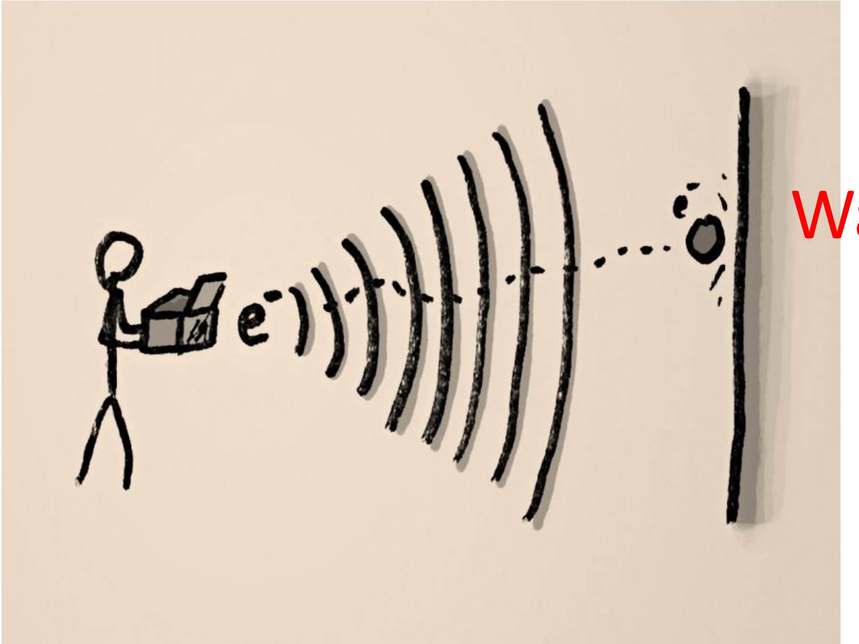
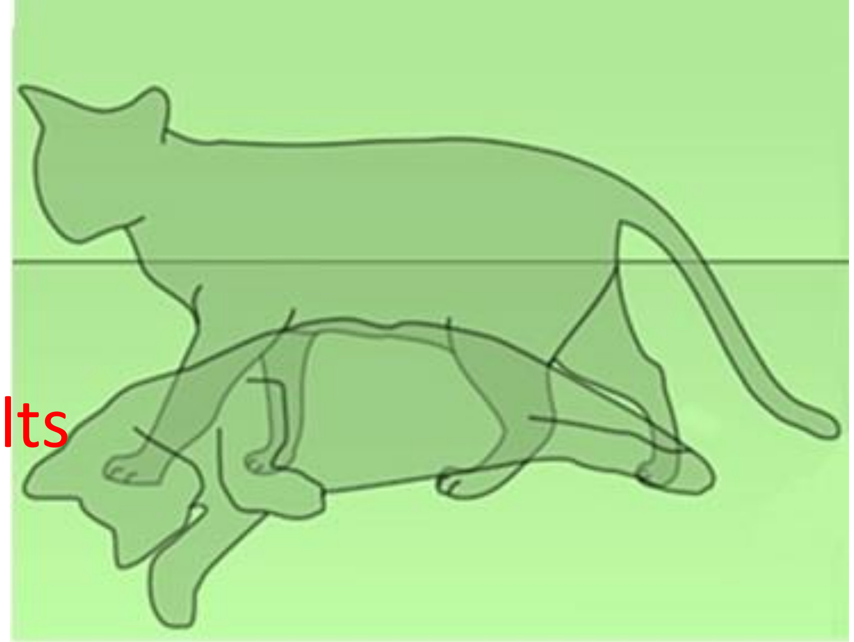


