# Quantum Mechanics

## Classical Point of View

- The laws are written in terms of PARTICLE TRAJECTORIES.
- A PARTICLE is an indivisible mass point object that has a variety of properties that can be measured (called observables).
- The observables specify the state of the particle (position and momentum).
- ❖ A SYSTEM is a collection of particles, which interact among themselves via internal forces, and can also interact with the outside world via external forces.
- ❖ The STATE OF A SYSTEM is a collection of the states of the particles that comprise the system.
- ❖ All properties of a particle can be known to infinite precision.

#### Conclusions:

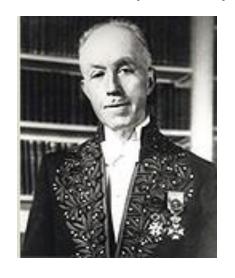
- TRAJECTORY → state descriptor of Newtonian physics,
- EVOLUTION OF THE STATE → Use Newton's second law
- PRINCIPLE OF CAUSALITY → Two identical systems with the same initial conditions, subject to the same measurement will yield the same result.

## Quantum Point of View

- ❖ Quantum particles can act as both particles and waves
  → WAVE-PARTICLE DUALITY
- ❖ Quantum state is a conglomeration of several possible outcomes of measurement of physical properties → Quantum mechanics uses the language of PROBABILITY theory (random chance).
- An observer cannot observe a microscopic system without altering some of its properties. Neither one can predict how the state of the system will change.
- QUANTIZATION of energy is yet another property of "microscopic" particles.

### de Broglie relation from relativity

Popular expressions of relativity: m<sub>0</sub> is the mass at rest, m in motion



$$\mathbf{m} = \frac{\mathbf{m}_0}{\sqrt{1 - \frac{\mathbf{v}^2}{\mathbf{c}^2}}} \qquad \text{and} \quad \mathbf{E} = \mathbf{m} \ \mathbf{c}^2$$

$$E^2 = m^2 e^4 (1 - \frac{v^2}{e^2}) + p^2 e^2 = m_0^2 e^4 + p^2 e^2$$

Application to a photon (m $_0$ =0) E=h
u

$$\mathbf{E} = \mathbf{pc} \rightarrow \mathbf{pc} = \mathbf{h}\mathbf{v}$$

$$|\mathbf{p} = \frac{\mathbf{h}\mathbf{v}}{\mathbf{c}}| = \frac{\mathbf{h}}{\lambda} = \frac{\mathbf{E}}{\mathbf{c}}$$

$$(\lambda = \frac{\mathbf{h}}{\mathbf{p}})$$

### De Broglie Hypothesis

- · We have seen that radiation has dual behavior:
  - Wave-like and particle-like.
- In 1924 de Broglie suggested that the same is true for matter.
- Specifically, he proposed that frequency and wavelength can be associated with an electron's energy and momentum.
  - Here, λ is the de Broglie wavelength.
- Recall for photon:

$$E = pc = hv = \frac{hc}{\lambda}$$

de Broglie relations hold for photon.

$$v = \frac{E}{h}$$
$$\lambda = \frac{h}{p}$$

Consider a particle with kinetic energy K. Its momentum is found from

$$K = \frac{p^2}{2m} \quad or \quad p = \sqrt{2mK}$$

Its wavelength is then

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}}$$

### de Broglie Wavelength in terms of V

Consider an electron of mass *m* and charge *q* accelerated through a potential difference of *V* volts

KE of the electrons is equal to the energy of the electron accelerated at

a potential of 
$$V$$
 volts 
$$\frac{1}{2}mv^2 = qV \rightarrow m^2v^2 = 2mqV \rightarrow p^2 = 2mqV$$

$$p = mv = \sqrt{2m\,qV}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m\,q\,V}}$$

de Broglie wavelength of electron q = e

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}} \qquad \lambda = \frac{12.28}{\sqrt{V}} \times 10^{-10} m$$

Calculate the wavelength of a electron and a bullet of mass 10 gram moving at 100 m/s.

