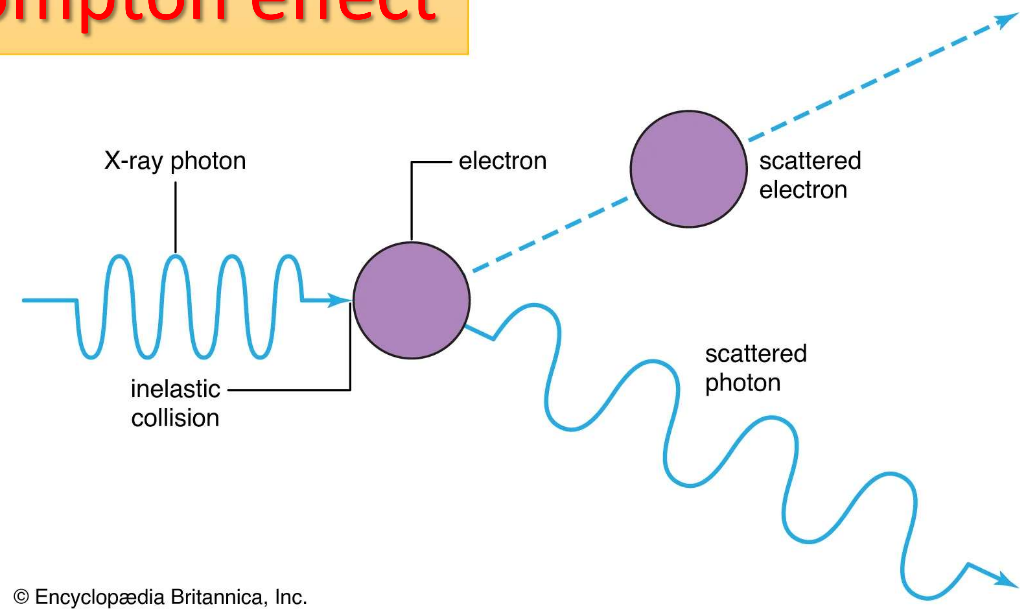
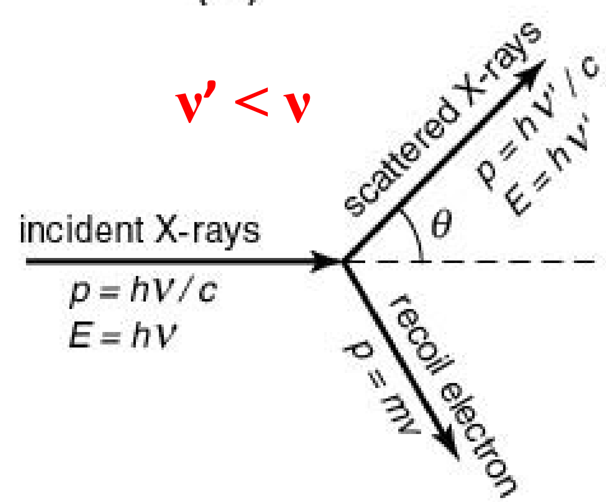
Compton effect

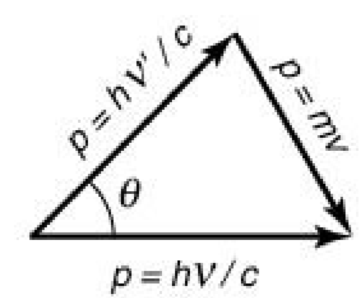


(A)

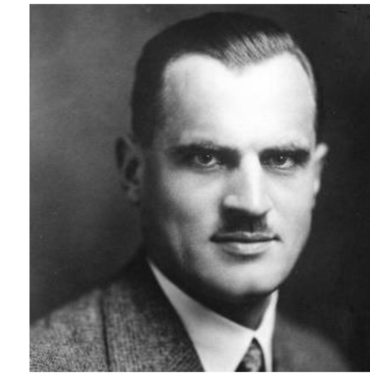
$\nu' < \nu$



(B)