Wave-particle duality

1



2

Probabilistic results

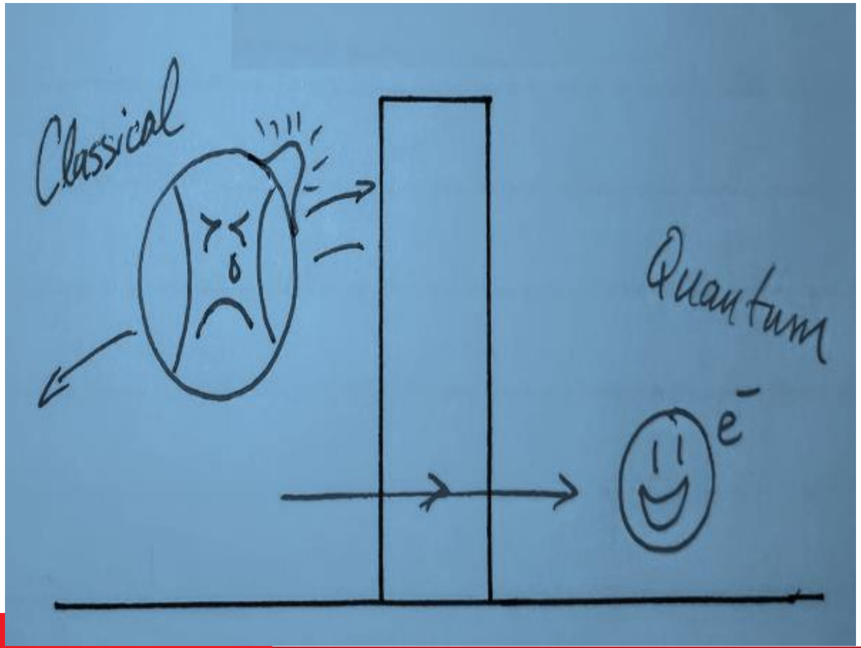
Module 3 Introductory Quantum Mechanics

Uncertainty principle

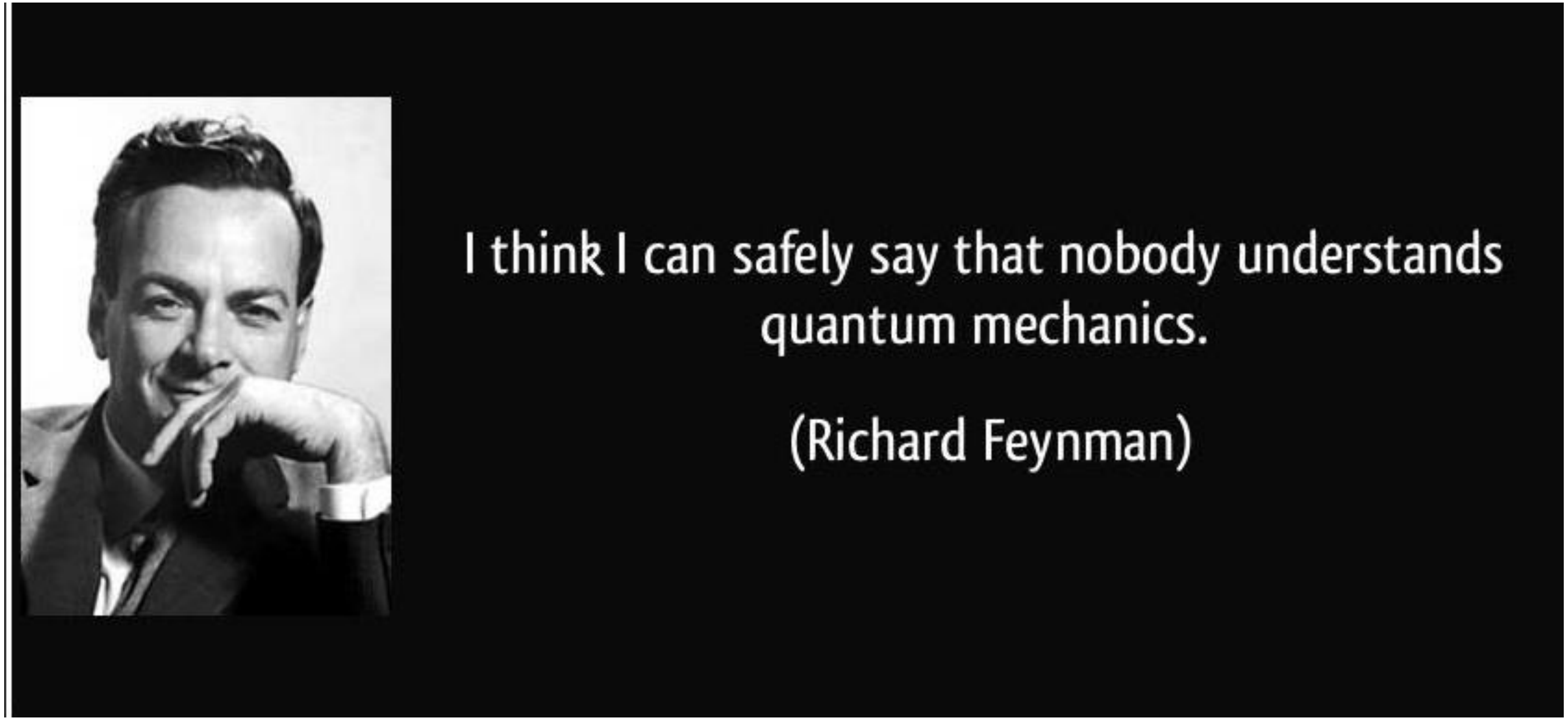
3

4

Tunnel effect



What is Quantum Mechanics?



1965; At the time of Nobel Prize Ceremony

The Role of Quantum Mechanics: Phase 1

Phase 1 (1900-1923) → Phase 2 (1923-1970s) → Phase 3 (1970s onwards)

What it did

Blackbody Radiation, Photoelectric Effect, Bohr's Theory of Hydrogen Atom, Einstein's theory of specific heats, Rutherford' model of atom, Radioactivity

Overcome some of the shortfalls of Classical Physics

Applications/ Areas benefited

Mechanical Engineering, Electrical Engineering, Civil Engineering, Automobile Engineering, Vacuum Tube-Electronics, Aviation, Chemistry, Materials Science etc.

The Role of Quantum Mechanics: Phase 2

Phase 1 (1900-1923) → Phase 2 (1923-1970s) → Phase 3 (1970s onwards)

What it did

de' Broglie's Hypothesis, Uncertainty Principle, Wave Mechanics, Nuclear and Particle Physics, Matter-Antimatter Theory, Quantum Electrodynamics, Unified Field Theory

Laid the foundations of modern science and technology as well as provided new inputs to areas such as philosophy

Applications/ Areas benefited

Materials science, Modern Chemistry, Biotechnology, Evolution of life, Medicine, Electronics, Nanotechnology, Computer Science, Astrophysics, Cosmology, Modern Philosophy

The Role of Quantum Mechanics: Phase 3

Phase 1 (1900-1923) → Phase 2 (1923-1970s) → Phase 3 (1970s onwards)

Grand unified theories, Standard model, Quantum gravity, String theories, Theory of Everything

What it did

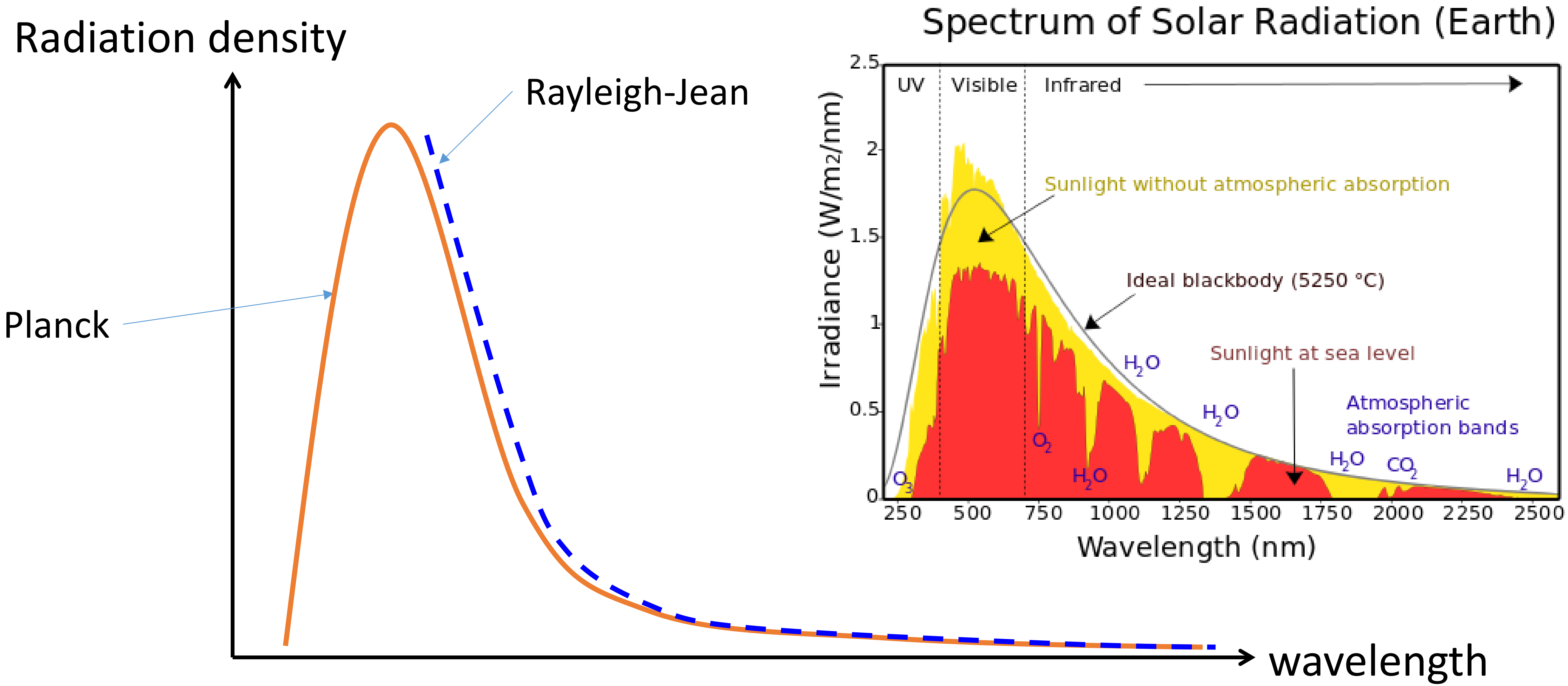
Frontiers areas of Physics research

Applications yet to occur

Contents

0. Shortfalls of Classical Physics and the Foundations of QM
1. de’ Broglie’s hypothesis
2. Wave-particle duality and the Wave packet
3. The Uncertainty principle
4. Wave function and the probabilistic interpretation of QM
5. Schrodinger’s equation - time dependent and time independent forms
6. The *particle in a box* problem – “Hello, World!" of QM
7. Basics of Quantum Computing (in separate slides)

Birth of Quantum Mechanics - Blackbody radiation catastrophe



Shortfalls of Classical Physics

Electron spin

Zeeman effect

Franck-Hertz Experiment

Planck's theory of blackbody radiation

splitting of spectral lines in magnetic field

Stark effect

Blackbody radiation catastrophe

stability of atoms

Mass-Energy conversion

Origin of magnetism

Bohr's theory of hydrogen atom

"old" quantum theory

superconductivity

radioactivity

wide range of magnetization

Constituents of matter

Nernst-Einstein theory of specific heats of solids

Stern-Gerlach Experiment

What produces X-rays

Specific heats of solids

Rutherford's model of atom

photoelectric effect

Wide range of conductivity of solids

Einstein's theory of photoelectric effect

Origin of atomic and molecular spectra

Origin of quantization of energy

Louis de’Broglie’s Hypothesis

- Energy
  - Radiation
    x-rays, γ-rays
    - Wave properties
      - Interference
        Diffraction
    - Particle properties
      - Photoelectric effect
        Compton effect
  - Matter
    Atoms, marbles
    - Particle properties
      (Newtonian mechanics)
      - Rectilinear motion
        Circular motion
        Projectile motion
        Oscillations
        Scattering
        Gravitation
    - Wave properties
      (Wave mechanics?)
      “Missing link”
      - New experiments!