Comment on the answers

#### For electron

$$\lambda e = h/mv = 6.63x10^{-34} / (9.1x10^{-31}) (100)$$

$$\lambda e = 7.28 \times 10^{-6} \text{ m}$$

#### measurable

#### for bullet

$$\lambda = h/mv = 6.6x10^{-34}/(0.01)(100)$$

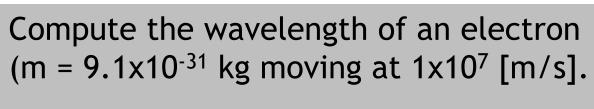
$$= 6.63 \times 10^{-34} \text{ m}$$

This is immeasureably small

For ordinary "everyday objects," we don't experience that

**MATTER CAN BEHAVE AS A WAVE** 

### But, what about small particles?



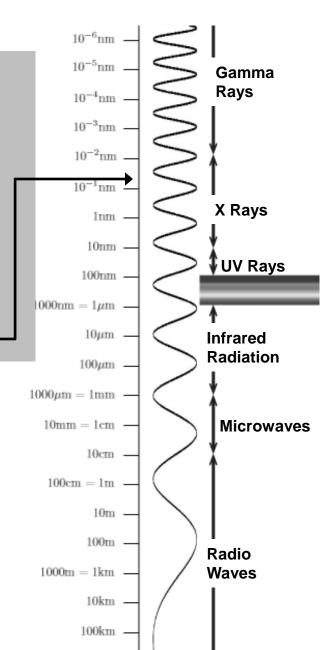
 $\lambda = h/mv$ 

=  $6.6 \times 10^{-34} [J s]/(9.1 \times 10^{-31} [kg])(1 \times 10^{7} [m/s])$ 

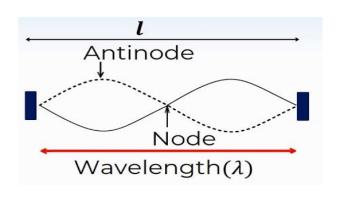
 $= 7.3 \times 10^{-11} [m].$ 

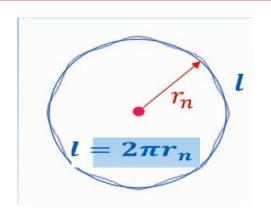
= 0.073 [nm]

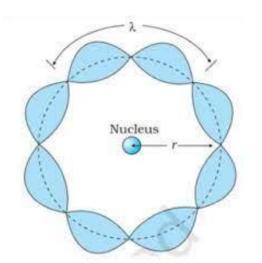
These electrons have a wavelength in the region of X-rays



### DE BROGLIE'S EXPLANATION OF BOHR'S SECOND POSTULATE OF QUANTIZATION







For an electron moving in  $n^{th}$  circular orbit of radius  $r_n$ ,  $2\pi r_n = n\lambda$ n = 1, 2, 3...

i.e., Circumference of orbit should be integral nultiple of de-Broglie wavelength of electron moving in nth orbit.

Also, we know, de Broglie wavelength;  $\lambda = \frac{h}{mv}$ Therefore

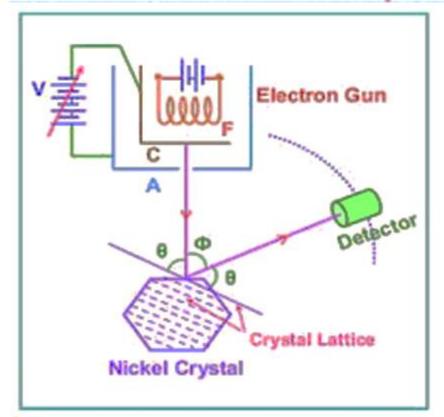
Therefore 
$$2\pi r_n = \frac{h}{mv_n}$$

$$\Rightarrow m v_n r_n = \frac{\eta h}{2\pi}$$

# **Davisson – Germer experiment**



### Davisson and Germer Experiment:



A beam of electrons emitted by the electron gun is made to fall on Nickel crystal cut along cubical axis at a particular angle.

The scattered beam of electrons is received by the detector which can be rotated at any angle.

The energy of the incident beam of electrons can be varied by changing the applied voltage to the electron gun.

Intensity of scattered beam of electrons is found to be maximum when angle of scattering is 50° and the accelerating potential is 54 V.

θ + 50° + θ = 180° i.e. θ = 65°

For Ni crystal, lattice spacing d = 0.91 Å

For first principal maximum, n = 1

Electron diffraction is similar to X-ray diffraction.

→ Bragg's equation 2dsinθ = nλ gives.

$$\lambda = 1.65 \text{ Å}$$

For Nickel crystal

$$d = 0.91 \text{ A}^{\circ}$$
  $\theta = 65^{\circ} n = 1$   
 $2 \times 0.91 \times \sin 65 = 1.65 \text{ A}^{\circ}$   
 $\lambda = 1.65 \text{ A}^{\circ}$ 

Hence, the De-broglie wavelength as obtained from the experiment is  $\lambda = 1.65 A^{\circ}$ 

Now we use De-broglie for theoretical calculation of  $\lambda$  as

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mev}}$$

$$= \frac{6.64 \times 10^{-34}}{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 54}$$

$$\lambda = 1.66 \text{A}^{\circ}$$

Hence the De-broglie wavelength of electron waves determined by Davisson and Germer experiment and those calculated from De-broglie hypothesis are found to be in close agreement. Thus the result of Davisson and Germer confirms the De-broglie concept of matter waves without any doubts.

### **Phase Velocity (Velocity of Matter wave)**

phase velocity

$$v_p = \lambda v$$

for a massive particle

$$v_p = \frac{h}{mv} \frac{mc^2}{h} = c \frac{c}{v} > c$$

for a massless particle

$$v_p = \frac{h}{p} \frac{E}{h} = \frac{1}{p} \frac{pc}{1} = c$$

phase velocity does not describe particle motion

# Properties of Matter Waves

- Associated with moving particles.
- Wavelength inversely proportional to mass and velocity.
- Independent of nature of charge.
- > Neither electromagnetic nor mechanical waves.
- > Associated with probability of finding particle.
- Phase velocity is not significant for the matter waves.
- > A velocity called group velocity is significant for the matter waves
- P Quantity associated is called wave function  $\Psi(x, y, z, t) = A + i B$
- $\triangleright |\Psi|^2$  is real and called probability of finding the particle.

