CHAPTER 1: Quantum Mechanics at a Glance for Beginners

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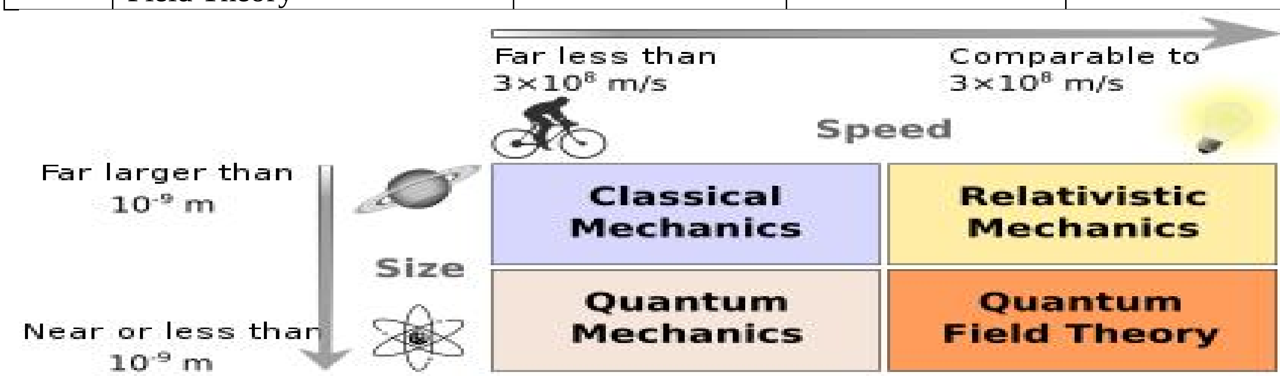
1.0 Introduction-

As we know that Mechanics is a branch of physics which deals the motion of objects. It is mainly divided into four types on the basis of size and speed of objects given in (Table- 1):

Table 1-

S.No.	Mechanics	Size of object	Speed of object v	Examples
1	Classical or Newtonian Mechanics	Macroscopic (i.e. size greater than that of atoms)	$v \ll$ Speed of light c $(\approx 3 \times 10^8\ m/s)$	Motion of bicycle, scooter, car, train. Aeroplane etc.
2	Quantum Mechanics	Microscopic (i.e. size comparable to atoms)	$v \ll c$	Motion of atom, molecule, electron, proton, neutron etc.
3	Relativistic Mechanics	Macroscopic	$v \approx c$	Motion of photon, meson etc.
4	Relativistic Quantum Mechanics or Quantum Field Theory	Microscopic	$v \approx c$	Motion of EM radiations



(Courtesy to Google website)

Recent Trends in Physics: Quantum Science & Technology

The Latin term for "how much" is where the word "quantum" originates. The study of atomic particle existence and interaction is known as quantum mechanics. In all quantum theories, discrete amounts of anything are always present. e.g. energy $E = n\,h\nu$, where $n = 0, 1, 2, 3, \cdots$ where $\boldsymbol{h}\,(= \mathbf{6.67 \times 10^{-34}}\,\boldsymbol{Js or}\,\mathbf{6.67 \times 10^{-34}}/1.6 \times \mathbf{10^{-19}} = \mathbf{4.1356677 \times 10^{-15}\ eV \cdot s}\,)$ is a fundamental physical constant occurring in quantum mechanics called **Planck constant**. The sign for the Dirac constant, also known as the reduced Planck constant, is = h/2. The two men who developed quantum physics, Niels Bohr and Max Planck, each won the Nobel Prize in Physics for their research on quanta.

