For progressive wave (the wave traveling with velocity $v$), $x \to (x - vt)$,

$$y(x,t) = A \sin k(x - vt). \qquad (k(x - vt) \text{ is known as phase of wave.})$$

The wave is periodic in both space and time. The spatial period is known as the wave length $\lambda$ (i.e., wavelength is the number of units of length per wave) and $\lambda = 2\pi/k$.

The temporal period '$\tau$' is the number of units of time per wave and inverse of it ($\tau$) is temporal frequency $\nu$, or the number of waves per unit of time. Thus, $\nu = 1/\tau$. Also the wave velocity $v$ is related with wavelength $\lambda$ and frequency $\nu$ by the relation $v = \nu\lambda$.

Two more relations:-

- Angular temporal frequency
  $\omega = 2\pi/\tau = 2\pi\nu$.
- Wave number or spatial frequency
  $\kappa = 1/\lambda$.

The various wave expressions using above mentioned relations,

- $y = A \sin k(x \mp vt)$
- $y = A \sin 2\pi \left(\frac{x}{\lambda} \mp \frac{t}{\tau}\right)$
- $y = A \sin 2\pi(\kappa x \mp \nu t)$
- $y = A \sin(kx \mp \omega t)$
- $y = A \sin 2\pi\nu \left(\frac{x}{v} \mp t\right)$

For further reading on this topic please refer to "*OPTICS Ed IV* by *Hetch and Ganesan*" chapter 2.

# 4 Wave particle duality

- Interference, diffraction and polarization
  $\Longrightarrow$ Explained by WAVE THEORY.
- Photoelectric effect, emission and absorption of light
  $\Longrightarrow$ Explained by QUANTUM THEORY or PARTICLE THEORY.

**De Broglie Concept of Matter Wave:** In 1924, Louis de Broglie proposed that the matter also possesses dual character like light. His concept about the dual nature of matter was based on the following facts, (a). Matter and light, both are form of energy and each of them can be transformed into each other.

(b). Both are governed by the space time symmetries of the theory of relativity.

**Statement:** "A moving matter particle is surrounded by a wave whose wavelength depends upon the mass of the particle and its velocity. The waves are known as *matter waves* or *de-Broglie waves.*" Mathematically,

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

where $h$ is Plank's constant and $p$ is momentum of particle.

**Proof:** $E = h\nu$ and $E = mc^2 \implies h\nu = mc^2 \implies mc = \frac{h\nu}{c}$.

$$\therefore \quad p = mc = \frac{h\nu}{c} = \frac{h}{\lambda} \qquad (\because c = \nu\lambda)$$

$$\therefore \lambda = \frac{h}{p}.$$

## Special cases:

- For a particle moving with non-relativistic velocity $v$, momentum $p = mv$,

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

  [Note: for relativistic velocity i.e., $v \to c$, $m = \frac{m_0}{\sqrt{1-v^2/c^2}}$.]

- Kinetic energy $E_K = \frac{1}{2}mv^2 = \frac{p^2}{2m} \implies p = \sqrt{2mE_K}$

$$\therefore \lambda = \frac{h}{\sqrt{2mE_K}}$$

- If a charged particle is accelerated through a potential difference of $V$ volt, then $E_K = qV$

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

- For case of electron,

$$\therefore \lambda = \frac{h}{\sqrt{2meV}} = \sqrt{\frac{150}{V}}\mathring{A}$$

- If a material particle is in thermal equilibrium at an absolute temperature $T$, then $E_K = \frac{3}{2}kT$,

$$\therefore \lambda = \frac{h}{\sqrt{3mkT}}$$

**Properties of Matter Waves or de-Broglie's Waves:** From the expression $\lambda_m = \frac{h}{mv}$, it is clear that,

1. $\lambda_m$ of heavy particle $<$ $\lambda_m$ of light weight particle.
2. $\lambda_m$ of fast moving particle $<$ $\lambda_m$ of slow moving particle.
3. if $v = 0$ then $\lambda_m = \infty$, i.e., the matter waves are associated with only moving particles.
4. The matter wave can be generated by charged particles as well as by neutralized particles, i.e., matter wave does not depend on charge of particle.
5. The velocity of matter wave is not constant but depends on velocity of materials.
6. Matter waves are not EMWs.