#### Wave functions

#### Waves of what?

#### "normal" waves

are a disturbance in space carry energy from one place to another often (but not always) will (approximately) obey the classical wave equation

#### "Matter" waves

disturbance is the wave function  $\Psi(x, y, z, t)$  probability amplitude  $\Psi$  probability density  $p(x, y, z, t) = |\Psi|^2$ 

### **Group Velocity**

$$\Psi_1 = A\cos(\omega t - kx)$$

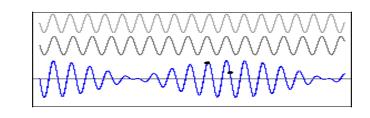
$$\Psi_2 = A\cos\left[\left(\omega + \Delta\omega\right)t - \left(k + \Delta k\right)x\right]$$

$$\Psi = \Psi_1 + \Psi_2$$

$$\Psi = 2A\cos\frac{1}{2}\left[\left(2\omega + \Delta\omega\right)t - \left(2k + \Delta k\right)x\right]\cos\frac{1}{2}\left[\left(\Delta\omega\right)t - \left(\Delta k\right)x\right]$$

with  $\Delta \omega \ll \omega, \ll k$ 

$$\Psi \cong 2A\cos\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right]\cos\left[\omega t - kx\right]$$



phase velocity = wave velocity of carrier:  $v_p = \frac{\alpha}{k}$ 

group velocity= wave velocity of envelope: 
$$v_g = \frac{\Delta \omega}{\Delta k}$$

for more than two wave contiributions  $v_g = \frac{d\omega}{dk}$ 

#### **Group Velocity**

$$\omega = 2\pi v = 2\pi \frac{E}{h} = 2\pi \frac{m_0 c^2}{h\sqrt{1 - (v/c)^2}}$$

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h} mv = \frac{2\pi}{h} \frac{m_0 v}{\sqrt{1 - (v/c)^2}}$$

$$v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv}$$

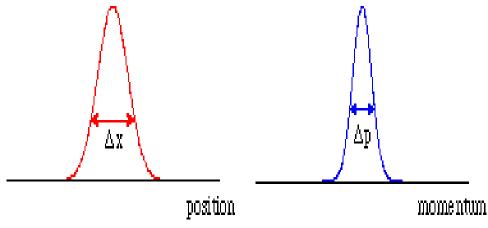
$$v_{g} = rac{d\omega}{dk} = rac{d\omega/dv}{dk/dv}$$
  $d\omega/dv = 2\pi rac{m_{0}c^{2}v}{h(1-(v/c)^{2})^{3/2}}$   $dk/dv = 2\pi rac{m_{0}c^{2}v}{h(1-(v/c)^{2})^{3/2}}$ 

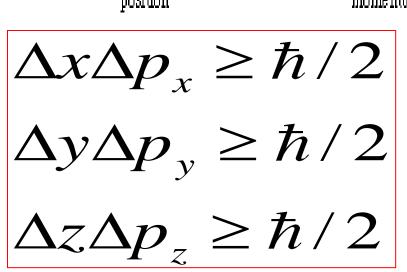
$$\Rightarrow v_g = v$$

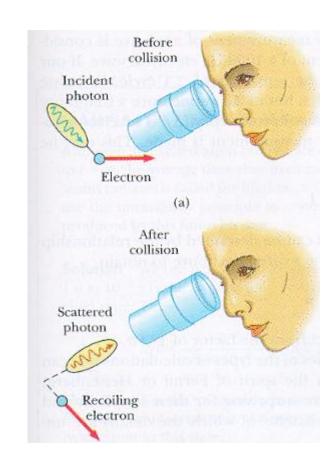
### Heisenberg's Uncertainty Principle

It is not possible to precisely specify a particle's position and momentum at the same time.









# *Implications*

- It is impossible to know both the position and momentum exactly, i.e.,  $\Delta x=0$  and  $\Delta p=0$
- These uncertainties are inherent in the physical world and have nothing to do with the skill of the observer

 $\hbar = 1.054 \times 10^{-34} \, [\mathrm{J \cdot s}]$  • Because h is so small, these uncertainties are not observable in normal everyday situations

# Example of Baseball

A pitcher throws a 0.1-kg baseball at 40 m/s

• So momentum is  $0.1 \times 40 = 4 \text{ kg m/s}$ 

 Suppose the momentum is measured to an accuracy of 1 percent, i.e.,

 $\Delta p = 0.01 p = 4 \times 10^{-2} \text{ kg m/s}$ 

# Example of Baseball (cont 'd)

 The uncertainty in position is then

$$\Delta x \ge \frac{h}{4\pi\Delta p} = 1.3 \times 10^{-33} \text{m}$$

 No wonder one does not observe the effects of the uncertainty principle in everyday life!