de'Broglie Equation

- For photons, we have

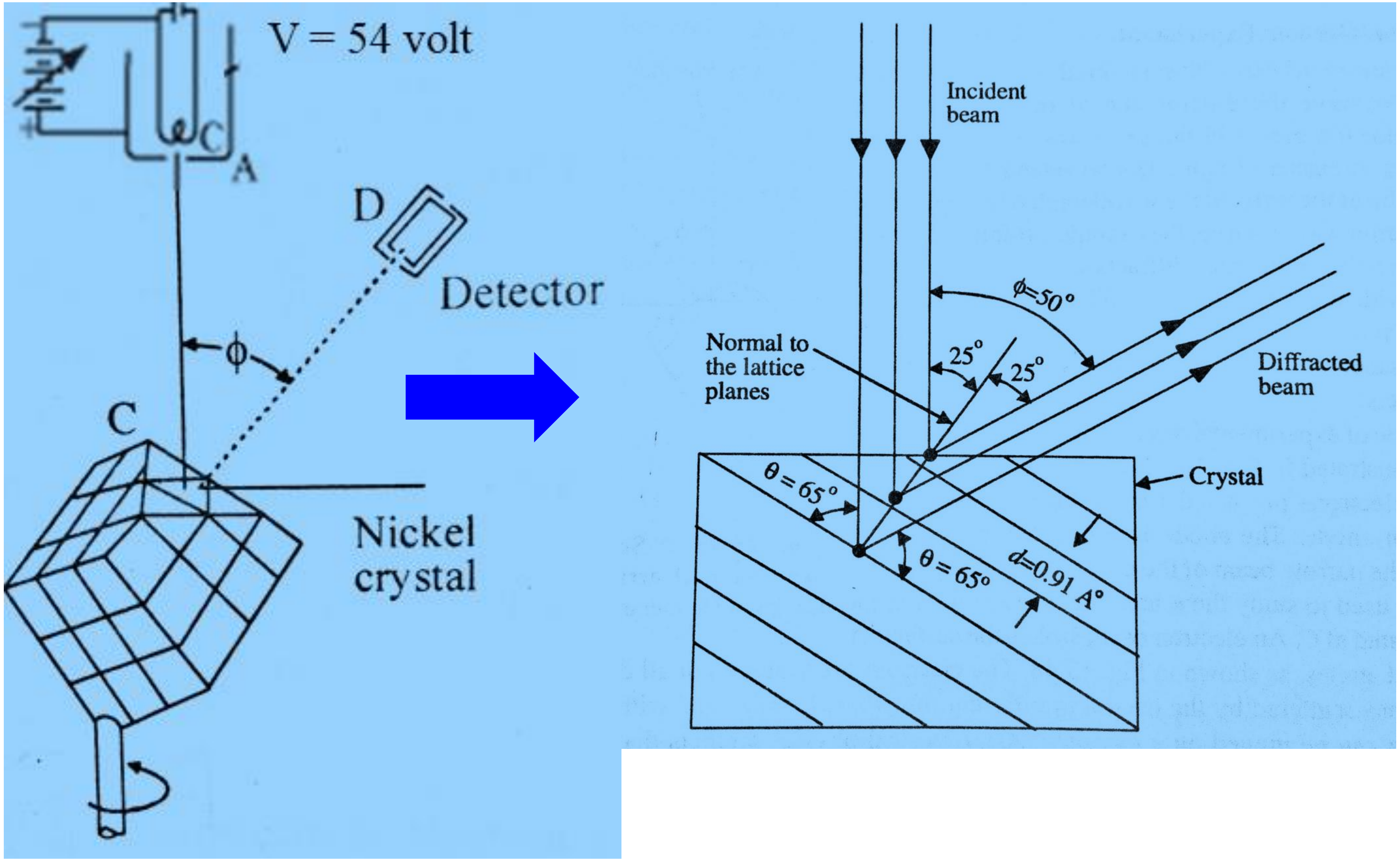
  $$E = h\nu = \frac{hc}{\lambda} \qquad \text{-------- (1)}$$

  and $E = mc^2$ -------- (2)

- Combining two equations gives $\lambda = \frac{h}{mc} = \frac{h}{p}$
- De' Broglie, proposed a similar equation for all material objects i.e.
- $\lambda = \frac{h}{p} = \frac{h}{mv}; v < c$ always, which follows from relativity theory

"All material objects possess wave nature and the associated wavelength is inversely proportional to its momentum"