Between 1900 and 1930, physics experiences a significant change. The study of matter and its interactions with energy at the level of atomic and subatomic particles is known as quantum mechanics. The Quantum Mechanics (QM) era was during this time. Micro particle behavior, including that of electrons, protons, neutrons, hydrogen atoms, potential wells, potential barriers, tunneling, etc., is explained using quantum mechanics (QM). Max Planck first proposed the concept of quantization in 1900 to describe the entire black-body spectrum. Albert Einstein (Photoelectric Effect), Arthur Holly Compton (Compton Effect), Werner Heisenberg (Heisenberg's uncertainty relations), Louis Victor de Broglie (Matter Waves or de Broglie Waves), Erwin Schrödinger (Schrödinger wave equations), Max Born (Wave functions), Paul Adrien Maurice Dirac (Dirac equation), and others are among the physicists who are credited with the majority of inventions. When a particle reaches a macroscopic size, quantum theory transforms into classical physics. Particles in quantum mechanics have wavelike characteristics, and the Schrödinger equation, a specific wave equation, determines how these waves behave under various conditions.

The first law of quantum physics asserts that everything is constituted of matter and energy and that the barrier between them is never stable or infinite. Different atomic levels show the interaction between matter and energy. The quanta of electromagnetic energy, the uncertainty principle, the Pauli exclusion principle, and the wave theory of matter particles are basically the four key principles of quantum mechanics that have been demonstrated experimentally and are relevant to the behavior of nuclear particles at close ranges.

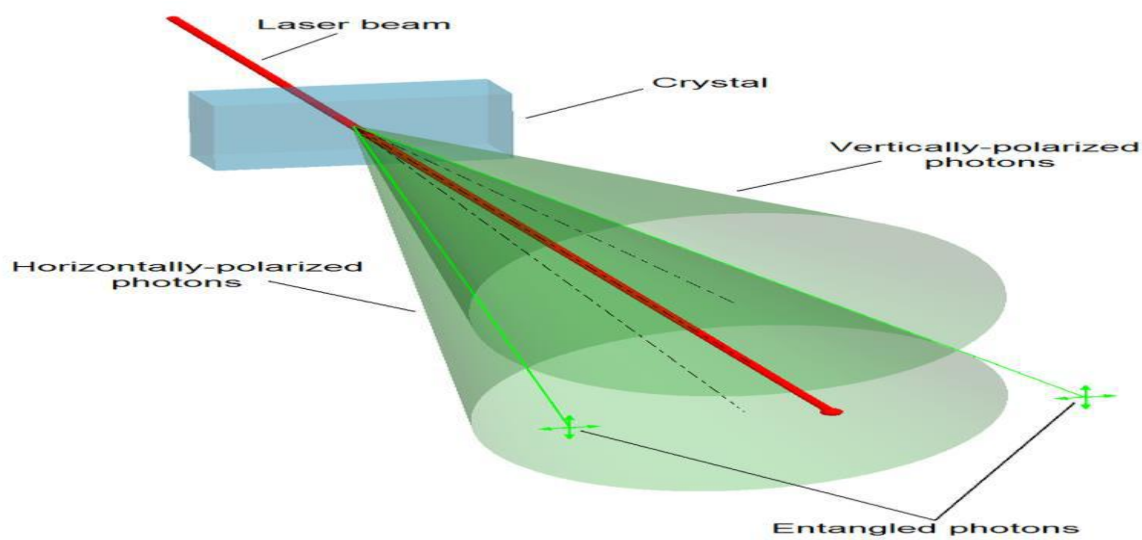
Lasers and integrated circuits are two examples of quantum phenomena that are used in quantum mechanics applications. Understanding how individual atoms are united by covalent bonds to form molecules relies heavily on quantum mechanics. Lasers, solar cells, electron microscopes, atomic clocks used in GPS, and MRI scanners for medical imaging are all examples of practical applications of quantum mechanics. Usually, it is used to describe microscopic systems like molecules, atoms, and subatomic particles. The discovery that waves could be quantized into tiny energy packets that resembled particles, or quanta, led to the development of the field of physics known as quantum mechanics, which studies atomic and subatomic systems.

Thus, the field of physics known as quantum mechanics studies how matter and energy behave on a scale smaller than that of atoms and subatomic particles or waves. Max Born initially used the term "quantum mechanics" in 1924.We'll talk about the Black Body radiation spectrum, the

Compton effect, the photoelectric effect, and their interpretations based on Max Planck's quantum theory in this chapter. Louis de Broglie's theory of matter waves and its experimental confirmation by the experiments conducted by Davisson-Germer and Thomson.