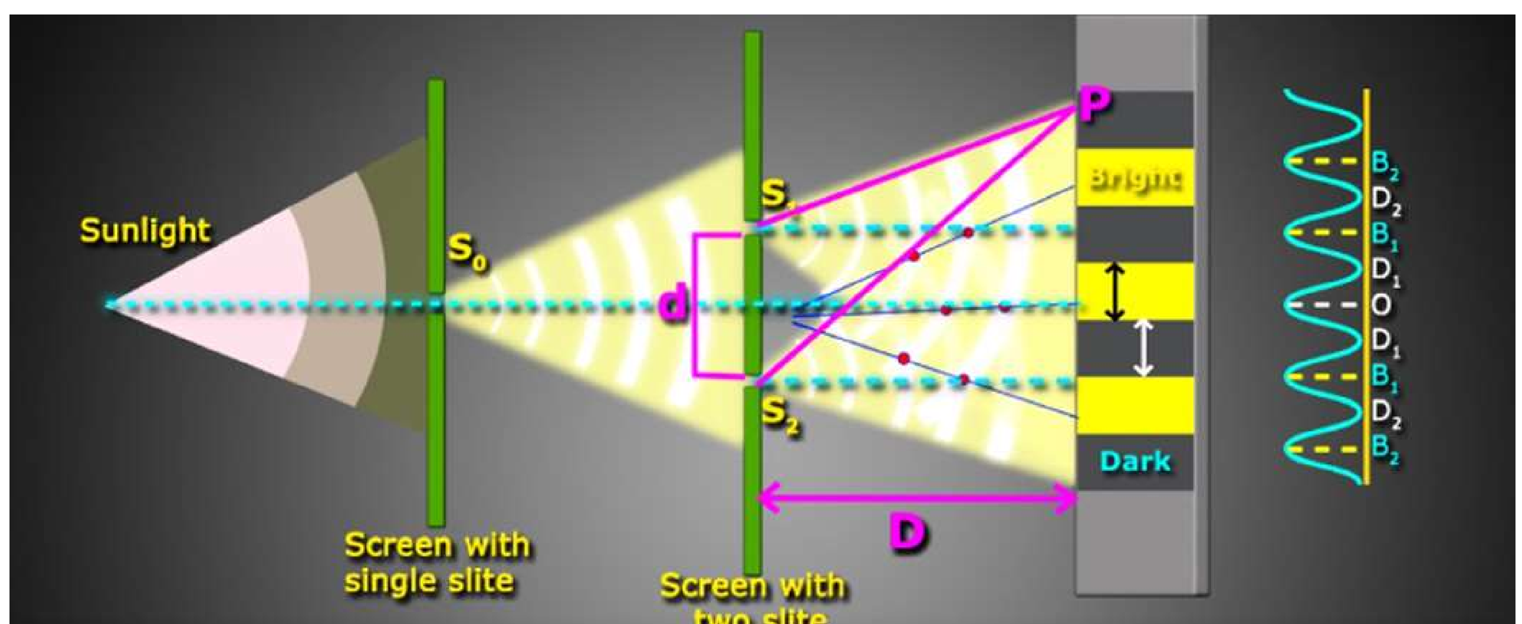
$$\Delta\lambda = \lambda' - \lambda = \frac{h}{mc}(1 - \cos\theta)$$



Arthur Holly Compton

This phenomena of change in the frequency of scattered X-ray is called ***Compton effect****.*

Young's double slit experriment



Thomas Young

de Broglie's hypothesis: Dual character of matter

Einstein pointed out: Light has both **particle** and **wave nature**
de Broglie expanded: All form of matters show dual character