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**Q.** Why matter waves are not EMW? Q

**Ans.** Because,

a. The matter waves are associated with only moving particles, irrespective of whether the particle is charged or not. Whereas EMWs are produced by only accelerated charges particles.

b. The velocity of matter waves is depends on the velocity of material particles but velocity of EMW is constant for a given medium.

**Q.** Prove that velocity of matter wave is greater than the velocity of light. Q

**Ans.** From de-Broglie concept,

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

The energy of particle is

$$E = h\nu \quad \Longrightarrow \nu = \frac{E}{h}.$$

But from mass-energy relationship $E = mc^2$

$$\therefore \quad \nu = \frac{mc^2}{h}$$

We know that $\qquad c = \nu\lambda$

The de-Broglie wave velocity $v_p$ is given as,

$$\begin{aligned} v_p &= \nu\lambda \\ &= \left(\frac{mc^2}{h}\right)\left(\frac{h}{mv}\right) \\ v_p &= \frac{c^2}{v}. \end{aligned}$$

Because $v < c$ always, hence *the matter wave always travels faster than light.*

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# 5 Concept of Wave packet

The velocity of de-Broglie wave is given by $v_p = c^2/v$, but no material particle can have velocity greater than $c$, also if velocity of de-Broglie wave is greater than the velocity of the particle then the particle will left behind. Hence, it has been concluded that instead of one wave, a wave packet is associated with particle. The wave packet is formed by superposition of several waves whose velocities and wavelengths are slightly different from each other. The amplitude and phase of the component waves are such that they interfere constructively in a region where the particle is found and outside the region they interfere destructively.

Thus, when several progressive waves of slightly different wavelengths travel along in one direction, the resultant wave obtained on superposition travel in form of group of waves which is called *wave packet*. The velocity of component waves of a wave packet is called the *wave velocity* or *phase velocity* $v_p$ and the velocity of wave packet is called the *group velocity* $v_g$.

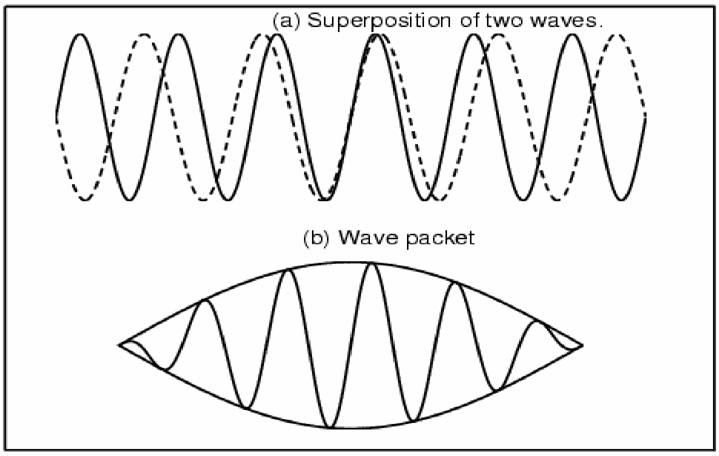


Figure 4: Formation of wave packet.

***Phase Velocity*** $v_p$ **&** ***group velocity*** $v_g$: Consider two progressive waves, whose amplitude is same but angular frequency and propagation constant differs by $\Delta\omega$ and $\Delta k$ respectively. Such wave can be written as,

$$y_1 = A\cos(\omega t - kx)$$
$$y_2 = A\cos[(\omega+\Delta\omega)t - (k+\Delta k)x]$$