In the honour of Max Planck the whole world celebrate **World Quantum Day on 14 April**, i.e. **a reference to 4.14** due to $\boldsymbol{h}\ (\mathbf{4.1356677} \times \mathbf{10^{-15}\ eV \cdot s}\ )$.World Quantum Day is an annual celebration for promoting public awareness and understanding of quantum science and technology around the world. Quantum Mechanics or Relativity (or both) is said to be Modern Physics.

When a group of particles are created, interact, or share spatial proximity in such a way that the quantum states of each particle of the group cannot be described independently of the states of the others, including when the particles are separated by a great distance, this phenomenon known as quantum entanglement (also known as Entangle Photons) takes place. When a system is in a "superposition" of several states, this is when quantum entanglement occurs. One key aspect of quantum physics that distinguishes it from classical mechanics is entanglement. A particular sort of superposition called entanglement involves two isolated locations in space.



(Courtesy to Google website)

It is possible to find instances where measurements of entangled particles' physical characteristics, such as position, momentum, spin, and polarization, are fully coupled. For instance, if a pair of entangled particles is created with known zero total spin, and one particle is discovered to have clockwise spin on a first axis, the other particle's spin is found to be anticlockwise when measured on the same axis.

Examples-

1-if a coin is tossed (or flipped) without being watched for the outcome. The man is aware that it will either be heads or tails. Simply put, the man is unsure which is which. Superposition indicates that until you look at it (take a measurement), it is not just unknown to the other person; it is also not even in its heads or tails condition. Similar to this, a photon might collide with a 50/50 splitter to cause the entanglement (superposition of two different places) of a collection of images. After the splitter, the photon could follow path A or path B. The superposition in this instance is between

- a photon in path A and no photon in path B
- no photon in path A and a photon in path B.

As a typical human being, the individual believes that it is just in one road or the other way, and that one simply is unaware of it. However, until you really measure it, it is in both. Once more, the average person wants to assert that if I measured it and discovered it along path A.

S.N.	**EM Wave** $\left(\lambda = \frac{hc}{E}\right)$	**Matter Wave** $\left(\lambda = \frac{h}{p}\right)$
1	An oscillating charged particle gives rise to the EM wave.	A matter wave is associated with a moving microscopic particle.
2	The speed of an EM wave is constant in a medium. Its speed is $c\left(=3\times10^{8}\ m/s\right)$ in vacuum.	Its speed is always greater than the speed of light.
3	Its wave length is inversely proportional to the energy of photon, i.e. $\lambda \propto \frac{1}{E}$.	Its wave length is inversely proportional to the momentum of microscopic particle, i.e. $\lambda \propto \frac{1}{p}$.
4	An EM wave can be radiated into space by an oscillating charged particle.	A Matter wave cannot be emitted by a moving microscopic particle.
5	In an EM wave its electric and magnetic fields oscillate $\perp$ to the direction of motion.	A de- Broglie wave is associated with neutral and charged microscopic particles. A charged moving microscopic particle has electric and magnetic fields.

1.1 **de-Broglie concept of matter waves-**

Prince Louis-Victor de Broglie [15th August, 1892 – 19th March, 1987]-In **1924**, French physicist first time introduced the idea of matter wave or de Broglie wave. In **1929**, de Broglie was awarded **Nobel Prize** for this discovery **'the wave nature of electron'**.**(Courtesy to Google website)**

A matter was regarded as a particle in nature up until 1923. All minuscule particles, such as electrons, protons, neutrons, alpha particles, etc., were included in de Broglie's expansion of the concept of the dual nature of light. The photons that make up light are said to be its constituents, according to the quantum hypothesis. De Broglie derived the relationship between particle and wave natures from Einstein's energy-mass relation for electromagnetic (EM) waves and Planck's energy formula.