Davison-Germer Experiment - Schematic



As per Bragg's law,

$2d \sin\theta = n\lambda$

$d = 0.91$ Å,

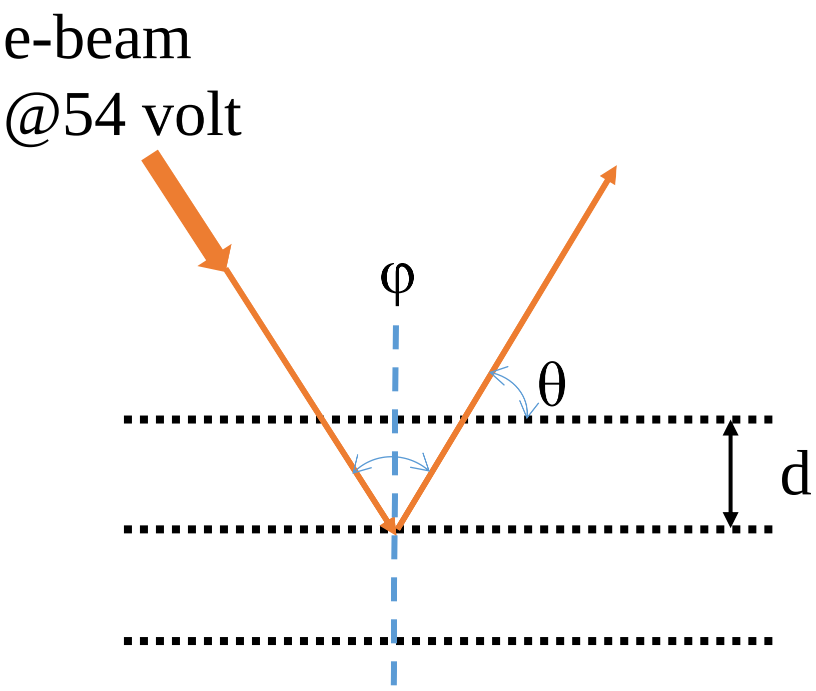
$n = 1$,

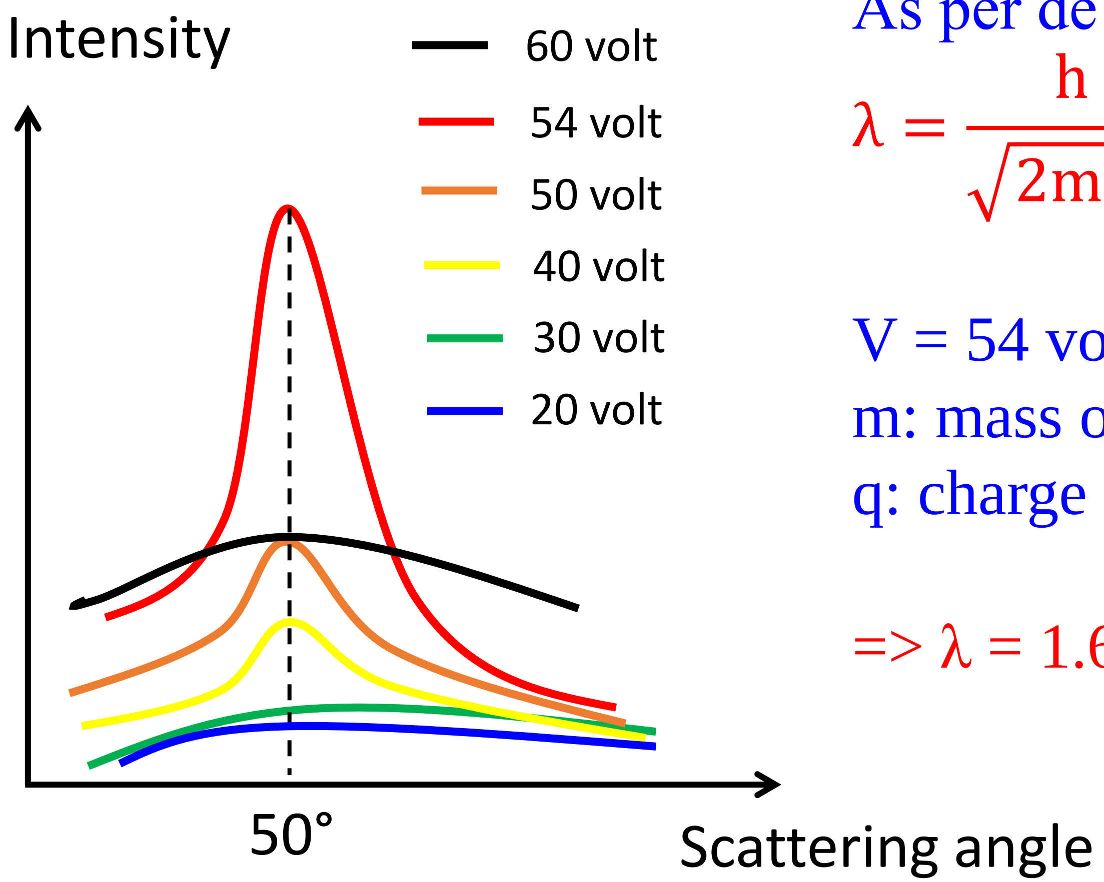
$\varphi = 50°$

$\theta = 90 - \varphi/2 = 65°$

=> $\lambda = 1.65$ Å

Davison-Germer Experiment - Observations





As per de'Broglie equation,

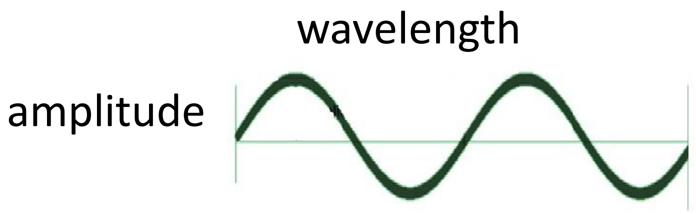
$$\lambda = \frac{h}{\sqrt{2mqV}}$$

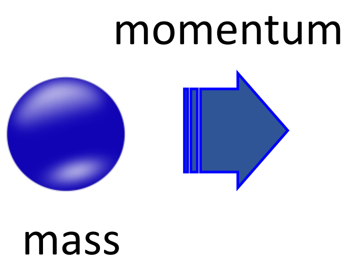
V = 54 volt,
m: mass of electron
q: charge on electron

=> λ = 1.67 Å

Importance of de'Broglie's Work

- It connects both the aspects which carry energy – waves and particle
- But waves and particles are completely complementary to each other





continuous

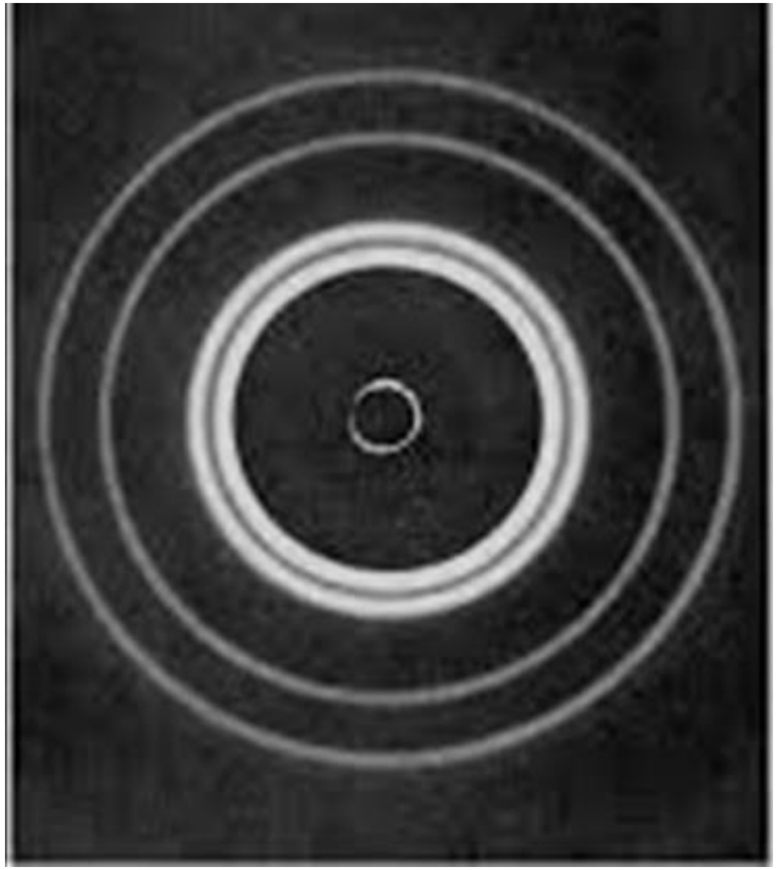
discrete

present at all points at a given time

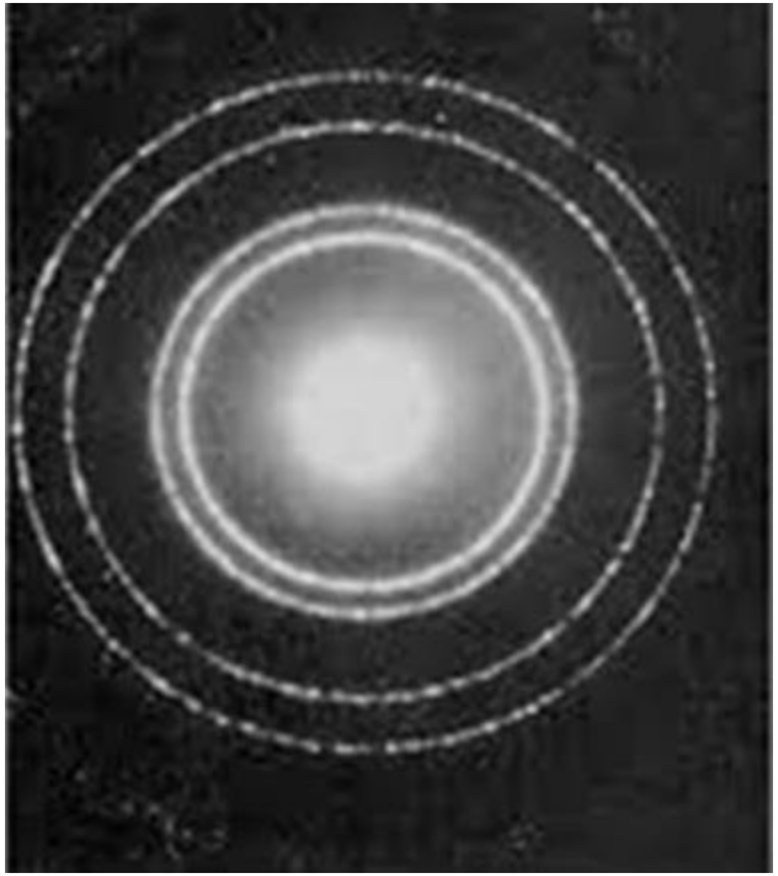
present at one point at a given time

De'Broglie hypothesis hints towards "*wave-particle duality*"