Louis de Broglie

Special theory of relativity: $E = mc^2$

Planck's equation: $E = h\nu = \dfrac{hc}{\lambda}$

Therefore, $mc^2 = \dfrac{hc}{\lambda}$

$$\lambda = \frac{h}{mc}$$

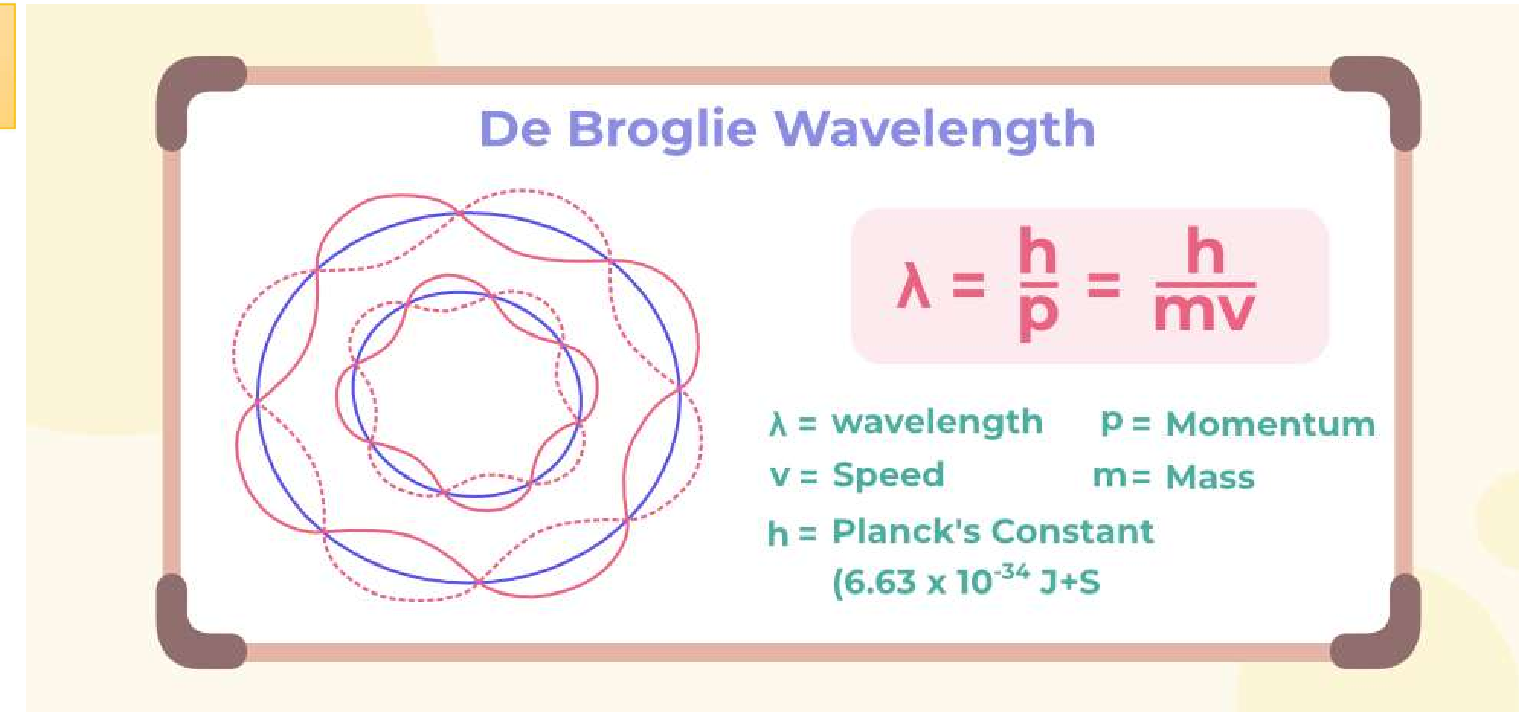
For, all matter other than light 'c' is replaced by 'v'

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

If an electron with charge e is accelerated with a potential V, then its kinetic energy,

$KE = \frac{1}{2}mv^2 = eV$

$\Rightarrow v = \sqrt{\dfrac{2eV}{m}}$



$\lambda = \dfrac{h}{\sqrt{\dfrac{2eV}{m}}}$; e = 1.6 x 10^{-19} C, m = 9.11 x 10^{-31} Kg

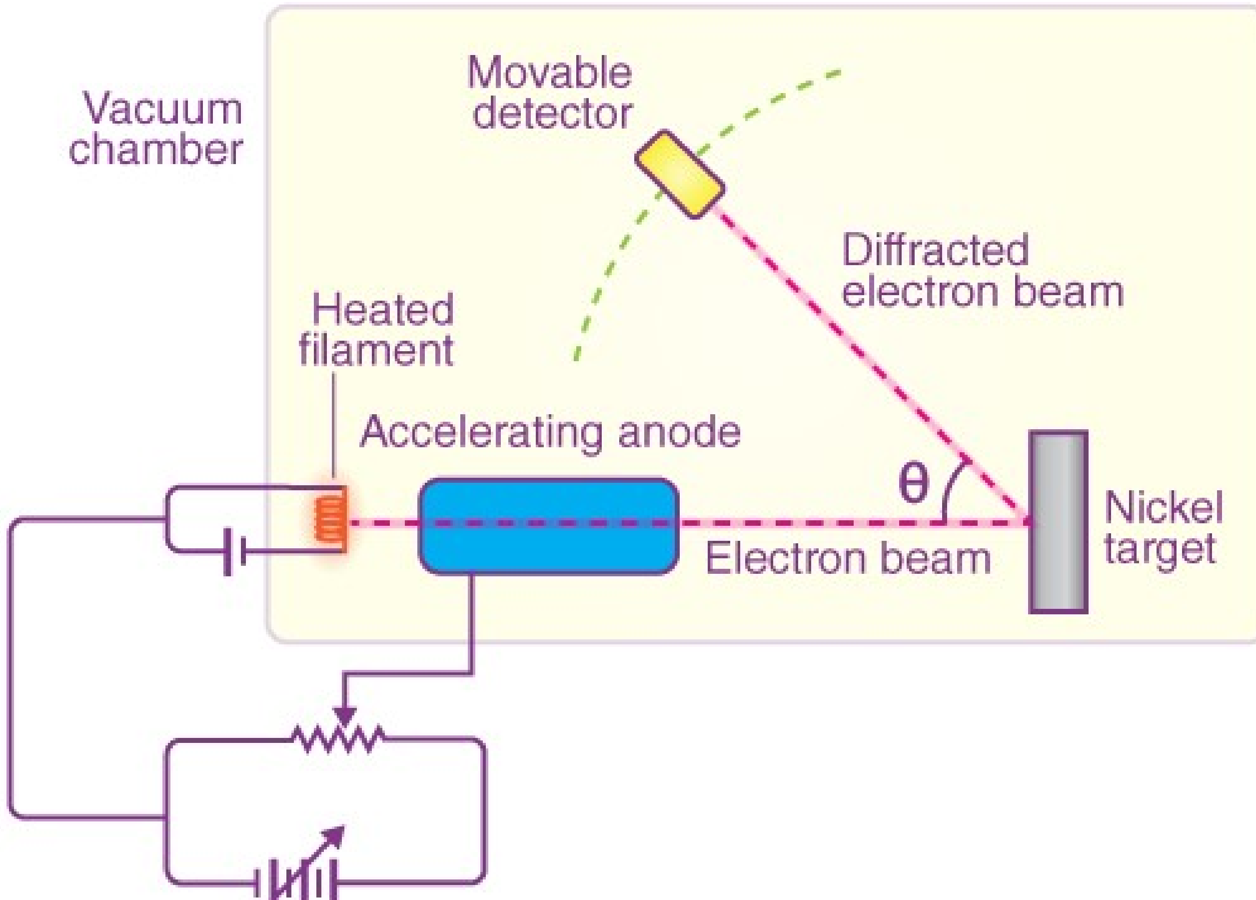
$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2V \times 1.6 \times 10^{-19} \times 9.11 \times 10^{-31}}}$$