$$E = h\nu = h\frac{c}{\lambda} \;.......(1.101)$$

where h is Planck's constant, ν is frequency of EM wave and λ is wavelength of EM wave

$$E = mc^2 \quad ....(1.102)$$

$$\therefore \quad \frac{hc}{\lambda} = mc^2 \text{ or, } \lambda = \frac{h}{mc} = \frac{h}{m\mathrm{v}(=\mathrm{c})} \;.......(1.103) \Rightarrow \quad \boxed{\lambda = \frac{h}{p}}$$

In contrast to and, which are characteristics of waves, E and P are characteristics of particles. Thus, the Planck's constant h establishes a relationship between the particle and wave natures, giving rise to the EM wave's (or light's) dual nature.

The de Broglie hypothesis, put out by Louis de Broglie, states that a moving particle is connected to a wave known as the de Broglie or matter wave. The mechanical motion of a moving macroscopic particle is represented by the symbol and the motion of a matter wave is represented by the symbol u.

From eqs. (1.201) and (1.202) we put the value of $\nu\left(=\frac{mc^2}{h}\right)$ and $\lambda\left(=\frac{h}{m\mathrm{v}}\right)$ from the formula of matter wave in equation.

$$\therefore \quad u = \frac{mc^2}{h}\frac{h}{m\mathrm{v}} = \frac{c^2}{\mathrm{v}} \qquad (1.204) \quad \Rightarrow u \rangle \mathrm{v} \text{ since } \mathrm{v} \langle \mathrm{c}.$$

Properties of matter waves-

1. These waves are generated only when microscopic particles are in motion. If speed v of the particle is zero (i.e. $\mathrm{v}=0$) then the wavelength of matter wave $\lambda\left(=\frac{h}{m\mathrm{v}(=0)}\right)=\infty$ on the other hand if $\mathrm{v}=\infty$ then $\lambda=\frac{h}{m\mathrm{v}(=\infty)}=0$.
2. These waves are independent of nature of microscopic particles, i.e. either the particles are charged or neutral.
3. Speed of matter waves is always greater than the speed of light $c\left(=3\times10^{8}\ m/s\right)$, i.e. $\mathrm{v_p} \rangle c$.

Note- A matter wave cannot be split as electromagnetic waves do this.

Davisson-Germer and G.P. Thomson provided the experimental evidence for the de Broglie wave for slow electrons, respectively. C.J. Davisson and G.P. Thomson shared the Nobel Prize in 1937 for their work confirming matter waves through experiment.

Application of de Broglie wave-

Bohr's condition for the quantization of angular momentum

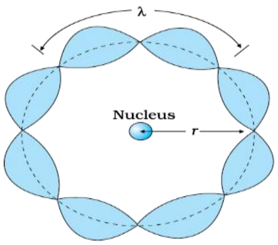
Let's say that an electron of mass is moving rapidly in the nth circular orbit of radius around the atom's nucleus (for example, a hydrogen atom). The de Broglie wave's wavelength can be calculated using the following formula:

$$\lambda_n=\frac{h}{m_e\,\mathrm{v_n}} \quad ....(ii)$$

Here, the motion of the electron can be thought as the wave of λ_n traveling along the circumference of the orbit. Thus, for a circular path its circumference is integral multiple of the wavelength, i.e.

$$2\pi r_n=n\lambda_n \quad ....(iii) \quad where\ n=1,2,3\cdots$$

$$2\pi r_n=n\frac{h}{m_e\,\mathrm{v_n}} \Rightarrow \boxed{J=m_e\,\mathrm{v_n}\,r_n=n\frac{h}{2\pi}=n\hbar}$$



(Courtesy to Google website) It represents Bohr's condition for the quantization of angular momentum

Example 1.101- Why do not we see the wave properties of a macroscopic object (e.g. baseball, cat, man, elephant, earth etc.)?

Solution 1.101- An object will appear wave like if it exhibits interference or diffraction pattern when its size 'a' is of the order of the wavelength λ, i.e. $a \approx \lambda$. But in case of macroscopic objects the essential condition of diffraction is not satisfied.

Example 1.102-Does, de Broglie hypothesis have any relevance to macroscopic matter?