only formula & concept, no derivation

According to principle of superposition,

$$\begin{aligned}
Y &= y_1 + y_2 \\
&= A\left[\cos(\omega t - kx) + \cos[(\omega+\Delta\omega)t - (k+\Delta k)x]\right] \\
&= 2A\cos\left[\frac{(2\omega+\Delta\omega)t - (2k+\Delta k)x}{2}\right]\cos\left[\frac{\Delta\omega t - \Delta k x}{2}\right] \\
&\qquad\left[\because \cos A + \cos B = 2\cos\left(\frac{A+B}{2}\right)\cos\left(\frac{A-B}{2}\right)\right] \\
&= \underbrace{2A\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)}_{amplitude}\cos(\underbrace{\omega t - kx}_{phase})
\end{aligned}$$

where $2\omega \approx 2\omega + \Delta\omega$ and $2k \approx 2k + \Delta k$. $\omega$ and $k$ are mean angular frequency and mean propagation constant respectively.

For phase of the wave to be constant

$$\omega t - kx = \text{Constant}$$

$\therefore$ Wave velocity $\quad v_p = \dfrac{dx}{dt} = \dfrac{\omega}{k}$

Now for the amplitude of wave packet to be constant,

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x = \text{constant.}$$

Hence the group velocity

$$\begin{aligned}
v_g &= \frac{dx}{dt} = \frac{\Delta\omega/2}{\Delta k/2} = \frac{\Delta\omega}{\Delta k} \\
&= \lim_{\omega_1\to\omega_2}\frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk}.
\end{aligned}$$

## 5.1 Relationship between group velocity $v_g$ and phase velocity $v_p$:

Wave velocity $\quad v_p = \dfrac{\omega}{k} \quad \Rightarrow \quad \omega = kv_p.$

$$\text{Group velocity} \quad v_g = \frac{d\omega}{dk} = v_p + k\frac{dv_p}{dk} = v_p + \left(\frac{2\pi}{\lambda}\right)\frac{dv_p}{d\left(\frac{2\pi}{\lambda}\right)}$$
$$= v_p - \lambda\frac{dv_p}{d\lambda}.$$

**Case I:** In the non-dispersive medium, i.e., $dv_p/d\lambda = 0$, then $v_g = v_p$. For example, EMW propagation in vacuum.

**Case II:** In the dispersive medium,

1. If $dv_p/d\lambda = +ve$ then $v_g < v_p$. For example, EMW propagation in dielectric substance.
2. If $dv_p/d\lambda = -ve$ then $v_g > v_p$. For example, propagation in electric conductors.

## 5.2 Phase velocity and group velocity of de-Broglie waves

### (a). associated with *a non relativistic free particle*:

The K.E. of the particle is $E = \dfrac{p^2}{2m}$
According de-Broglie hypothesis,

Only results.

$$\lambda = \frac{h}{p} \quad \Rightarrow \quad p = \frac{h}{\lambda}$$

$$\therefore \quad E = \frac{(h/\lambda)^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{h^2k^2}{8\pi^2 m} \qquad (\because k = 2\pi/\lambda)$$

But, $\quad E = h\nu = \dfrac{h\omega}{2\pi} \qquad (\because \nu = 2\pi/\omega)$

Hence, wave velocity,

$$v_p = \frac{\omega}{k} = \frac{hk}{4\pi m} = \frac{p}{2m} = \frac{mv}{2m} = \frac{v}{2} = \textbf{Half the velocity of the particle.}$$

Thus *the wave velocity of the matter wave is less than the particle velocity*, hence the matter wave will be left behind, which is wrong because there will be no relationship between the particle and the matter wave. Thus for matter waves, the *wave velocity has no physical significance.*

Group velocity

$$v_g = \frac{d\omega}{dk} = \frac{2hk}{4\pi m} = \frac{h}{m\lambda} = \frac{h}{m(h/mv)} = v = \textbf{particle velocity}.$$

Thus, the group velocity of the de-Broglie wave associated with a non-relativistic free particle is equal to the particle velocity i.e., *the de-Broglie waves travels with the particle velocity.* Hence, a moving particle is equivalent to a wave packet.