$$\Rightarrow \lambda = \frac{12.27 \times 10^{-10}}{\sqrt{V}} \text{ meter}$$

$$\text{(or) } \lambda = \frac{12.27}{\sqrt{V}} \text{ Å}$$

When V = 10 -10,000 Volt, λ = 3.877 to 0.1226 Å

Davisson–Germer experiment

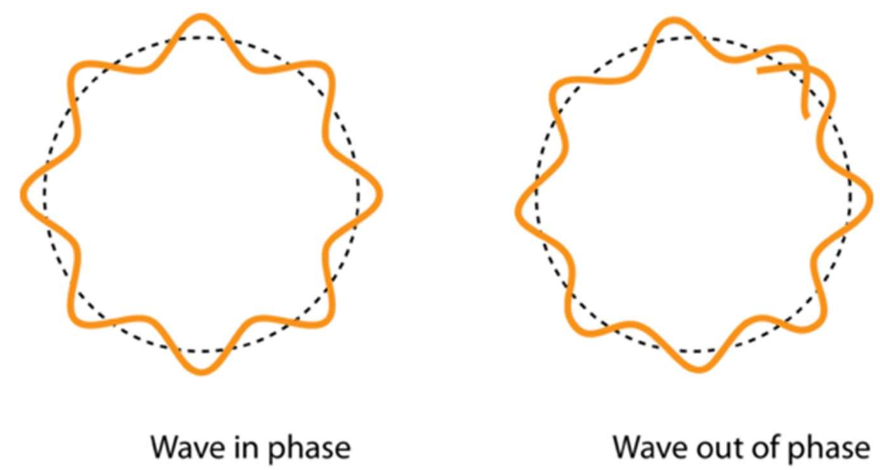


Clinton Davisson (left) and Lester Germer (right)

Bohr said, "*The electron is bound in a circular orbit around the nucleus such that the angular momentum is quantized in integral units of Planck's constant*"

$$\boldsymbol{mvr} = \frac{\boldsymbol{nh}}{\boldsymbol{2\pi}}; \text{m} = \text{mass of electron, v} = \text{velocity of electron, r} = \text{radius of the orbit}$$

Electron behaves as a **stationary wave** which extends round the nucleus and always **in phase**.



therefore, $2\pi r = n\lambda$

$$\Rightarrow \lambda = \frac{2\pi r}{n}$$

Now, according to de Broglie $\boldsymbol{\lambda} = \dfrac{\boldsymbol{h}}{\boldsymbol{mv}}$

Combining, $mvr = \dfrac{nh}{2\pi}$

Significance of de Broglie's concept

- The wave character of a **large object** in motion, **has no practical significance**, since their wavelength is too small to be observed and hence cannon be measured.
- The wave character of a **small object** in motion has practical significance, since their wavelength is **easily observed in electromagnetic spectrum**.

