$\lambda = L\,;\, k = \frac{2\pi}{L}$$

$$\lambda = 2L\,;\, k = \frac{\pi}{L}$$

Energies of confined states

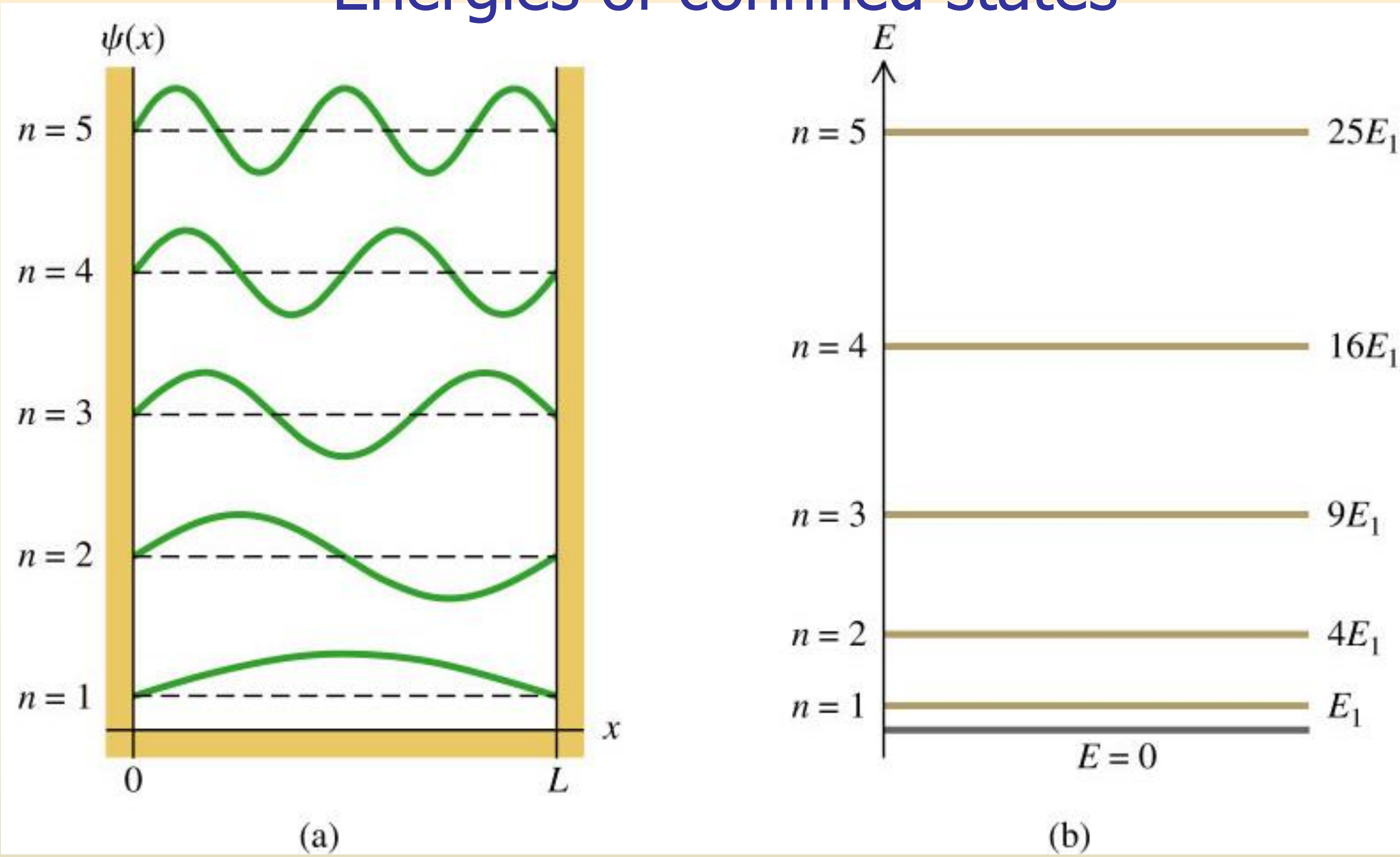


$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

$$E_n = n^2 E_1$$

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$$

Energies of confined states



$$E_n = n^2 E_1$$

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$$

Particle in a box: wave functions

From Lecture 4, standing wave on a string has form:

$$y(x,t) = (A\sin kx)\sin(\omega t)$$

Our particle in a box wave functions represent STATIONARY (time independent) states, so we write:

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

A is a constant, to be determined……………

Interpretation of the wave function

The wave function of a particle is related to the *probability density* for finding the particle in a given region of space:

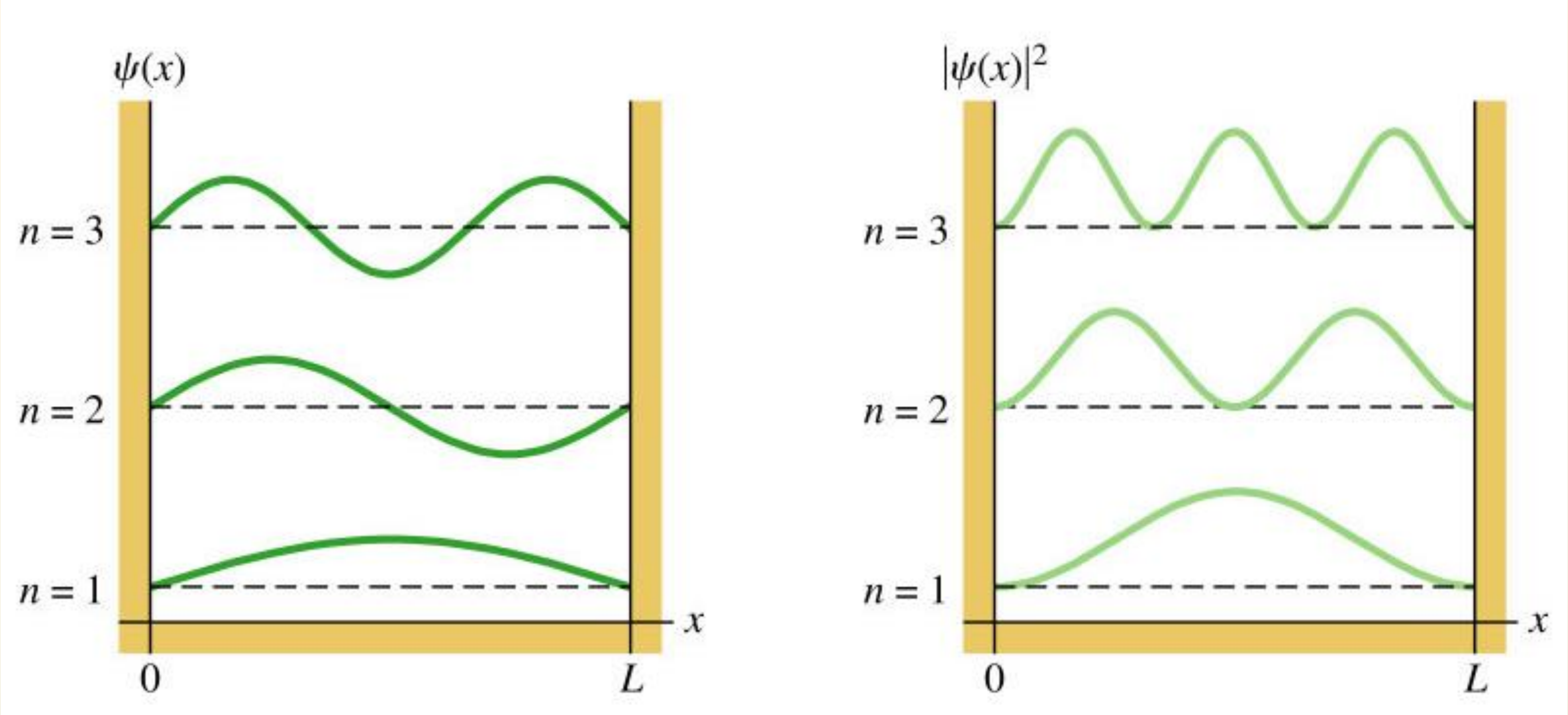
Probability of finding particle between x and x + dx:

$$\left|\psi(x)\right|^2 dx$$

Probability of finding particle *somewhere* = 1, so we have the NORMALISATION CONDITION for the wave function:

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

Interpretation of the wave function



(a) (b)

Interpretation of the wave function

Normalisation condition allows unknown constants in the wave function to be determined. For our particle in a box we have WF:

$$\psi(x) = A\sin kx = A\sin\frac{n\pi x}{L}$$

Since, in this case the particle is confined by INFINITE potential barriers, we know particle must be located between x=0 and x=L →Normalisation condition reduces to :

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

Particle in a box: normalisation of wave functions

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

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

$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

Some points to note…………..