Radiation and Matter - Seemingly Parallel Effects



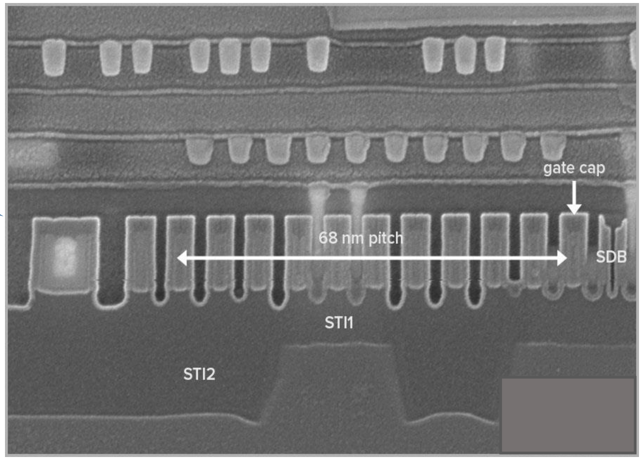
X-rays @ 1 nm



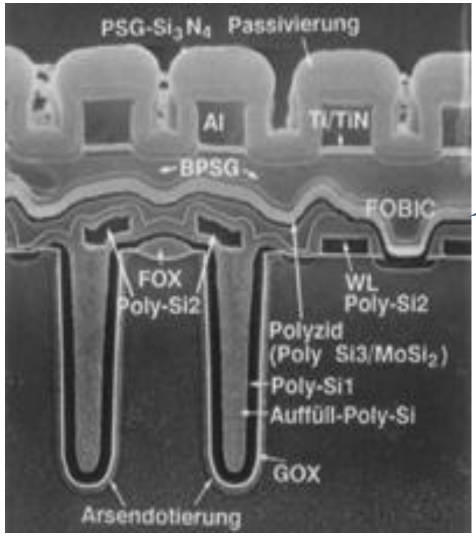
E-beam @ 50 keV

Applications in Use

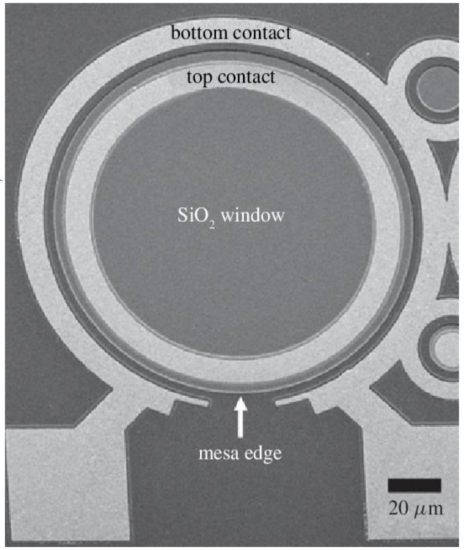
RAM



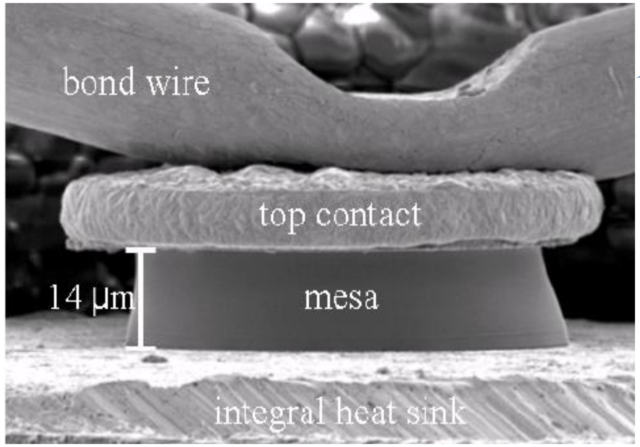
FinFET (microprocessor)



IR Sensor



Laser diode

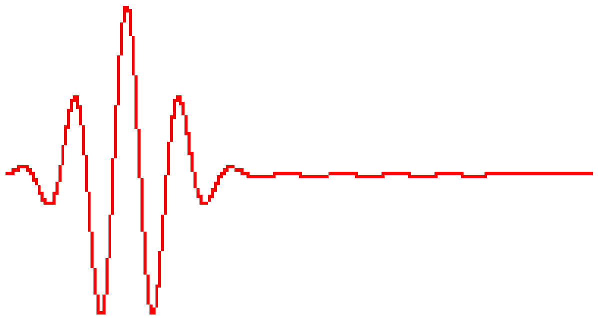


Electron Microscope images;
Principle:
de’Broglie hypothesis

Double Slit Experiment with Electrons

Particle as a Wave Packet and Wave-Particle Duality

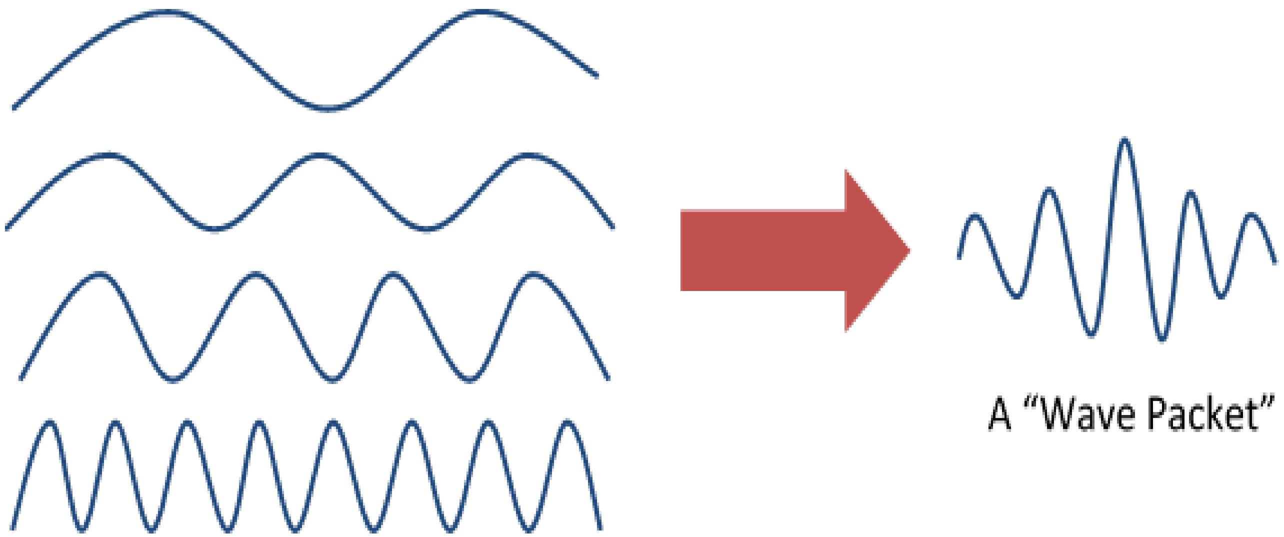
- In QM, each material object is represented by a wave packet
- A wave packet can be reduced to a perfect particle or a perfect wave
- Thus, the wave packet is supposed to carry "wave-particle duality"