## (b.) associated with *a relativistic free particle*:

$$\text{The angular frequency} \quad \omega = 2\pi\nu = \frac{2\pi mc^2}{h} \qquad [\because \quad E = mc^2 \quad \& \quad E = h\nu]$$
$$= \frac{2\pi m_0 c^2}{h\sqrt{1-\frac{v^2}{c^2}}}$$

$$\& \quad \text{The propagation constant} \quad k = \frac{2\pi}{\lambda} = \frac{2\pi mv}{h} = \frac{2\pi m_0 v}{h\sqrt{1-\frac{v^2}{c^2}}}$$

only results.

Hence phase velocity,

$$v_p = \frac{\omega}{k} = \frac{2\pi m_0 c^2}{h\sqrt{1-\frac{v^2}{c^2}}} \times \frac{h\sqrt{1-\frac{v^2}{c^2}}}{2\pi m_0 v} \implies \boxed{v_p = \frac{c^2}{v}.}$$

and group velocity $\quad v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv}$

$$\frac{d\omega}{dv} = \frac{d}{dv}\left[\frac{2\pi m_0 c^2}{h}\sqrt{1-\frac{v^2}{c^2}}\right]$$
$$= \frac{2\pi m_0 c^2}{h}\left[-\frac{1}{2}\left(1-\frac{v^2}{c^2}\right)^{-3/2}\left(-\frac{2v}{c^2}\right)\right]$$
$$= \frac{2\pi m_0 c^2}{h}\left[\frac{v}{c^2}\left(1-\frac{v^2}{c^2}\right)^{-3/2}\right]$$

$$\frac{dk}{dv} = \frac{d}{dv}\left(\frac{2\pi m_0 v}{h\sqrt{1-\frac{v^2}{c^2}}}\right), \qquad \text{(after differentiation,)}$$
$$= \frac{2\pi m_0}{h}\left(1-\frac{v^2}{c^2}\right)^{-3/2}$$

$$\therefore \quad v_g = \frac{2\pi m_0 c^2}{h}\left[\frac{v}{c^2}\left(1-\frac{v^2}{c^2}\right)^{-3/2}\right] \Big/ \left[\frac{2\pi m_0}{h}\left(1-\frac{v^2}{c^2}\right)^{-3/2}\right] = v$$

Thus,

(a). As $c > v$, hence $v_p > c$, i.e., phase velocity has no physical significance.

(b). The de-Broglie wave packet associated with a moving body travels with the velocity of the moving particle.

[Note: In above derivations, for relativistic motion $E = mc^2$ and for non relativistic motion $E = p^2/2m$. ]

# 7 Heisenberg's Uncertainty Principle, 1927

**Statement:** "It is impossible to determine the exact position and momentum of a particle simultaneously."

**Proof:** As per de-Broglie hypothesis, any moving particle is surrounded by packet of matter waves. See the figure (4). Now let consider this wave packet is formed due to superposition of two sinusoidal waves of different angular frequencies $\omega_1$ & $\omega_2$ and propagation constant $k_1$ & $k_2$ traveling along X-axis. The equations are,

$$\psi_1 = A\sin(\omega_1 t - k_1 x)$$
$$\psi_2 = A\sin(\omega_2 t - k_2 x)$$

no derivati

Using superpostion principle,

$$\begin{aligned}\psi = \psi_1 + \psi_2 &= A\sin(\omega_1 t - k_1 x) + A\sin(\omega_2 t - k_2 x)\\ &= 2A\cos\left(\frac{\delta\omega}{2}t - \frac{\delta k}{2}x\right)\sin(\omega t - kx),\end{aligned}$$

$$\text{where,}\quad \omega = \frac{\omega_1+\omega_2}{2},\quad k = \frac{k_1+k_2}{2},\quad \delta\omega = \omega_1-\omega_2,\ \text{and}\ \delta k = k_1 - k_2.$$

The error in the measurement of the position of the particle is equal to the distance between two nodes. These nodes are formed when $\cos\left(\frac{\delta\omega}{2}t - \frac{\delta k}{2}x\right) = 0$, i.e., $\left(\frac{\delta\omega}{2}t - \frac{\delta k}{2}x\right) = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots$ .