# Example of Electron

 Same situation, but baseball replaced by an electron which has mass 9.11 x 10<sup>-31</sup> kg traveling at 40 m/s

• So momentum =  $3.6 \times 10^{-29} \text{ kg m/s}$ and its uncertainty=  $3.6 \times 10^{-31} \text{ kg m/s}$ 

The uncertainty in position is then

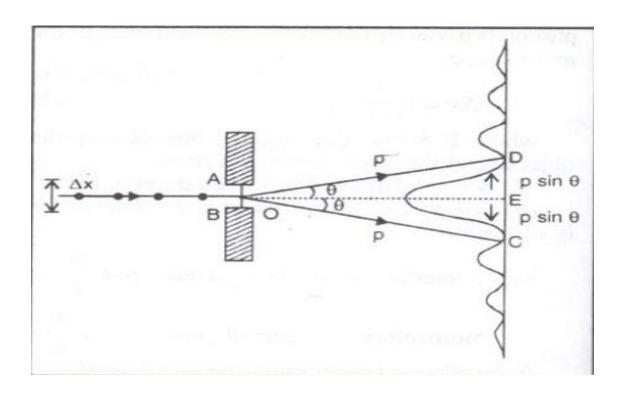
$$\Delta x \ge \frac{h}{4\pi\Delta p} = 1.4 \times 10^{-4} \text{m}$$

# Diffraction of Electron by a slit

electrons. Before entering the slit, the electron has a definite momentum p and after passing through the slit the electron gets diffracted.

For first minima

$$\Delta x$$
.  $\sin \theta = \lambda$ , ....(1)  
[:  $d \sin \theta = n\lambda$ ]



## **Electron Diffraction - Continued**

... uncertainty in the measurement of position of electrons at which the electron beam enters the slit

$$\Delta x = \frac{\lambda}{\sin \theta}$$
 ....(2)

Since the electron can be anywhere in the diffraction pattern from angle  $-\theta$  to  $+\theta$ , so the component of momentum perpendicular to the initial direction can have momentum  $p \sin \theta$  and  $p \sin (-\theta)$ 

$$[=-p\sin\theta)]$$

:. Uncertainty in momentum of electron

$$\Delta p = p \sin \theta - (-p \sin \theta) = 2p \sin \theta$$

or 
$$\Delta p = \frac{2h}{\lambda} \sin \theta$$
 ....(3)

## **Electron Diffraction - Continued**

From Eq. (2) & (3), we have

$$\Delta x \cdot \Delta p = \frac{\lambda}{\sin \theta} \cdot \frac{2h}{\lambda} \sin \theta = 2h$$
  
 $\Delta x \cdot \Delta p \ge h$ 

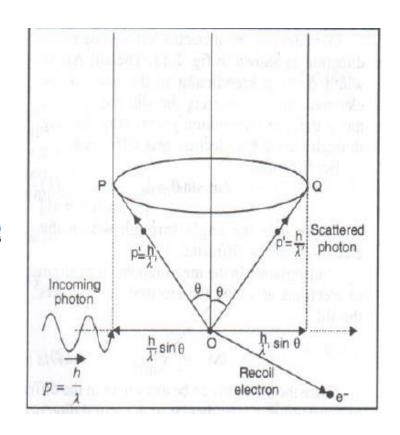
or

# Gamma Ray Microscope

(a)Limitation in determing the position of electron

$$\Delta x = \frac{\lambda'}{2\sin\theta} - -(1)$$

 $\lambda' = wavelenth of scattered photon$  $\theta=half angle subtended by the objective at the object i.e. electron$ 



(b)Limitation in determining the momentum of the electron

Let momentum of the Incident photon 
$$p = \frac{n}{\lambda}$$

momentum of the scattered photon 
$$p' = \frac{h}{\lambda'}$$

photon is scattered along OQ,Then

Momentum of the scattered Photon along 
$$X - axis = \frac{h}{\lambda'} \sin \theta$$

Momentum imparted to the electron along 
$$X - axis = \frac{h}{\lambda} - \frac{h}{\lambda'} \sin \theta$$

If photon is scattered along OP, then

Momentum of the scattered Photon along  $X - axis = -\frac{h}{\lambda'} \sin \theta$ 

Momentum imparted to the electron along  $X - axis = \frac{h}{\lambda} - (-\frac{h}{\lambda'}\sin\theta) = \frac{h}{\lambda} + \frac{h}{\lambda'}\sin\theta$ 

Thus an electron can have momentum  $\left(\frac{h}{\lambda} + \frac{h}{\lambda'} \sin \theta\right)$  and  $\left(\frac{h}{\lambda} - \frac{h}{\lambda'} \sin \theta\right)$ 