Heisenberg's uncertainty principle

It is not possible to determine simultaneously and precisely both position and momentum (or velocity) of a microscopic moving particle (e.g. Proton, neutron or electron)

$$\textbf{Mathematically},\ \Delta x \times \Delta p \geq \frac{h}{4\pi}$$

Δx = uncertainty in position
Δp = uncertainty in momentum

$$\text{Alternatively},\ \Delta x \times (m \times \Delta v) = \frac{h}{4\pi}$$

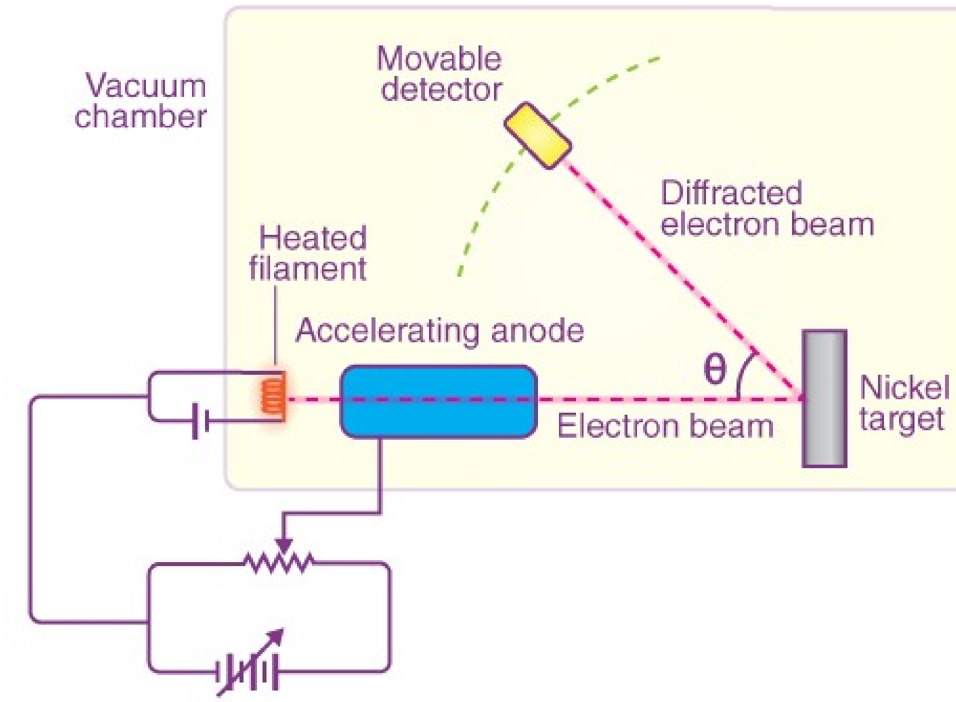
Q. Weight of a cricket ball is 200 g and uncertainty of position is 5pm. What is the uncertainty in velocity?
Q. Uncertainty position of electron is 5 pm. What is the uncertainty of velocity? Mass of electron = 9.1×10^{-31} kg.

Uncertainty & Bohr's theory

- Heisenberg's principle tells that, we cannot describe the exact path on an electron due to its wave nature.
- Thus Bohr theory, **which tells that electrons move in a fixed path**, **is no longer correct**.
- At most, **we can predict the probability of locating the electron with a probable velocity in a particular region of space round the nucleus.**

Schrodinger Wave Equation

Recollecting Davisson–Germer experiment…



Electron is a Wave!!!

- Bohr's theory violates two fundamental laws:
  Dual nature of matter and **uncertainty principle**

Time-independent wave equation

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}+\frac{8\pi^2 m}{h^2}(E-V)\Psi=0$$

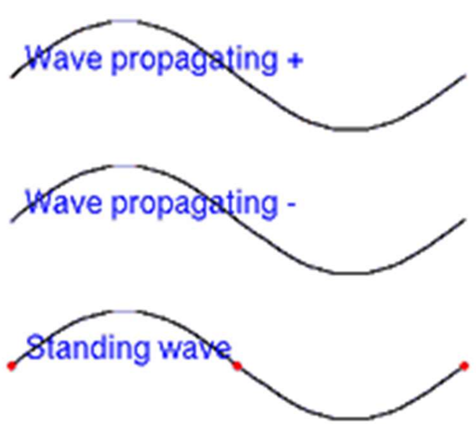
$$\Rightarrow \nabla^2\,\Psi+\frac{8\pi^2 m}{h^2}(E-V)\Psi=0$$

$\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$ is called Laplacian operator