Let $x_1$ and $x_2$ are the position of any two successive nodes at any time $t$, then

$$\begin{aligned}\frac{\delta\omega}{2}t - \frac{\delta k}{2}x_1 &= (2n+1)\frac{\pi}{2}\\ \text{and}\quad \frac{\delta\omega}{2}t - \frac{\delta k}{2}x_2 &= (2n+3)\frac{\pi}{2}\end{aligned}$$

on substraction,

$$\begin{aligned}&\Longrightarrow \quad \frac{\delta k}{2}(x_2 - x_1) = \pi\\ &\Longrightarrow \quad \Delta x = x_2 - x_1 = \frac{2\pi}{\delta k}\\ &\Longrightarrow \quad \Delta x = \frac{2\pi}{\delta k} = \frac{2\pi}{\Delta\left(\frac{2\pi}{\lambda}\right)} = \frac{1}{\Delta\left(\frac{p}{h}\right)} = \frac{1}{\Delta p}\\ &\Longrightarrow \quad \Delta x.\Delta p = h\\ &\Longrightarrow \quad \Delta x.\Delta p \geq \hbar \ \left(=\frac{h}{2\pi}\right)\end{aligned}$$

$$\Longrightarrow \quad \boxed{\Delta x.\Delta p \geq \hbar}$$

## 7.1 Energy and time uncertainty principle

We know that group velocity $v_g$ is equal to particle velocity $v_x$. Let the wave packet moves $\Delta x$ distance in $\Delta t$ time. Since $\Delta x$ is the uncertainty in the x-coordinate and $\Delta t$ is the uncertainty in time, hence

$$v_g = \frac{\Delta x}{\Delta t} \qquad \Longrightarrow \qquad \Delta t = \frac{\Delta x}{v_g}. \tag{11}$$

$$\text{As energy} \quad E \equiv E(p_x)$$
$$\Delta E = \frac{\partial E}{\partial p_x}.\Delta p_x.$$
$$\text{But} \qquad \frac{\partial E}{\partial p_x} = v_x = v_g \qquad [\because \ E = \frac{1}{2}mv^2 \quad \longrightarrow \quad \frac{\partial E}{\partial v} = \frac{1}{2}2mv \quad \longrightarrow \quad \frac{\partial E}{\partial p} = v.]$$
$$\therefore \quad \Delta E = v_g.\Delta p_x \tag{12}$$

Using Eqs (11) and (12),

$$\Delta E.\Delta t = v_g.\Delta p_x.\frac{\Delta x}{v_g} = \Delta p_x.\Delta x \geq \hbar \qquad \text{[Using Heisenberg's uncertainty principle]}$$
$$\Longrightarrow \quad \boxed{\Delta E.\Delta t = \hbar}$$

## 7.2 Applications of Heisenberg's uncertainty principle

### 7.2.1 Non-exitance of electron in nucleus

Since size of nucleus = $10^{-14}m$, hence uncertainty in position inside the nucleus = $2 \times 10^{-14}m$.

From Heisenberg's uncertainty principle,

$$\Delta p_x = \frac{\hbar}{\Delta x} = \frac{1.055 \times 10^{-14} J - sec}{2 \times 10^{-14}} m = 5.275 \times 10^{-21} Kg - m/s.$$

Since the magnitude of momentum is relativistic compare to the mass of the electron, then using relativistic mass formula for energy of electron,

$$E^2 = p^2c^2 + m_0^2c^4$$
$$E^2 = p^2c^2 \qquad [\because \quad m_0^2c^4 = 0.511MeV \ll p^2c^2]$$
$$E = pc = (5.275 \times 10^{-21}) \times (3 \times 10^8)J$$

$$= \frac{(5.275 \times 10^{-21}) \times (3 \times 10^8)}{1.6 \times 10^{-19}} eV = 10Mev.$$

Thus if the electron resides in the nucleus, it should have an energy of the order of $10MeV$. However, electrons emitted during $\beta$-decay have energies of the order of $3MeV$. Hence we conclude that electron do not reside in the nucleus.