Solution 1.102-de Broglie relation can be applied to both microscopic and macroscopic. For example A car (i.e. a macroscopic object) of mass 100 Kg is moving at a speed of 100 m/s then it will have de- Broglie Wavelength $\lambda = \frac{6.63\times10^{-34}}{100 \times100} = 6.63 \times 10^{-30} m$

The automobile is made up of very short wavelengths that match high frequencies. Particle-antiparticle annihilation occurs in waves below a given wavelength or above a certain frequency to produce mass. De Broglie wavelength or wave nature are therefore not apparent in macroscopic materials.

1.2 Phase velocity (or wave velocity) $\vec{v}_p$ **-** The velocity with which a point of constant phase moves is referred to as the phase velocity when a single wave with a fixed wavelength passes through a medium.

The formula for wave propagation along the positive x-axis is:

$$\psi\left(\vec{r}, t\right) = \psi_0 e^{\left(\omega t - \vec{k}\cdot\vec{r}\right)} \quad ....(1.201)$$

where ψ_0 is amplitude of the wave, $\vec{k}$ is wave vector, $\vec{r}$ is position vector and ω is angular frequency of the wave.

The phase of the wave is $\phi = \omega t - \vec{k}\cdot\vec{r}$

When the phase is constant at a point then $\omega t - \vec{k}\cdot\vec{r} = \phi_0$ (constant)

Or, $\vec{r} = \frac{\omega}{k} t - \phi_0 \quad ....(1.202)$

Thus, phase velocity $\vec{v}_p$ is given by:

$$\vec{v}_p = \frac{d\vec{r}}{dt} = \frac{\omega}{k}\hat{k} \quad ....(1.203) \Rightarrow \boxed{V_p = \frac{\omega}{k}}$$

The term "non-dispersive" (or "dispersive") media" refers to a medium in which a wave's wavelength is higher (or lower) than the distance between two adjacent particles in that medium. It is constant in a non-dispersive medium, meaning that waves of various frequencies and wavelengths move at the same speed. Examples- (i) Electromagnetic waves cannot disperse in empty space. (ii) Sound waves cannot disperse in the air. (iii) Transverse waves generated in a continuous string cannot disperse in it. Not continuous in a non-dispersive medium.

Group velocity (or particle velocity $\vec{v}$) $\vec{v}_g$ -From the relation between particle velocity $\vec{v}$ and de Broglie wave velocity $\vec{u}\left(=\vec{v}_p\right)$ we have:

$$u\left(=v_p\right) = \frac{c^2}{v} \quad \Rightarrow \quad v_p \rangle\, c \quad \left(\text{Since } v \langle\, c \text{ always.}\right)$$

The above term makes it very evident that a material particle cannot be compared to a single wave. Erwin Schrödinger was able to overcome this challenge. He made the assumption that the moving material particle is equivalent to a wave packet rather than a single wave. A collection of waves is known as a wave packet. The wavelength and speed of each wave are marginally different. Each wave's amplitude is selected in such a way that, within a limited area of space where the particle can be localized, they interfere constructively, and outside of this area, they interfere destructively. As a result, the amplitude of the resulting waves rapidly decreases to zero.

A wave packet is a discrete area of constructive interference created by superimposing two or more waves with similar amplitudes but slightly differing angular frequencies. Assume that these waves are traveling along the x-axis while having the same amplitude but slightly varying angular frequencies and wave numbers. Suppose that these two waves are represented mathematically as:

$$y_1 = a\sin\left(\omega t - kx\right) \quad ....(1.204)$$

$$y_1 = a\sin\left\{\left(\omega \pm \Delta\omega\right)t - \left(k \pm \Delta k\right)x\right\} \quad ....(1.205)$$

Applying the principle of superposition we have:

$$y = y_1 + y_2 = a\sin(\omega t - kx) + a\sin\{(\omega \pm \Delta\omega)t - (k \pm \Delta k)x\}$$