Ψ *is called wave function*

$$\Psi(x)=A\sin\frac{2\pi x}{\lambda}$$

E = total energy, V = potential energy



$$\varphi(x,t)=A\sin\frac{2\pi x}{\lambda}\cos 2\pi\nu t$$
$$=\Psi(x)f(t)$$

Erwin Schrödinger

$$\Psi(x) = A \sin \frac{2\pi x}{\lambda}$$

$$\Rightarrow \frac{d\Psi}{dx} = \left(A \cos \frac{2\pi}{\lambda}\right)\left(\frac{2\pi}{\lambda}\right) = \left(\frac{2\pi A}{\lambda}\right) \cos \frac{2\pi}{\lambda}$$

$$\Rightarrow \frac{d^2\Psi}{dx^2} = \frac{d}{dx}\left(\frac{d\Psi}{d^x}\right) = \left(\frac{2\pi A}{\lambda}\right)\left(- \sin \frac{2\pi x}{\lambda}\right)\left(\frac{2\pi}{\lambda}\right) = -\frac{4\pi^2}{\lambda^2}\left(A \sin \frac{2\pi x}{\lambda}\right) = -\frac{4\pi^2}{\lambda^2}\Psi$$

Kinetic energy, $T = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{h^2}{2m\lambda^2}$ $\quad [\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\boldsymbol{mv}}]$

$$\Rightarrow \frac{1}{\lambda^2} = \frac{2m}{h^2}T = \frac{2m}{h^2}(E - V)$$ [total energy(E) = kinetic energy(T) + potential energy(V)]

$$\frac{\partial^2\Psi}{\partial x^2} = -\frac{8\pi^2 m}{h^2}(E - V)\Psi$$

$$\Rightarrow \frac{\partial^2\Psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$$

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$$

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}+\frac{8\pi^2 m}{h^2}(E-V)\Psi=0$$

$$\Rightarrow \frac{h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi+(E-V)\Psi=0$$

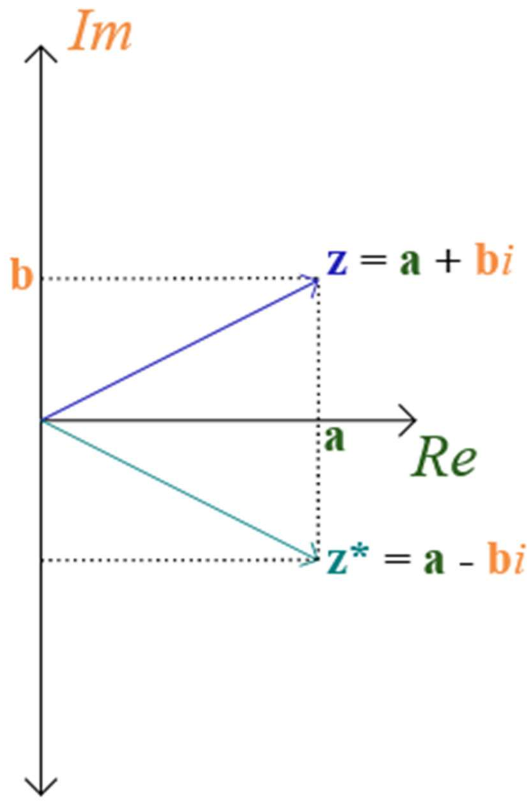
$$\Rightarrow \frac{h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi-V\Psi=-E\Psi$$

$$\Rightarrow -\left[\frac{h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)-V\right]\Psi=E\Psi$$

$$\Rightarrow \hat{H}\Psi=E\Psi$$

$-\frac{h^2}{8\pi^2 m}\nabla^2+V=\hat{H}$, **Hamiltonian Operator**

Significance of Wave Function



Ψ and Ψ^*

Ψ is imaginary but $\Psi\Psi^*$ is real.