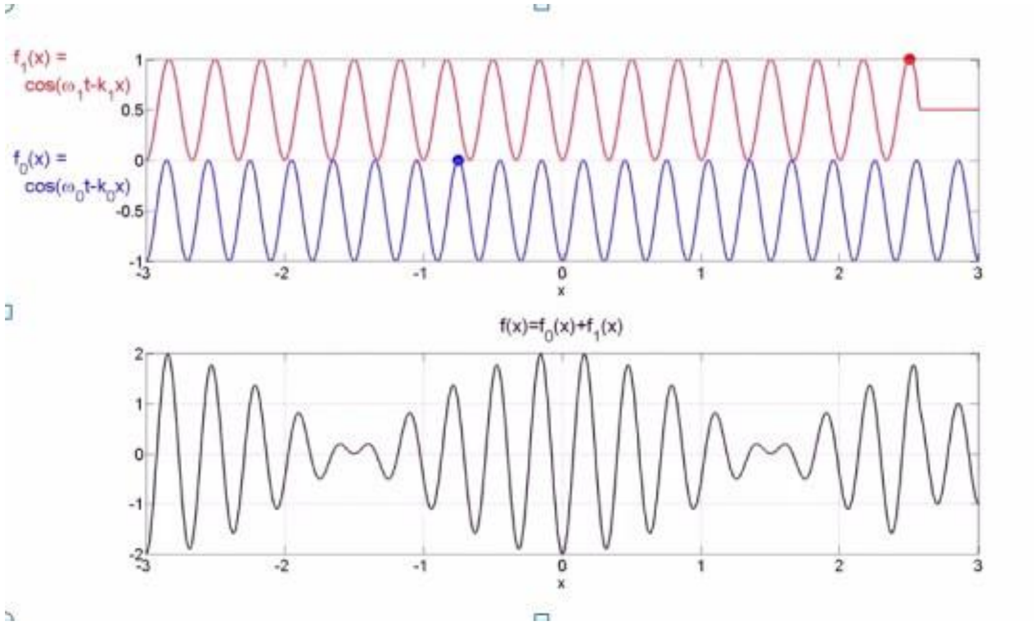
- Before any sort of detection, wave nature of particle is preserved (duality)
- Detection i.e. a measurement breaks this duality
- Detection is a kind of "interaction"
- On detection, only one nature is manifested

Wave Velocity, Group Velocity and the Wave Packet

- Wave velocity or phase velocity is given by: $\mathrm{v_{ph}} = \nu\lambda = \frac{\omega}{\mathrm{k}}$
- Group velocity is velocity of the wave packet given by: $\mathrm{v_g} = \frac{\mathrm{d}\omega}{\mathrm{dk}}$
- Particle moves with a velocity equal to group velocity
- $\mathrm{v_{particle}} \neq \mathrm{v_{ph}}$ rather $\mathrm{v_{particle}} = \mathrm{v_g}$

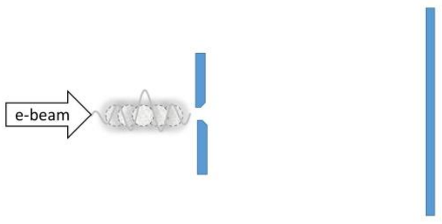


A "Wave Packet"

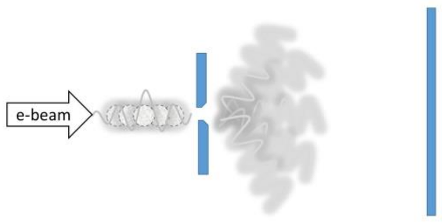


Measurement and the “Collapse” of Wave-Particle Duality

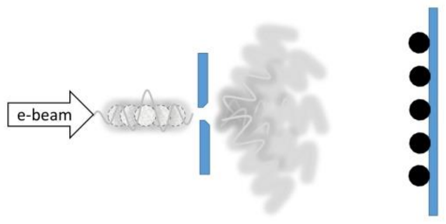
Frame 1



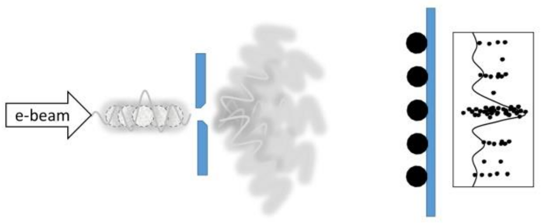
Frame 2



Frame 3



Frame 4



Frame 1: beam of electrons incident on a single slit

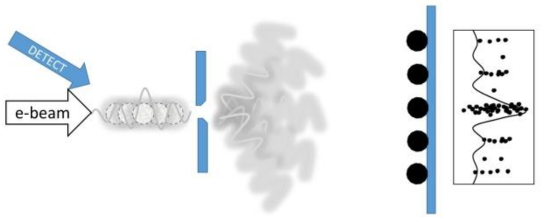
Frame 2: If electrons are “wave”, they will diffract like waves

Frame 3: When detected on screen, electrons appear as “particles”

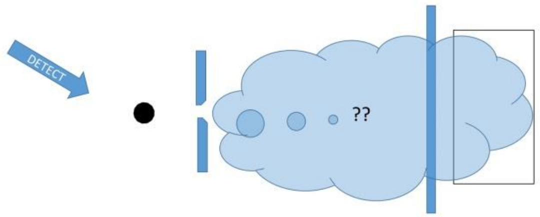
Frame 4: However, since electrons behaved as waves before detection, they arrive at specific locations on the screen, which can be described by single slit diffraction pattern due to some kind of waves

Measurement and the “Collapse” of Wave-Particle Duality

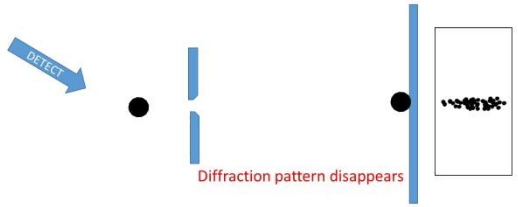
Frame 5



Frame 6



Frame 7



Frame 5: Since electrons showed wave property i.e. diffraction, we conclude they possess wave nature so we try to verify their wave nature by placing a detector before the slit

Frame 6: When we try to detect electrons, they pop up as particles. Then it is not certain what would be their nature after passing through the slit

Frame 7: But now, the diffracting pattern disappears and we get a pattern as if electrons have particle nature!

This effect is famously described as “collapse of wave function” in QM. Any kind of measurement breaks the wave-particle duality

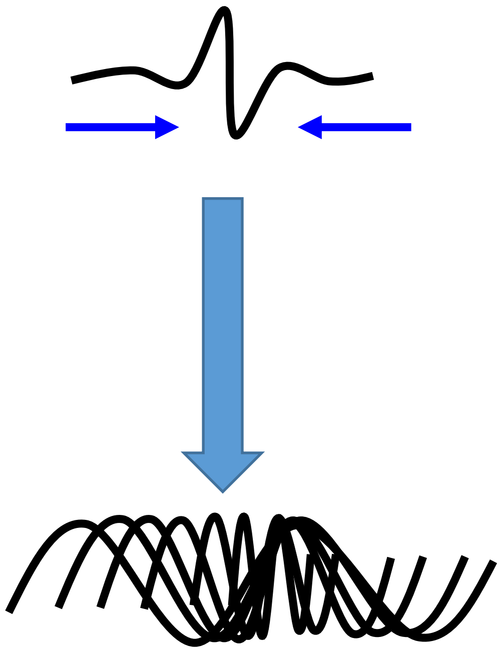
Matter waves

- Matter waves are waves associated with material objects
- However, a matter wave is not a separate physical entity
- It is an abstract quantity which carries the wave nature of matter
- A resultant of all such matter waves is noting but the **wave packet**

- Consequence of calling particles as wave packet:
- Wave properties of matter can be explained
- “uncertainty” is introduced in measurements

Wave Packet and the Uncertainty Principle

- Start with a wave packet that is highly localized as shown:
- This wave packet is close to the concept of a "perfect particle"
- Uncertainty in position is almost zero for this i.e. $\Delta x \rightarrow 0$