Uncertainty in Momentum of the electron along  $X - axis \ \Delta px = \frac{h}{\lambda} + \frac{h}{\lambda'} \sin \theta - (\frac{h}{\lambda} - \frac{h}{\lambda'} \sin \theta)$ 

$$\Delta px = \frac{2h}{\lambda'} \sin \theta - - - -(2)$$

from 1 and 2  $\Delta x \Delta p x = \frac{\lambda}{2 \sin \theta} X \frac{2h}{\lambda'} \sin \theta = h$ 

$$\Delta x \Delta p x \ge h$$

# Applications of Heisenberg uncertainty Principle Non existence of electron in the nucleus

Size of Nucleus =  $10^{-14}$  m

If electron is present in the nucleus uncertainty in the position of electron is =  $10^{-14}$  m

$$\Delta p \ge \frac{h}{\Delta x} = \frac{1.055 \times 10^{-34}}{10^{-14}} \text{ kg ms}^{-1}$$

$$\Delta p = 1.05 \times 10^{-20} \text{ kg ms}^{-1}$$

# The minimum momentum of the electron must be at least equal to uncertainty in momentum

$$p = \Delta p = 1.05 \times 10^{-20} \text{ kg ms}^{-1}$$
  
 $E = \sqrt{p^2 c^2 + m_0^2 c^4}$ 

Since for electron, 
$$m_0^2 c^4 \ll p^2 c^2$$
, so it is neglected, hence  

$$E = pc$$

$$E \approx (1.05 \times 10^{-20}) \times (3 \times 10^8) \text{ J}$$

$$\approx \frac{(1.05 \times 10^{-20}) (3 \times 10^8)}{1.6 \times 10^{-13}} \text{ MeV}$$

$$= .20 \text{ MeV}$$

# Kinetic energy

Classical 
$$T = \frac{p^2}{2m}$$
 quantum operator  $\mathbb{P}^2 = \frac{-h^2}{2m} \frac{\partial^2}{\partial \mathbb{X}^2}$ 

In 3D: 
$$\mathbb{T} = \frac{-h^2}{2m} \ (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}) = \frac{-h^2}{2m} \ \triangle$$

Calling 
$$\triangle = (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial y^2})$$
 the laplacian



Pierre Simon, Marquis de Laplace (1749 -1827)



#### **Time-dependent Schrödinger Equation**

Without potential E = TWith potential E = T + V

$$ih\frac{\partial \Psi(\mathbf{r},t)}{\partial t} = -\frac{h^2}{2m} \Delta \Psi(\mathbf{r},t)$$

$$ih\frac{\partial\Psi(\mathbf{r,t})}{\partial t}~=-\frac{h^2}{2m}~\Delta\Psi(\mathbf{r,t})~+~V(\mathbf{r,t})\Psi(\mathbf{r,t})$$

Erwin Rudolf Josef Alexander Schrödinger Austrian
1887 –1961



### Schrödinger Equation for stationary states

$$ih\frac{\partial \Psi(\mathbf{r},t)}{\partial t} = -\frac{h^2}{2m} \Delta \Psi(\mathbf{r},t) + V(\mathbf{r},t)\Psi(\mathbf{r},t)$$

$$\begin{split} \Psi(\textbf{r},\textbf{t}) &= \Psi(\textbf{r}).\Psi(\textbf{t}) = A \exp(\frac{-iEt}{h}) \ \Psi(\textbf{r}) \\ ih \frac{\partial \Psi(\textbf{r}).\Psi(\textbf{t})}{\partial \textbf{t}} &= -\frac{h^2}{2m} \ \Delta \Psi(\textbf{r}).\Psi(\textbf{t}) \ + V(\textbf{r})\Psi(\textbf{r}).\Psi(\textbf{t}) = E \ \Psi(\textbf{r}).\Psi(\textbf{t}) \\ -\frac{h^2}{2m} \ \Delta \Psi(\textbf{r}) \ + V(\textbf{r})\Psi(\textbf{r}) = E \ \Psi(\textbf{r}) \end{split}$$
 Potential energy



### Schrödinger Equation for stationary states

$$-\frac{\hbar^2}{2m} \Delta \Psi(\mathbf{r}) + V(\mathbf{r})\Psi(\mathbf{r}) = E \Psi(\mathbf{r})$$

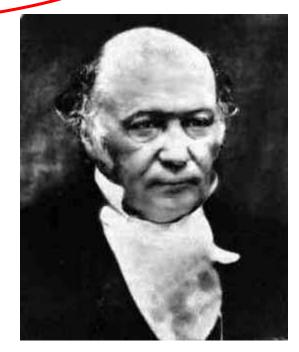
Remember

$$\mathbb{H} \Psi(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \mathbb{E} \Psi(\mathbf{x}, \mathbf{y}, \mathbf{z}) \quad \text{with} \quad \mathbb{H} = -\frac{h^2}{2m} \triangle + \mathbb{V}$$

#### H is the hamiltonian



Half penny bridge in Dublin



Sir William Rowan Hamilton Irish 1805-1865

### Schrodinger's equation applied to free particle

- Consider a particle of mass m moving along positive x-axis.
- Particle is said to be free if it is not under the influence of any field or force.
- Therefore for a free particle potential energy can be considered to be constant or zero.
- > The Schrodinger wave equation for a free particle is given by.

