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Quantum Mechanics Revision

(i) de-Broglie hypothesis and

$$\lambda = \frac{h}{p} = \frac{h}{mv} , \quad E = \frac{p^2}{2m}$$

$$p = \sqrt{2mE} , \quad E = \frac{1}{2}mv^2 = eV ,$$

$$E = \frac{3}{2}kT \; ; \quad E = kT , \quad E = \frac{1}{2}kT$$

(diff. cases to find E & hence v & p)

(ii) de-Broglie waves are waves of mathematical probability.
These are not em waves or soundwave

(iii) de-Broglie waves can travel with speed faster than the speed of light (in vaccum/free space).

$$u = \frac{c^2}{v} > c$$

(iv) Concept of wave packet → superimposition of infinite waves associated with moving material particle and leads to the concept of group velocity.
Individual monochromatic wave is infinite whereas group of waves or wave packet will be finite in its existence.

Discuss the intereference of $\Psi_1 = A\sin(\omega t - kx)$
$\Psi_2 = A\sin[(\omega + d\omega)t - (k+dk)x]$

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Final wave function $\Psi = \Psi_1 + \Psi_2$

or $\Psi(x,t) = R \sin(\omega t - kx)$

where $R = 2A\cos\left(\frac{d\omega}{2}t - \frac{dk}{2}x\right)$

In individual wave, A is constant where as in wave packet R is variable.

(V) Phase velocity – velocity of individual wave — v_p or u

$\omega = 2\pi\nu$

$v_p = u = \nu\lambda = \frac{\omega}{k}$ $\quad k = \frac{2\pi}{\lambda}$

or $= \frac{E}{p}$ $\quad E = h\nu$

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

Clearly $u = \frac{c^2}{v} > c$ $\quad E = mc^2$

$p = mv$

(vi) Group velo. – Average vel of the group of waves or vel with which wave packet is moving ahead — $v_g = \frac{d\omega}{dk} = \frac{dE}{dp}$

Remember velocity of particle = group velocity

i.e $\underline{v = v_g}$ & $v \neq v_p$ (or u)

If particle's speed is $<<< c$, $E = \frac{p^2}{2m} \Rightarrow \frac{dE}{dp} = \frac{p}{m} = v$ (v_g)

if $v \to c$, $E^2 = p^2c^2 + m_0^2c^4$

$\Rightarrow \frac{dE}{dp} = \frac{pc^2}{E} = \underline{v}$ $\quad (p = mv,\ E = mc^2)$

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$u << c \rightarrow$ non relativistic speeds
$u \rightarrow c \rightarrow$ relativistic speeds

(vii) Dispersion relation (relation b/w phase velocity & group velocity)

$$v_p \text{ (or } u) = \frac{w}{k} \Rightarrow w = v_p \cdot k$$

$$v_g = \frac{dw}{dk} = \frac{d(v_p \cdot k)}{dk}$$

$$\Rightarrow v_g = v_p + k\frac{dv_p}{dk}$$

$$\Rightarrow v_g = v_p + k\frac{dv_p}{d\lambda} \cdot \frac{d\lambda}{dk}$$

Now $k = \frac{2\pi}{\lambda}$

$$\frac{dk}{d\lambda} = -\frac{2\pi}{\lambda^2}$$

$$\boxed{\therefore v_g = v_p - \lambda\frac{dv_p}{d\lambda}} \rightarrow \text{dispersion relation.}$$

if $\frac{dv_p}{d\lambda}$ is +ve $v_g < v_p$
Normal dispersion

if $\frac{dv_p}{d\lambda} = 0$ $v_g = v_p = c \rightarrow$ no dispersion
(only case, speed of light in free space)

if $\frac{dv_p}{d\lambda}$ is −ve, $v_g > v_p$, Anomalous dispersion.

P is prob. density.

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Max Born's interpretation of wave fn.