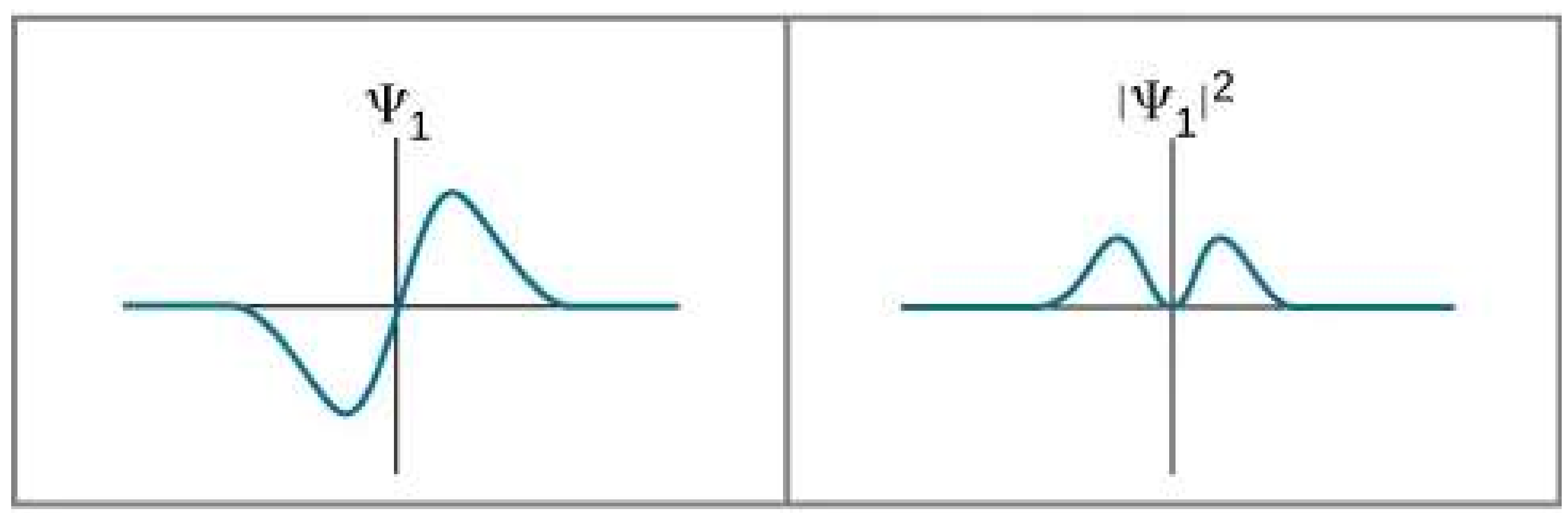
Complex conjugate **Ψ = a + ib**

Ψ^*= a -ib

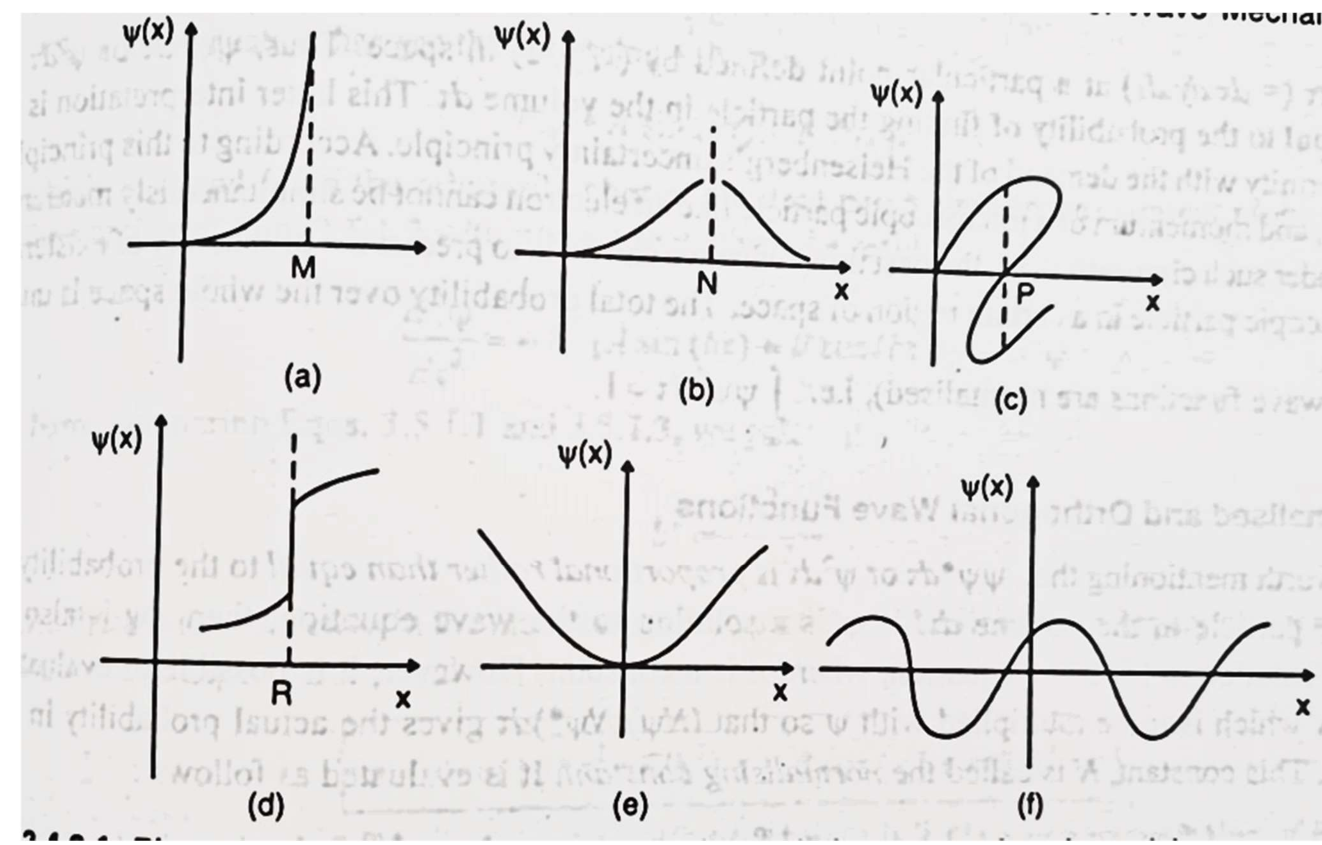
$|\Psi|^2$ *or* $\Psi\Psi^*$ *is proportional to the probability of finding a particle at a given time*