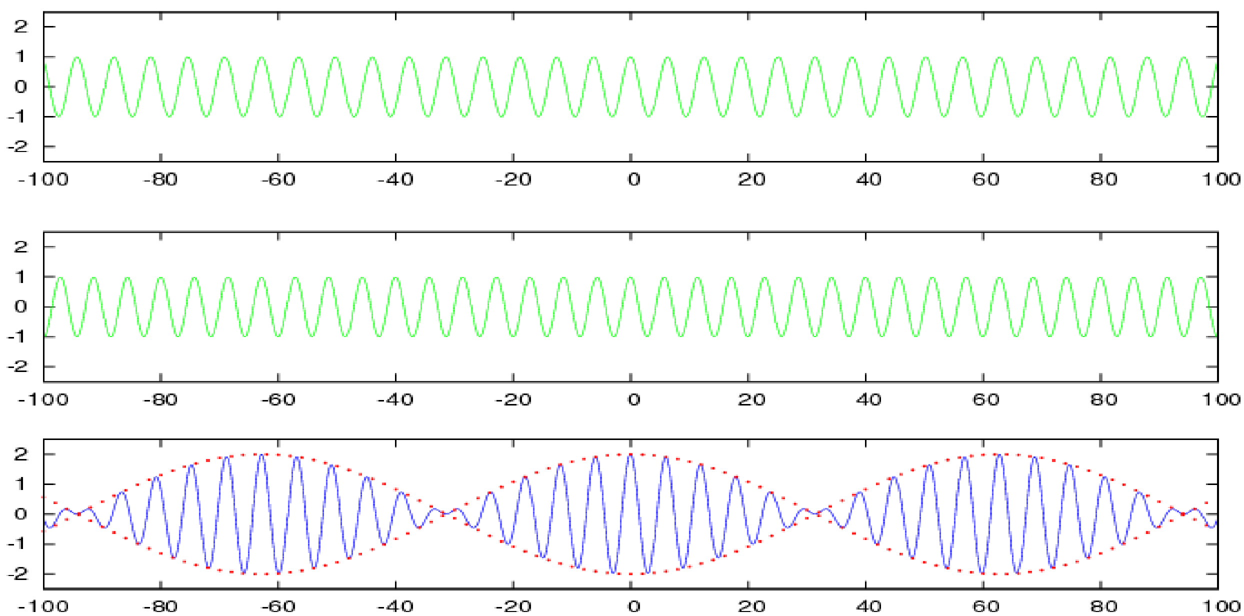
$$= 2a\sin\left[\frac{(\omega t - kx) + \{(\omega \pm \Delta\omega)t - (k \pm \Delta k)x\}}{2}\right]\cos\left[\frac{(\omega t - kx) - \{(\omega \pm \Delta\omega)t - (k \pm \Delta k)x\}}{2}\right]$$

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

Since $d\omega$ and dk are very small quantities, then $\omega + \frac{\Delta\omega}{2} \approx \omega$ and $k + \frac{\Delta k}{2} \approx k$. Thus, above equation becomes as:

$$y \approx 2a\sin[\omega t - kx]\cos\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right] = A\sin[\omega t - kx] \qquad \text{.........(1.206)}$$

where $A = 2a\cos\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right]$ is the amplitude of the wave packet. It changes both in space and time by a very slow-moving envelope of frequency $\frac{\Delta\omega}{2}$ and wave number $\frac{\Delta k}{2}$. It forms a standing wave which can be imagined by combining two identical waves moving in opposite directions. This represents <u>beats</u>. The phase of the wave packet is $[\omega t - kx]$



(Courtesy to Google website)

The observed velocity of the wave group or wave packet is called **group velocity** v_g. It is defined as:

$$\mathrm{v_g} = \frac{\Delta\,\omega/2}{\Delta k/2} = \frac{\Delta\,\omega}{\Delta k} \qquad \text{(For superposition of the two waves to form a wave packet.)}$$

(i) Relation between phase and group velocities- From the formula of phase velocity, we have the angular frequency $\omega = \mathrm{v_p}\, k$.