(viii) $\Psi \rightarrow$ wave fn $|\Psi|^2 \rightarrow$ probability density

3-D case $\rightarrow \frac{\text{prob.}}{\text{vol.}}$ then units of ψ will be of $L^{-3/2}$

2-D $\longrightarrow \frac{\text{prob.}}{\text{area}} \rightarrow$ " " $L^{-2/2}$ or L^{-1}

1-D $\rightarrow \frac{\text{prob.}}{\text{length}} \rightarrow$ " " $L^{-\frac{1}{2}}$

(IX) Conditions for wave fn Ψ to be acceptable or well behaved (a) normalizable i.e

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P\,dV = 1 \longrightarrow \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\Psi|^2 dV = 1 \quad (3\text{-D})$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P\,dA = 1 \longrightarrow \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\Psi|^2 dA = 1 \quad (2\text{-D})$$

$$\int_{-\infty}^{\infty} P\,dx = 1 \longrightarrow \int_{-\infty}^{\infty} |\Psi|^2 dx = 1 \quad (1\text{-D})$$

(b) should be single valued, finite valued & continuous

(c) $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}, \frac{\partial\psi}{\partial z}$ " " " " " " "

(d) as $x \rightarrow \pm\infty$, $\Psi(x) \rightarrow 0$.

(x) Normalization means total prob. to locate particle in universe is 1.

do numericals based on Normalization.

When we say normalize the wave fn, this means we have to find the value of 'A' in $\Psi = A\sin(\omega t - kx)$.

(xi) If $\int_{-\infty}^{\infty} P\,dx = 0 \Rightarrow \int_{-\infty}^{\infty} |\Psi|^2 dx = 0 \Rightarrow$ particle is not present in this universe.

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$ is Laplacian

(xii) Schrodinger eqn. gives the eqn. of motion of the particle moving in a region. It is analogous to Newton's second law of motion the only difference is Newton's laws are for macroscopic bodies/objects and Schrodinger eqn. is for microscopic particles.
Similarity b/w the two is both are for $u << c$, non relativistic speeds.

(xiii) Free particle → only K.E.
Restricted particle → K.E + P.E.

(xiv) Time Independent Sch. Eqn (1-D)

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}(E-U)\psi(x)=0 \quad (1)$$

$U \to$ P.E.

if free particle $U=0$

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

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

which is same as eq. of motion of SHM → $\frac{d^2x}{dt^2}+\omega_0^2 x=0$; $\omega_0^2=\frac{k}{m}$

Soln. is $\psi(x)=A\sin kx+B\cos kx$

For 3-D case, replace $\frac{d^2\psi}{dx^2}$ with $\nabla^2\psi$

(XV) Time dependent Sch. Eqn.
E will not be constant, rather it will have to be replaced by operator $i\hbar\frac{\partial}{\partial t}$

$$E\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U\psi$$

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

(XVI) $\hat{X} \to$ any operator, $f \to$ any fn.
then if

$$\hat{X} f = A f \to \text{eigen eqn.}$$

$\hat{X}$ → eigen op.
f → eigen fn.
A → constant eigen value of op.

eg. $\frac{d}{dx} e^{2x} = 2 \cdot e^{2x}$

$\frac{d}{dx}$ → eigen op.
e^{2x} → eigen fn.
2 → eigen value

(XVII) Time independent Schrodinger eqn. can be expressed in eigen eqn. form.
From ① (XIV)

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

$$\Rightarrow E\psi(x) = \underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U\right]}_{\hat{H}}\psi(x)$$

$$\Rightarrow \boxed{E\psi(x) = \hat{H}\psi(x)}$$

$\hat{H}$ is known as Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U \quad (1\text{-}D)$$

for total energy of the particle if motion is time independent.

If 3-D motion

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U$$

(xviii) Do remember

$$\hat{x} = x \quad \text{(position op.)}$$

$$\hat{E} = \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U \quad \text{(1-D, time independent)}$$

$$\hat{E} = i\hbar\frac{\partial}{\partial t} \quad \text{(time dependent motion)}$$

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

$$(\hat{K.E.}) = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \quad (1\text{-}D)$$

$$(\hat{P.E.}) = \hat{U} = U$$

($\wedge$ means operator).

(xix) Example of Application of Time Independent Sch. Eqn. is motion of Particle in a box along 1-D, usually known as 1-D box.

Eigen wave fn. $\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$

$n = 1, 2, 3$

& energy eigen values ($n \neq 0$)

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2 m L^2}$$

$m \rightarrow$ mass of the particle

$L \rightarrow$ width of the box

$\hbar = \frac{h}{2\pi}$ = reduced Planck's constant

$h = 6.62 \times 10^{-34}$ Js.