i.e. probability of an electron finding in a box of length dx, width dy, and height dz is

$$P \propto \Psi\Psi^* \mathrm{dxdydz} = \Psi\Psi^* \partial\tau$$



Well behaved or acceptable wave function



1. Ψ must be single valued.
2. Ψ and its first derivative must be continuous.
3. Ψ must be finite; i.e. for all possible values of x, y and z, $\int \Psi\Psi^* \partial\tau$ must exist.

Example 2.2. Which of the following functions are acceptable in quantum mechanics ?

(i) $\sin x$, (ii) $\tan x$, (iii) $\operatorname{cosec} x$, (iv) $\cos x + \sin x$; for $0 \le x \le \pi/2$

(v) e^{-ax}, (vi) $x\,e^{-ax}$; for $x \ge 0$ and (vii) e^{-bx^2} ($viii$) e^{-ax} ; for $x \le 0$

When x lies between 0 and $\pi/2$, the function (i) and (iv) are acceptable while (ii) and (iii) are not acceptable because (ii) tends to infinite at $x \to \pi/2$ and (iii) tends to infinite at $x \to 0$.

When $x \ge 0$ (v) is acceptable while (vi) is not acceptable because it tends to infinite as $x \to \infty$.

When $x \le 0$ (vii) is acceptable while ($viii$) is not acceptable.

Normalised and Orthogonal function

The probability of finding a particle in the whole space must be unity.

$$\int_{-\infty}^{+\infty} \Psi^2 \, d\tau = 1$$

$$\int_{-\infty}^{+\infty} \Psi\Psi^* \, d\tau = 1$$

Ψ and Ψ^* are each other complex conjugate

If Ψ fulfils the above condition then it is called **normalised.**

For two wavefunctions Ψ_1 and Ψ_2, if

$$\int_{-\infty}^{+\infty} {\Psi_1}^* \psi_2 \, d\tau = 0$$

Ψ_1 and Ψ_2 are called **orthogonal** to each other.

Example 2.3. Normalise the functions $\psi = x^2$ over the interval $0 \le x \le k$ (k is a constant).

Let the normalised function be Nx^2. Therefore, by (2.15)

$$\int_0^k (N\psi)^2\,dx = \int_0^k N^2 x^4\,dx = 1$$

or
$$N^2 \int_0^k x^4\,dx = 1$$

or
$$N^2 \left[\frac{x^5}{5}\right]_0^k = 1$$

$$N = \left[\frac{5}{k^5}\right]^{1/2}$$

Hence the normalised function is $\left(\frac{5}{k^5}\right)^{1/2} x^2$

Example 2.4. Show that $\psi_1 = x$ and $\psi_2 = x^2$ are orthogonal over the interval $-k \le x \le k$ [k is a constant].

By the condition (2.19)

$$\int_{-k}^{k} \psi_1 \psi_2\,dx = \int_{-k}^{k} x^3\,dx$$

$$\Rightarrow \quad \left[\frac{x^4}{4}\right]_{-k}^{k} = \left[\frac{1}{4} - \frac{1}{4}\right]k^4 = 0$$

Thus, the wavefunction ψ_1 and ψ_2 are orthogonal over the interval $-k \le x \le k$.

Significance of Schrodinger Wave Equation

Total energy = Kinetic energy + Potential energy

$$\Rightarrow E\Psi = \hat{K}\Psi + \hat{V}\Psi$$

$$\hat{H}\Psi = E\Psi \qquad \hat{H} = \hat{K} + \hat{V} \qquad \hat{H} = -\frac{h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V$$

$$\hat{K} = -\frac{h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

From classical mechanics, $\hat{k} = \frac{1}{2}mv^2 = \frac{1}{2m}\ mv\ ^2 = \frac{p^2}{2m} = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right)$

$$p_x^2 = -\hbar^2\frac{\partial^2}{\partial x^2} = \left(\pm i\hbar\frac{\partial}{\partial x}\right)^2 \qquad \mathrm{i} = \sqrt{-1}$$

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \qquad \hat{p}_x^* = i\hbar\frac{\partial}{\partial x}$$

$$\hat{p}_y = -i\hbar\frac{\partial}{\partial y} \qquad \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$$