# 8 The wave function '$\Psi$'

The wave function describes the wave properties of the moving particle. It is denoted by '$\Psi$'and is complex in nature, i.e., $\Psi = a + ib$, where $a$ and $b$ are real numbers.

## 8.1 Properties or physical significance of wave function

1. $\Psi$ must be continues and single values everywhere.
2. $\frac{\partial\Psi}{\partial x}, \frac{\partial\Psi}{\partial y}, \frac{\partial\Psi}{\partial z}$ also must be continues and single values everywhere.
3. $\Psi$ must be normalized, i.e., $\Psi = 0$ as $x \to \pm\infty$, $y \to \pm\infty$, $z \to \pm\infty$, i.e.,

$$\int_{-\infty}^{\infty} |\Psi|^2 \mathrm{d}V = 1.$$

4. $|\Psi|^2 = \Psi\Psi^*$ defines probability density and is at any particular place and time is proportional to the probability of finding the particle at that place on that time.

$$\text{Probability density} \qquad |\Psi|^2 = \Psi\Psi^*.$$

5. Probability $\quad P_{x_1 x_2} = \int_{x_1}^{x_2} |\Psi|^2 \mathrm{d}x.$
6. The expectation values: It is defined as,
   Position expectation values,

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x|\Psi|^2 \mathrm{d}x}{\int_{-\infty}^{\infty} |\Psi|^2 \mathrm{d}x} = \int_{-\infty}^{\infty} x|\Psi|^2 \mathrm{d}x. \qquad \text{[for normalized function.]}$$

Energy expectation values,

$$\langle E\rangle = \frac{\int\limits_{-\infty}^{\infty} E|\Psi|^2 \mathrm{d}x}{\int\limits_{-\infty}^{\infty} |\Psi|^2 \mathrm{d}x} = \int\limits_{-\infty}^{\infty} E|\Psi|^2 \mathrm{d}x. \qquad \text{[for normalized function.]}$$

# 9 The Schrödinger wave equation

In 1925, Schrödinger gave a wave equation using the concept of de-Broglie hypothesis and Plank's quantum mechanics, which is called *the Schrödinger wave equation.* This equation has same significance in quantum mechanics as Newton's laws of motion has in classical mechanics.

## 9.1 Time independent Schrödinger wave equation

Consider a system of stationary particle associated with the particle. Let $\Psi(r,t)$ be the wave function for the de-Broglie wave at any location $\vec{r} = i\,x + j\,y + k\,z$ at time $t$. Then 3D wave equation can be written as,

$$\nabla^2\Psi = \frac{1}{u^2}\frac{\partial^2\Psi}{\partial t^2} \quad \text{or} \quad \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} = \frac{1}{u^2}\frac{\partial^2\Psi}{\partial t^2}, \tag{13}$$

where $u->$ wave velocity.

The solution of Eqn (13) can be written as,

$$\Psi\,(r,t) = \Psi_0(r)\;e^{-i\,\omega t} \tag{14}$$

where $\Psi_0$ is the amplitude of wave at the point considered.

Differentiating Eqn (14) twice w.r.t. $t$,

$$\begin{aligned}
\frac{\partial\Psi}{\partial t} &= -i\,\omega\Psi_0(r)\;e^{-i\,\omega t},\\
\frac{\partial^2\Psi}{\partial t^2} &= (-i\,\omega)^2\;\Psi_0(r)\;e^{-i\,\omega t} = -\omega^2\;\Psi_0(r)\;e^{-i\,\omega t},\\
&= -\omega^2\;\Psi(r,t) \qquad (15)
\end{aligned}$$

Substituting (15) into (13),

$$\nabla^2\Psi = -\frac{\omega^2}{u^2}\Psi,$$

$$\begin{aligned}
\because \omega &= 2\pi\nu\\
&= \frac{2\pi u}{\lambda} \qquad (\because\; u = \nu\lambda)
\end{aligned}$$