$$\mathrm{v_g} = \frac{d\,\omega}{d\,k} = \frac{d\,\mathrm{v_p}\,k}{d\,k} = \mathrm{v_p} + k\,\frac{d\,\mathrm{v_p}}{d\,k}$$

$$= \mathrm{v_p} + \frac{2\pi}{\lambda}\frac{d\,\mathrm{v_p}}{d\left(\frac{2\pi}{\lambda}\right)} = \mathrm{v_p} + \frac{2\pi}{\lambda}\frac{d\,\mathrm{v_p}}{\left(\frac{-2\pi}{\lambda^2}\right)d\,\lambda} \quad ....(1.06C) \quad \Rightarrow \quad \boxed{\mathrm{v_g} = \mathrm{v_p} - \lambda\frac{d\,\mathrm{v_p}}{d\,\lambda}}$$

For normal dispersive medium $\frac{d\,\mathrm{v_p}}{d\,\lambda}$ is positive. This shows that $\mathrm{v_g} \langle \ \mathrm{v_p}$.

For anomalous dispersive medium $\frac{d\,\mathrm{v_p}}{d\,\lambda}$ is negative. This shows that $\mathrm{v_g} \rangle \ \mathrm{v_p}$.

For non- dispersive medium $\frac{d\,\mathrm{v_p}}{d\,\lambda}$ is zero. This shows that $\mathrm{v_g} = \mathrm{v_p}$.

(ii) Relation between particle 'v', phase '$\mathrm{v_p}$' and group '$\mathrm{v_g}$' velocities- According to de Broglie hypothesis, a moving microscopic particle consists of a group of waves. The total energy 'E' and momentum 'p' of the particle are given

Case (i) relativistic mechanics: Total energy 'E' is given by

$$E = m\,c^2 \ \text{ or, } \ h\nu = \frac{m_0}{\sqrt{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2}}c^2 \quad \rightarrow \quad \nu = \frac{m_0}{h\sqrt{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2}}c^2 \qquad ....(1.207)$$

Angular frequency ω is given as:

$$\omega = 2\pi\nu = 2\pi\,\frac{m_0}{h\sqrt{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2}}c^2 = \frac{m_0\,c^2}{\hbar\sqrt{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2}} \quad ....(1.208), \qquad \text{where } \hbar = \frac{h}{2\pi}$$

$$\therefore \quad d\,\omega = \frac{m_0\,c^2}{\hbar}\frac{\left(-\frac{1}{2}\right)\left(\frac{-2\,\mathrm{v}}{c^2}\right)}{\left\{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2\right\}^{3/2}}\,d\,\mathrm{v} = \frac{m_0\,\mathrm{v}\,d\,\mathrm{v}}{\hbar\left\{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2\right\}^{3/2}} \qquad ....(1.209)$$

$$p = m\,\mathrm{v} = \frac{m_0\,\mathrm{v}}{\sqrt{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2}} \qquad ....(1.210)$$

Wave number k is given as:

$$k = \frac{2\pi}{\lambda} = \frac{2\pi\,p}{h} = \frac{m_0\,\mathrm{v}}{\hbar\sqrt{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2}} \qquad ....(1.211)$$

$$\therefore \quad d\,k = \frac{m_0}{\hbar}\left[\frac{\mathrm{v}\left(-\frac{1}{2}\right)\left(\frac{-2\,\mathrm{v}}{c^2}\right)}{\left\{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2\right\}^{3/2}}\,d\,\mathrm{v} + \frac{\mathrm{v}}{\sqrt{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2}}\,d\,\mathrm{v}\right] = \frac{m_0}{\hbar\left\{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2\right\}^{3/2}}\left[\left(\frac{\mathrm{v}}{c}\right)^2 + 1 - \left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2\right]$$

$$= \frac{m_0}{\hbar\left\{1-\left(\frac{\mathrm{v}}{\mathrm{c}}\right)^2\right\}^{3/2}}\,d\,\mathrm{v} \qquad ....(1.212)$$