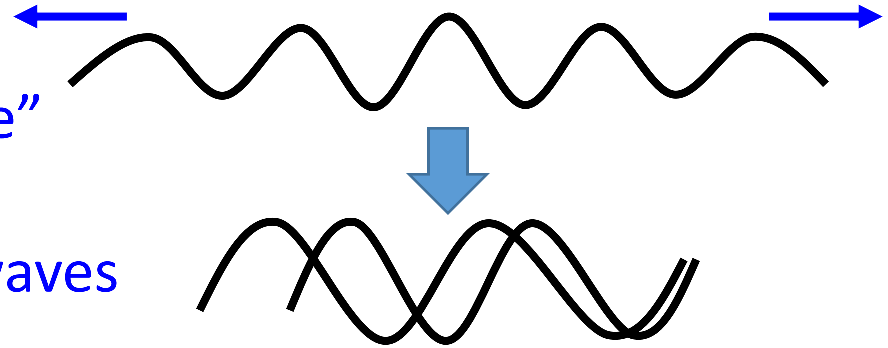


But …

- Such a wave packet is formed by combining a large number of waves
- Many waves means many wavelengths and hence many momentum
- Uncertainty in momentum is very large for this i.e. $\Delta p \rightarrow \infty$

Wave Packet and the Uncertainty Principle

- Next, Start with a wave packet that is spread over a long distance as shown:



- This wave packet is close to the concept of a "perfect wave"
- Such a wave packet is formed by a very small number of waves
- Less number of waves means lesser variation in wavelength and hence in momentum
- Uncertainty in momentum is almost zero for this i.e. $\Delta p \rightarrow 0$

But …

- There are a large number of possibilities for the position of this wave packet
- It becomes difficult to know its exact location due to the long extent
- Uncertainty in position is very large for this i.e. $\Delta x \rightarrow \infty$

The Uncertainty Principle

It states that
"It is impossible to determine certain pairs of physical quantities (such as position and momentum) with simultaneous accuracy and the product of their uncertainties is always greater than or at least equal to $h/4\pi$"

In mathematical form (3-dimensions), $\Delta x \Delta p \geq \frac{h}{4\pi}$

- Uncertainty principle puts the fundamental limit of measurement
- Certain pairs of physical quantities are "non-commutative"
- Uncertainty principle applies to all such pairs like x and p, E & t, L and θ etc.

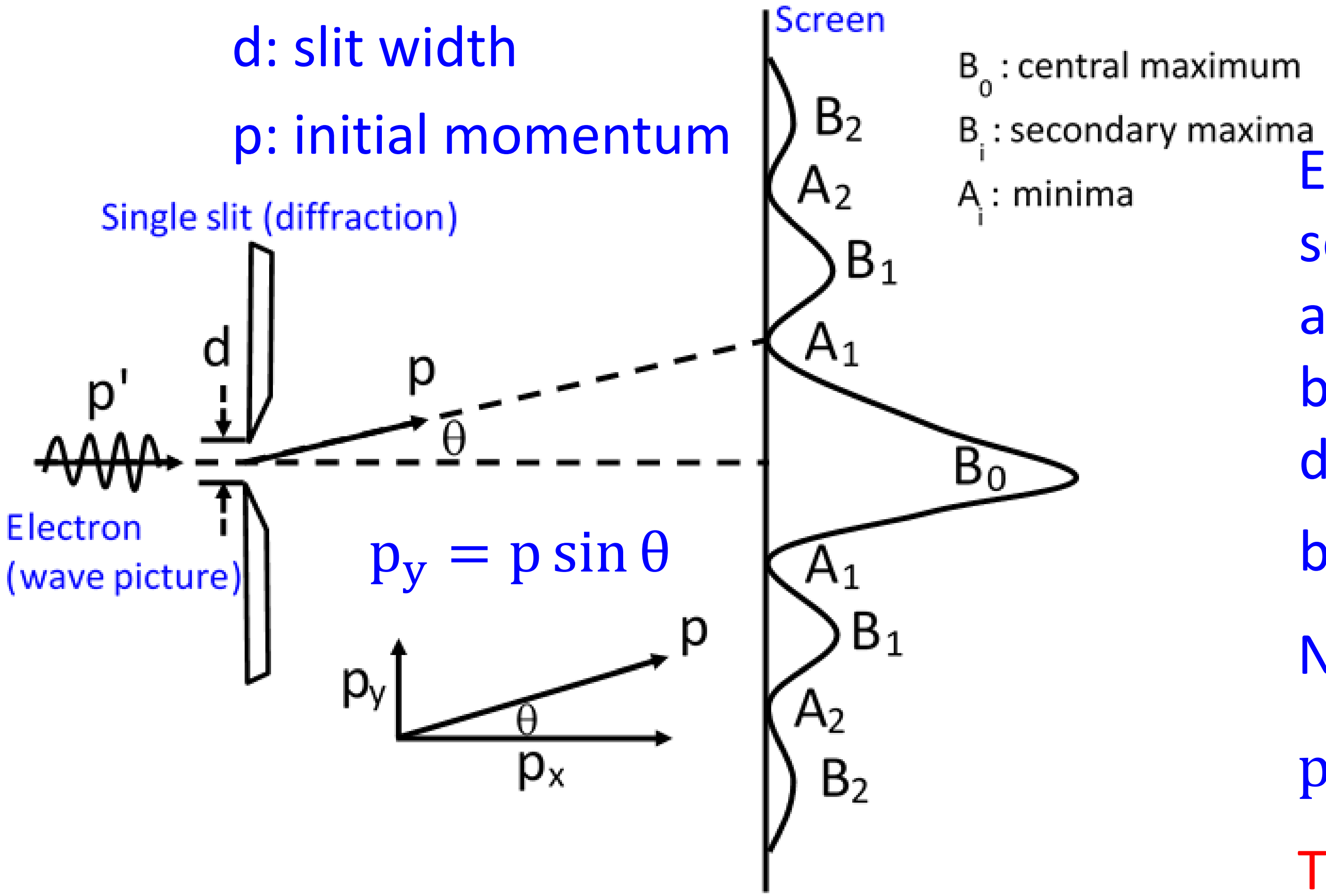
Uncertainty Principle – Proof-of-concept Derivation

1. Single slit diffraction of electrons

(via wave nature of electron)

d: slit width

p: initial momentum



$p_y = p \sin\theta$

An electron can pass from anywhere through the slit of width "d" so we take uncertainty in position $\Delta y \approx d$

Electrons form a diffraction pattern on the screen. Let any arbitrary electron reaching at some location say A_1, which happens to be the first minimum. According to diffraction theory, first minimum is given by $\sin\theta = \frac{\lambda}{d}$

Now, let $\Delta p_y \approx p_y \approx p \sin\theta$

$p \sin\theta \approx \frac{h}{\lambda}\frac{\lambda}{d} \therefore \Delta p_y \approx \frac{h}{d}$

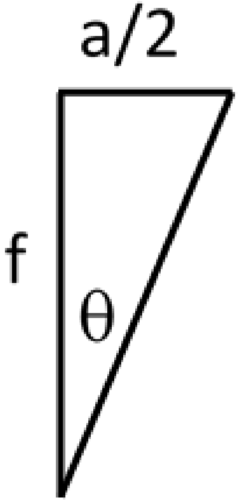
Thus, $\Delta y \Delta p_y \approx h$ as required