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi = E\Psi$$

$$V = 0$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$

$$\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + E\Psi = 0$$

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m}{\hbar^2} E \Psi = 0$$

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} E \Psi = 0 \qquad \text{let } k^2 = \frac{8\pi^2 m E}{h^2}$$

$$\frac{\partial^2 \Psi}{\partial x^2} + k^2 \Psi = 0$$

### The Solution of this equation is

$$\Psi = A e^{ikx} + B \bar{e}^{ikx}$$

#### The solution of the equation is of the form

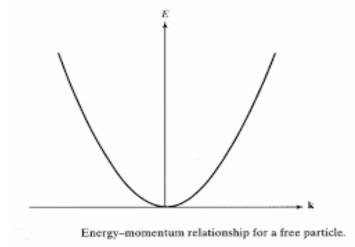
$$\Psi = A \cdot e^{ikx} + B \cdot \bar{e}^{ikx}$$

Where A and B are unknown constants to be determined. Since there are no boundary conditions A, B and k can have any values.

$$\mathbf{k^2} = \frac{8\pi^2 m \, \mathrm{E}}{h^2}$$

Energy of the particle is given by

$$E = \frac{k^2 h^2}{8\pi^2 m}$$



- Since there is no restriction on "k" there is no restriction on "E."
- ❖ Therefore energy of the free particle is not quantized. i.e., free particle can have any value of energy.

# MOTION OF AN ELECTRON IN ONE DIMENSIONAL POTENTIAL WELL (PARTICLE IN A BOX)

Consider a particle (like electron) of mass **m**, moving along positive x-axis between two walls of infinite height, one located at **x=0** and another at **x=L** 

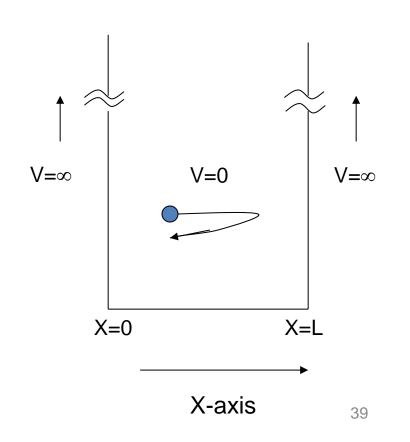
Let potential energy of the electron is assumed to be zero in the region inbetween the two walls and infinity in the region beyond the walls.

$$V = 0$$
 for  $0 \le x \le L$   
 $V = \infty$  for  $x < 0$  &  $x > L$ 

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\psi = E\psi$$

$$V = 0$$
 for  $0 \le x \le L$ 

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$



$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + E \Psi = 0$$

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m}{\hbar^2} E \Psi = 0$$

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} E \Psi = 0 \qquad \text{let } k^2 = \frac{8\pi^2 m E}{h^2}$$

$$\frac{\partial^2 \Psi}{\partial x^2} + k^2 \Psi = 0$$

### The Solution of this equation is

$$\Psi = A e^{ikx} + B e^{ikx}$$

$$at \ x = 0 \ , \ \psi = 0 \ ....(I)$$

and at 
$$x = L$$
,  $\psi = 0$  ..... (II)

#### Therefore correct solution of the equation can be written as

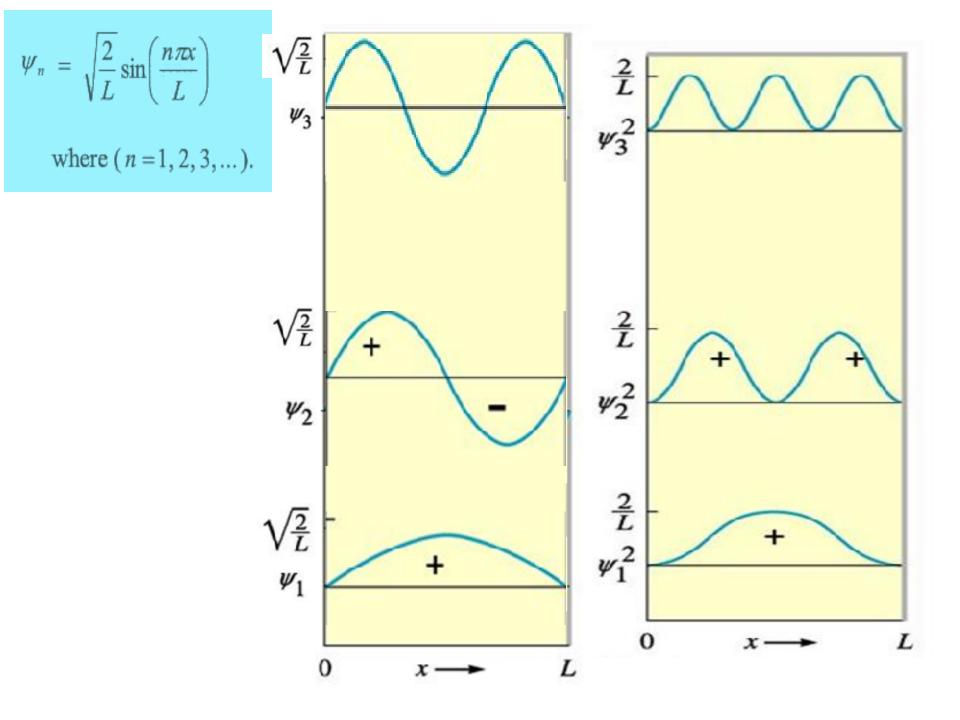
$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

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

The possible values of  $\psi$  are called eigen functions

$$E_n = \frac{n^2 h^2}{8mL^2}$$

The possible values of energy are called Eigenvalues.