So far we have only treated a very simple one-dimensional case of a particle in a completely confining potential.

In general, we should be able to determine wave functions for a particle in all three dimensions and for potential energies of any value

Requires the development of a more sophisticated "QUANTUM MECHANICS" based on the SCHRÖDINGER EQUATION…………………

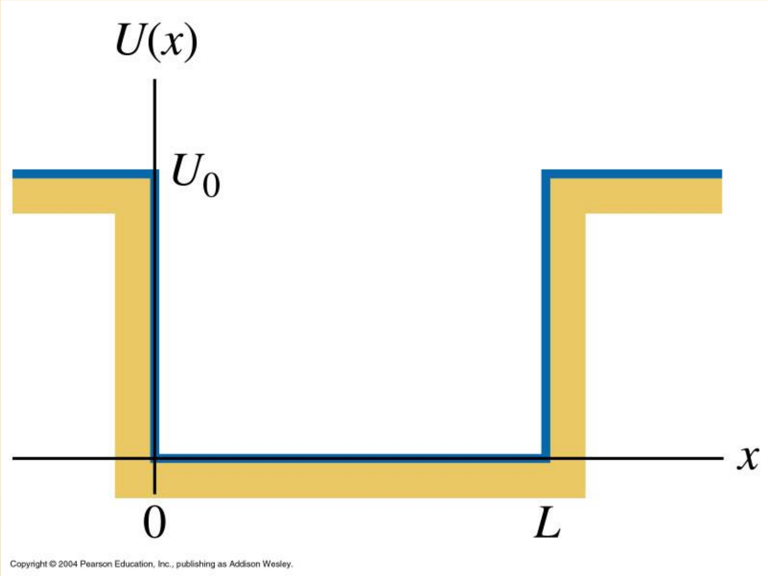
The Schrödinger Equation in 1-dimension (time-independent)

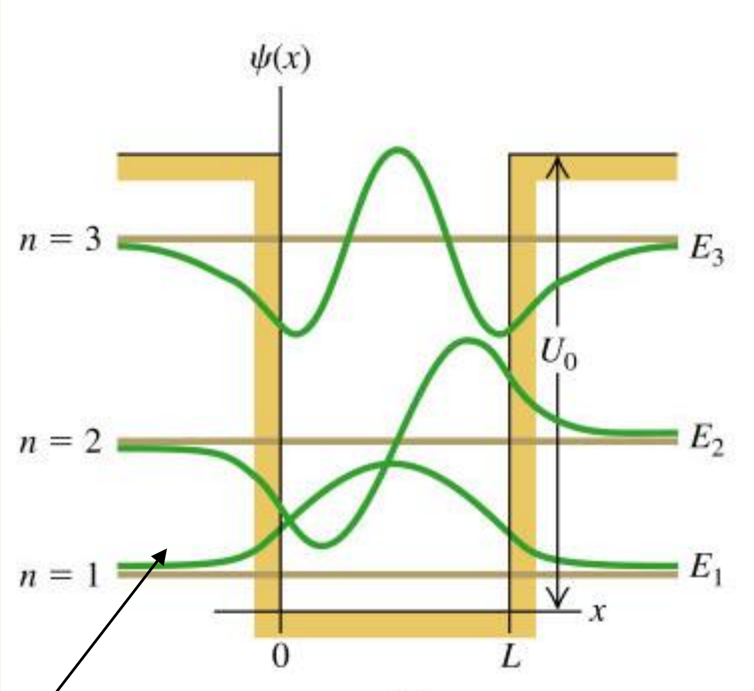
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