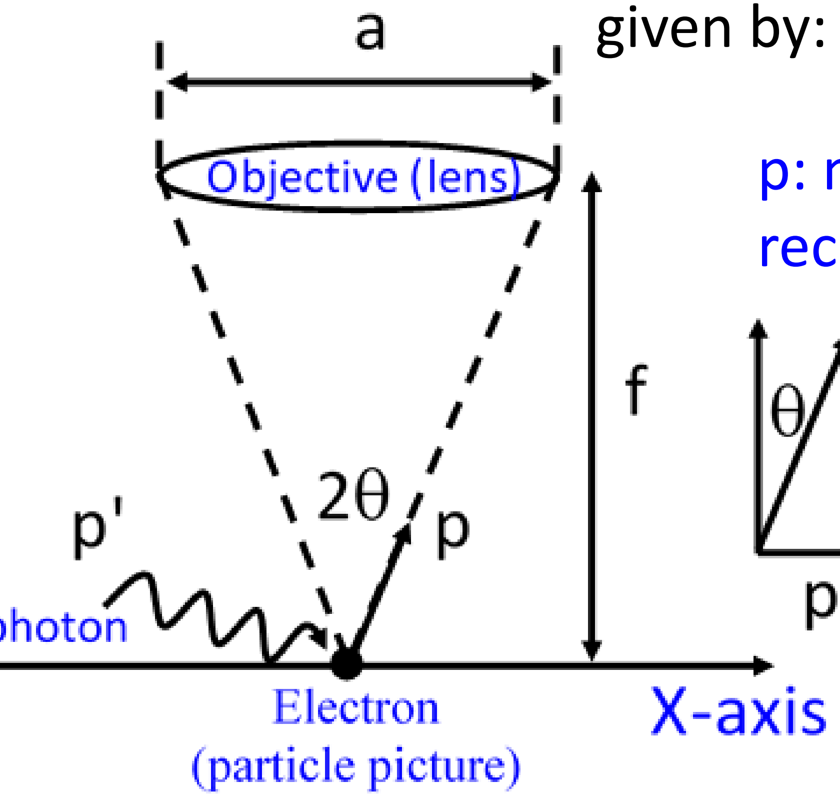
Uncertainty Principle – Proof-of-concept Derivation

2. Seeing an electron with γ-ray microscope
(via particle nature of electron)

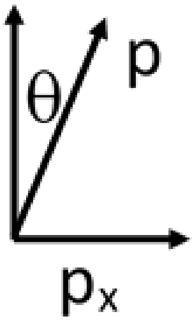
a: microscope aperture
f: focal length of objective

"field of view" of microscope is given by: $\frac{\lambda f}{a}$





p: momentum of recoiled photon



Let uncertainty in position

$$\Delta x \approx \frac{\lambda f}{a}$$

Let photon imparts all of it's X-component of momentum to the electron ($p_x = p\sin\theta$) and let $\Delta p_x \approx p_x \approx p\sin\theta$

$$p\sin\theta \approx \frac{h}{\lambda} \times \frac{\frac{a}{2}}{\sqrt{\left(\frac{a}{2}\right)^2 + f^2}}$$

$$\approx \frac{h}{\lambda}\frac{a}{2f} \approx \frac{h}{\lambda}\frac{\lambda}{2\Delta x}$$

For HR microscopes, $a \ll f$

Thus, $\Delta x \Delta p_x \approx \frac{h}{2}$ as required

Wave function and the probabilistic interpretation of QM

- It is the mathematical form of wave packet
- The wave function carries the wave-particle duality of material objects
- Wave function carries all the “information” about the particle

Characteristics of a wave function $\psi(x, t)$ of QM:

- It is a complex function (of real variables)
- It is defined over space and time
- It is continuous (hence differentiable), finite, well-behaved, normalizable
- **Square of wave function i.e. $\psi^*\psi$ or $|\psi|^2$ gives the probability factor**

Schrodinger Equation

- Central equation of quantum mechanics
- It is a scalar equation
- It is an energy equation
- if follows linear superposition

  - One dimensional time-dependent wave equation is given by

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

  - One possible solution of above equation is of the form: $\psi(x, t) = Ae^{i(kx-\omega t)}$
  - Three dimensional equation is $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = \hat{H}\psi$

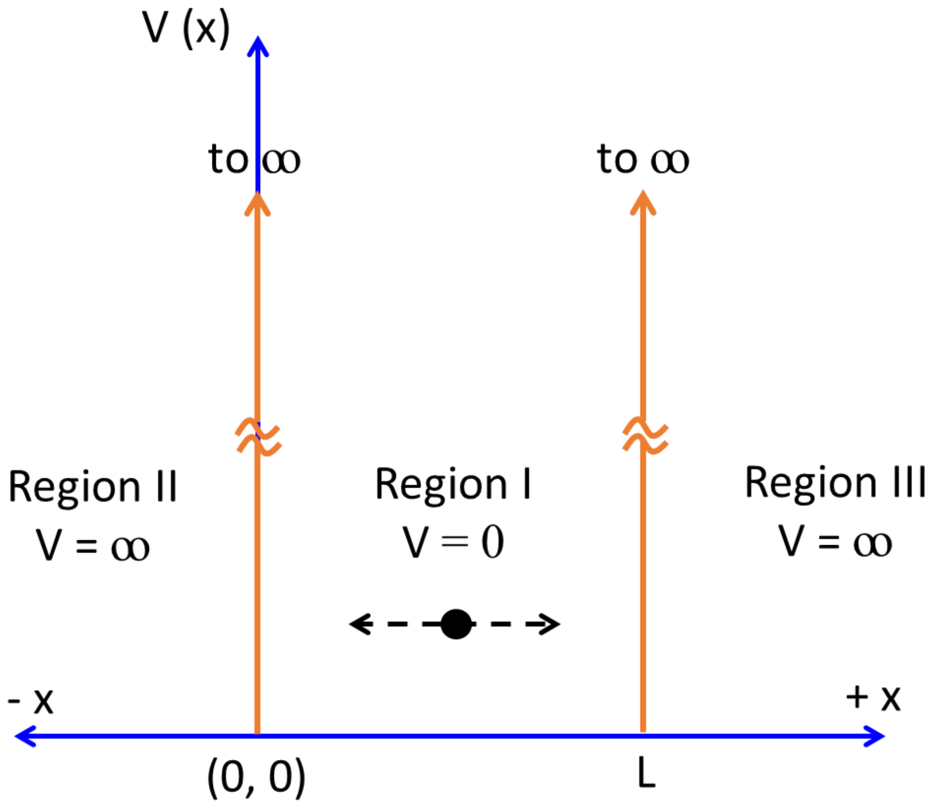
$\hat{H} \equiv \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)$ is called the “Hamiltonian operator” due to its analogy in classical mechanics

Schrodinger Equation v/s Newton's Equation

Schrodinger equation	Newton's equation (2nd law of motion)
It is regarded as the central equation of (non-relativistic) quantum mechanics	It is regarded as the central equation of classical mechanics (i.e. non-quantum)
General (time-dependent) form is $i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$	General form is $\vec{F} = \frac{d\vec{p}}{dt}$
It describes both, wave and particle properties of matter	It describes only particle properties of matter
It obeys principle of linear superposition	It does not fit into the context of linear superposition
It is an energy equation	It is a force equation
It is a scalar equation	It is a vector equation
It applies to both, microscopic as well as macroscopic scales	It applies only at macroscopic scales
Newton's 2nd law of motion can be derived from Schrodinger's equation	Schrodinger's equation cannot evolve from Newton's equations of motion

Schrodinger Equation – Case Study: "Particle in a box"

- Energy of particle trapped in one-dimensional infinite potential well
- "Hello, World" problem of QM
- Used to learn basic context of applying SE to quantum systems



The potential function is given by:

$$V(x) = 0; \quad \text{for } 0 < x < L$$
$$= \infty; \quad \text{for } x \le 0, \text{and } x \ge L$$

Schrodinger equation:

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

Wave function for infinite potential well

The Schrödinger's equation for region I can be written as

$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = E\varphi(x)$; As V = 0.

$\therefore \frac{d^2\varphi}{dx^2} = -\frac{2mE}{\hbar^2}\varphi = -k^2\varphi$; Where, $k = \frac{\sqrt{2mE}}{\hbar} = \frac{2\pi}{\lambda}$

This is a 2nd order DE $\frac{d^2\varphi}{dx^2} + k^2\varphi = 0$, whose solution is of the form:

$\varphi(x) = A\sin kx + B\cos kx;$

Where, A and B are constant to be evaluated.

For region II and III, $\varphi(x) = 0$ identically for all values of x as the particle cannot exist in region II.

Quantization of energy and momentum

The complete wavefunction of 1-D infinite potential well is given by

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

Energy $E = \frac{n^2h^2}{8mL^2}$; n = 1, 2, 3, …

Momentum $\vec{p} = \pm\frac{nh}{2L}\hat{\imath}$

Thanks