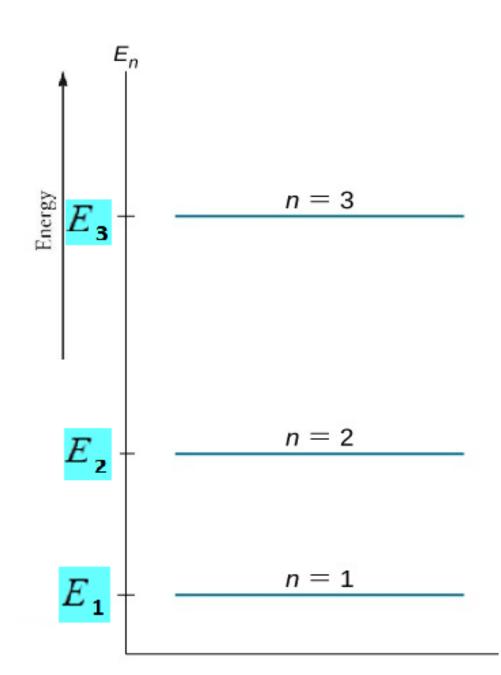


$$E_n = \frac{n^2 h^2}{8mL^2}$$

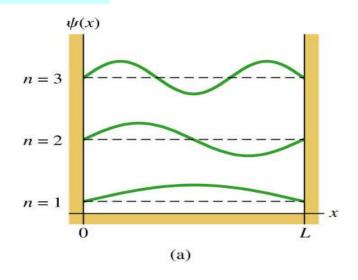
$$E_1 = \frac{h^2}{8mL^2}$$

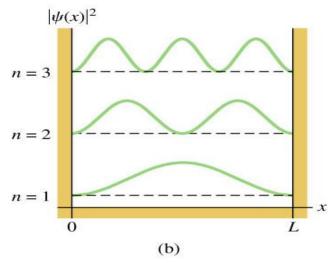
$$E_2 = \frac{4 h^2}{8mL^2}$$

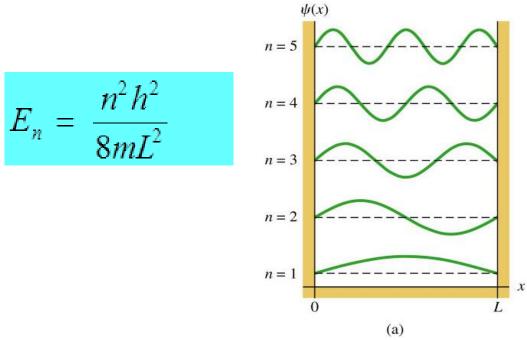
$$E_3 = \frac{9h^2}{8mI^2}$$

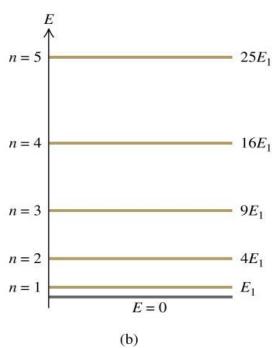


$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}n\right)$$

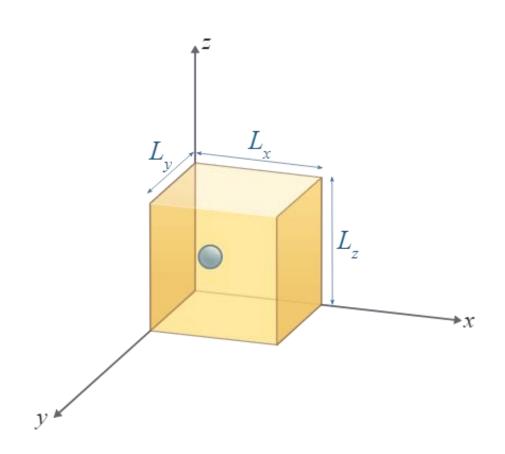








# The 3D infinite potential well



### The 3D infinite potential well

It's easy to show that:

$$\psi(x, y, z) = A\sin(k_x x)\sin(k_y y)\sin(k_z z)$$

where:

$$k_x = \pi n_x / L_x$$

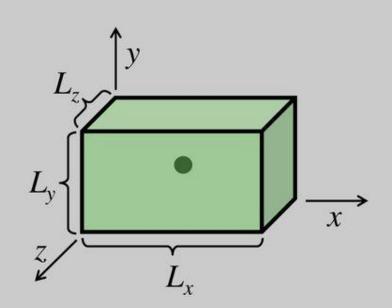
$$k_x = \pi n_x / L_x$$
  $k_y = \pi n_y / L_y$   $k_z = \pi n_z / L_z$ 

$$k_z = \pi n_z / L_z$$

and: 
$$E = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$

When the box is a cube:

$$E = \frac{\pi^2 \hbar^2}{2mL^2} \left( n_x^2 + n_y^2 + n_z^2 \right)$$



### Wave functions and energies for particle in a 3D box:

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n_x \pi x}{L}\right)$$

$$n_x = \{1, 2, 3, ...\}$$

$$m_y = \{1, 2, 3, ...\}$$

$$m_y = \{1, 2, 3, ...\}$$
eigenfunctions

$$\psi(y) = \sqrt{\frac{2}{L}} \sin\left(\frac{n_y \pi y}{L}\right)$$

$$\psi(z) = \sqrt{\frac{2}{L}} \sin(\frac{n_z \pi z}{L})$$
  $n_z = \{1, 2, 3, ...\}$ 

$$n_x = \{1, 2, 3, \ldots\}$$

$$n_y = \{1, 2, 3, \ldots\}$$

$$n_z = \{1, 2, 3, \dots\}$$

$$E_x + E_y + E_z = E = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$
 eigenvalues

$$E = \frac{\hbar^2 \pi^2}{2 m L^2} (L_x^2 + L_y^2 + L_z^2)$$
 = eigenvalues if  $L_x^2 = L_y^2 = L_z^2 = L$ 

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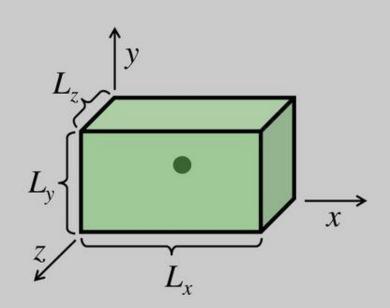
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### **Degeneracy**

- ❖ The energy level is said to be degenerate if it corresponds to two or more different measurable states of a quantum system.
- Conversely, two or more different states of a quantum mechanical system are said to be degenerate if they give the same value of energy upon measurement.



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degeneracy = 5

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non-degenerate (ground state)

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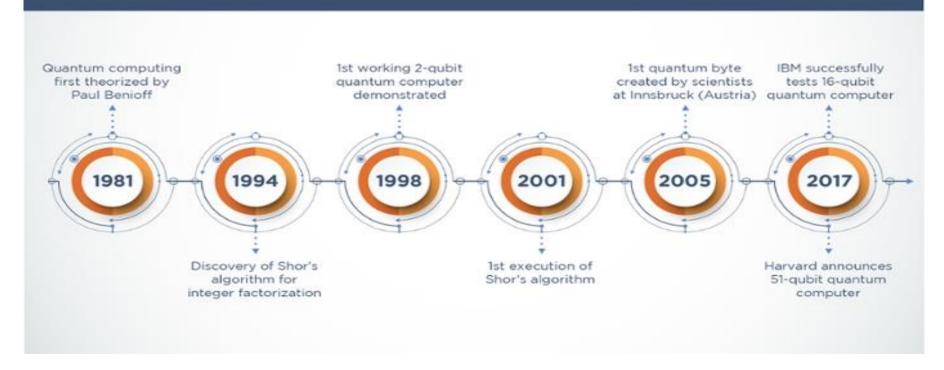
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### QUANTUM COMPUTING TIMELINE



#### **September 28, 2018**

# **Atom Computing and Bleximo Land Venture Funding of \$5 Million and \$1.5 Million Respectively**

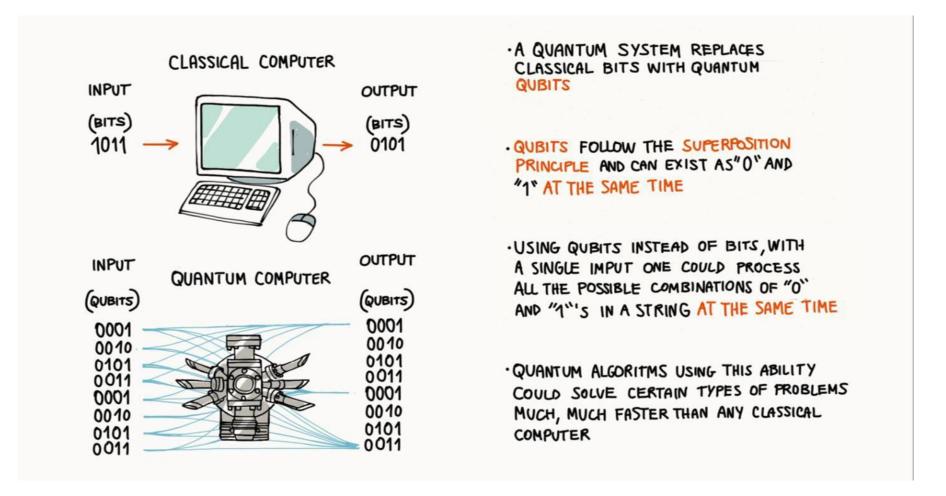
Two Berkeley, California based quantum startups with founders who are alumni of Rigetti Computing have raised seed funding rounds to develop distinctly different varieties of quantum machines. Atom Computing has raised \$5M in a seed round led by Venrock and Bleximo's seed round of \$1.5 million was led by Eniac Ventures.

## Quantum Computing

A classical computer encodes information as a string of binary digits, or bits.

Quantum computers supercharge processing power because they use quantum bits, (qubits)

This exist in a superposition of states, qubits can be both "1" and "0" at the same time.



#### **OUTPUT**