KE Term

PE Term

Finite potential well



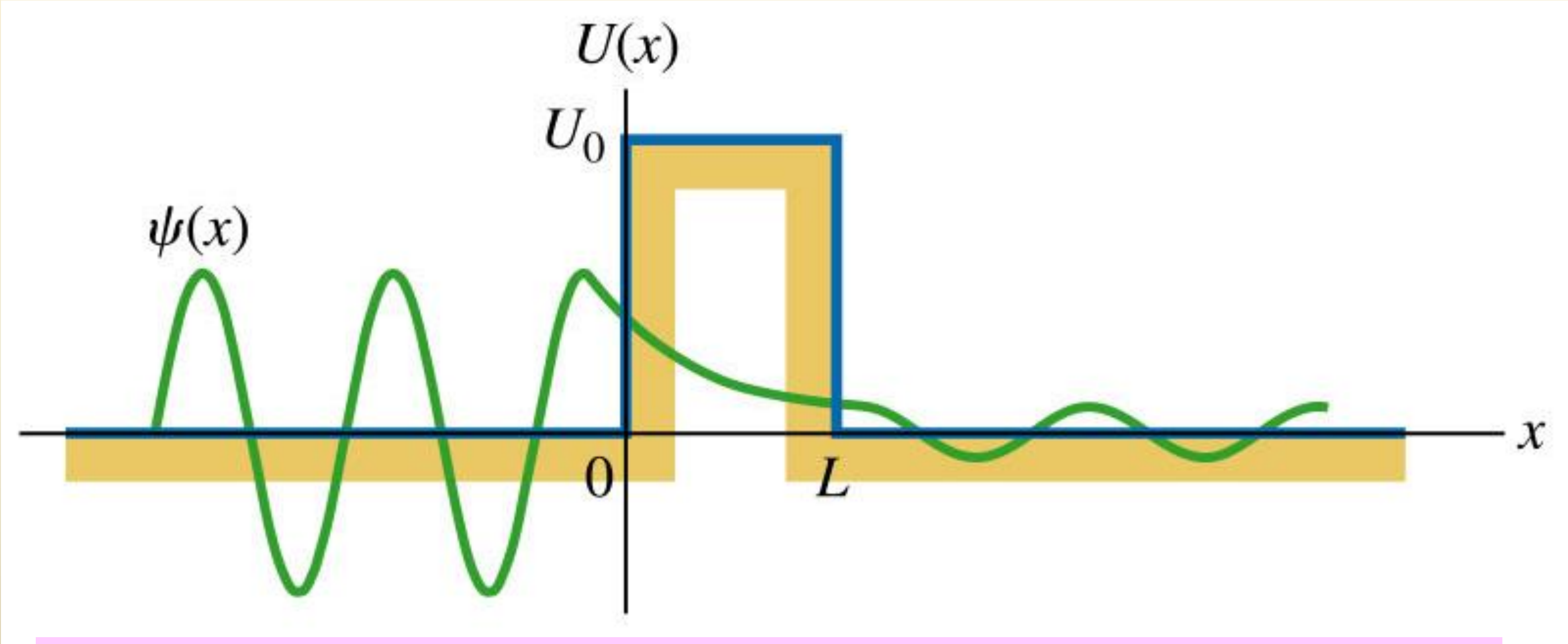


(a)

WF “leakage”, particle has finite probability of being found in barrier: CLASSICALLY FORBIDDEN

Solving the Schrodinger equation allows us to calculate particle wave functions for a wide range of situations (See Y2 QM course)…….

Barrier Penetration (Tunnelling)



Quantum mechanics allows particles to travel through “brick walls”!!!!

Solving the SE for particle in an infinite potential well

$$V(x) = 0 \qquad\qquad 0 < \mathrm{x} < \mathrm{L}$$

So, for 0<x<L, the time independent SE reduces to:

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

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE\psi(x)}{\hbar^2} = 0$$

General Solution:

$$\psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{1/2} x + B\cos\left(\frac{2mE}{\hbar^2}\right)^{1/2} x$$

$$\psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{1/2} x + B\cos\left(\frac{2mE}{\hbar^2}\right)^{1/2} x$$

Boundary condition: ψ(x) = 0 when x=0:→B=0

$$\psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{1/2} x$$

Boundary condition: ψ(x) = 0 when x=L:

$$\psi(0) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{1/2} L = 0 \quad \longrightarrow \quad E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$\psi(x) = A\sin\frac{n\pi x}{L}$$

In agreement with the “fitting waves in boxes” treatment earlier………………..

Thank You