On dividing eq. (1.211) from eq. (1.212), we have phase velocity

$$\boxed{\mathrm{v}_{\mathrm{g}} = \frac{d\,\omega}{d\,k} = \mathrm{v}}$$

$$\mathrm{v}_{\mathrm{p}} = \frac{\omega}{k} = \frac{2\pi\nu}{\frac{2\pi}{\lambda}} = \nu\,\lambda = \frac{m\,c^2}{h}\,\frac{h}{m\,\mathrm{v}\left(=\mathrm{v}_{\mathrm{g}}\right)} \Rightarrow \quad \boxed{\mathrm{v}_{\mathrm{p}}\,\mathrm{v}_{\mathrm{g}} = c^2}$$

Case (ii) In Non- relativistic mechanics: Total energy $'E'$ is given by

$$E = h\nu = \frac{1}{2}m\,\mathrm{v}^2 \quad \rightarrow \nu = \frac{m\,\mathrm{v}^2}{2\,h} \qquad ....(1.213)$$

From de Broglie concept, we have:

$$\lambda = \frac{h}{p} = \frac{h}{m\mathrm{v}(= \mathrm{v_g})} \quad ....(1.214)$$

The phase velocity is given by:

$$\mathrm{v_p} = \frac{\omega}{k} = \frac{2\pi\nu}{\frac{2\pi}{\lambda}} = \nu\lambda = \frac{m\,\mathrm{v_g}^2}{2\,h}\frac{h}{m\mathrm{v}_g} \Rightarrow \boxed{\mathrm{v_p} = \frac{\mathrm{v}_p}{2}}$$

Ex. 1.201- Calculate the phase velocity given by $\boldsymbol{E_x = E_0 \cos(\omega t - kz)\, A/m}$ with a frequency of 5 GHz and a wavelength in the material medium of 3.0 cm is

Sol. 1.201- Given: $\nu = 5\ GHz = 5\ X10^9 Hz, \lambda = 3.0\ cm$ & $c = 3\ X10^8\ m/s$

$$\mathbf{v}_{\boldsymbol{p}} = \frac{\boldsymbol{\omega}\ (= \boldsymbol{2\pi\nu})}{\boldsymbol{k}\ (= \frac{\boldsymbol{2\pi}}{\lambda})} = \boldsymbol{\nu}\lambda = 5X10^9\ X\ .03 = \mathbf{1.5\ X10^8 \boldsymbol{m/s} = \boldsymbol{c}/2}$$

Ex. 1.202- Estimate the phase velocity of a wave having a group velocity of 6 x 10^6 is

Sol. 1.202- Given: $\mathrm{v}_g = 6\boldsymbol{X}\ \mathbf{10^6}\ m/s$

$$\mathrm{v}_p\mathrm{v}_g = c^2\ or\ \mathrm{v}_p = \frac{c^2}{\mathrm{v}_g} = \frac{(3X\ 10^8)^2}{6X\ 10^6} = \frac{3X\ 10^{10}}{2} = 1.5\ X\ 10^{10} = \mathbf{150\ \boldsymbol{X}\ 10^8\ \boldsymbol{m/s}}$$

Q.1.203 1 MHz plane wave travelling in a dispersive medium has a phase velocity $\mathbf{3 \times 10^8} \boldsymbol{m/s}$. The phase velocity as a function of wavelength is given by$\mathbf{v}_{\boldsymbol{p}} = \boldsymbol{K}\sqrt{\boldsymbol{\lambda}}$, where K is a constant. Calculate the group velocity.

Sol. 1.203 -Given: f = 1 MHz, $\mathrm{v}_p = 3 \times 10^8\ m/s$&$\mathrm{v}_p = K\sqrt{\lambda}$

$$\mathrm{v}_g = \mathrm{v}_p - \lambda\frac{d\mathrm{v}_p}{d\lambda} = K\sqrt{\lambda} - \lambda\frac{dK\sqrt{\lambda}}{d\lambda} = K\sqrt{\lambda} - \lambda K\frac{1}{2}\frac{1}{\sqrt{\lambda}} = \frac{K\sqrt{\lambda}}{2}$$

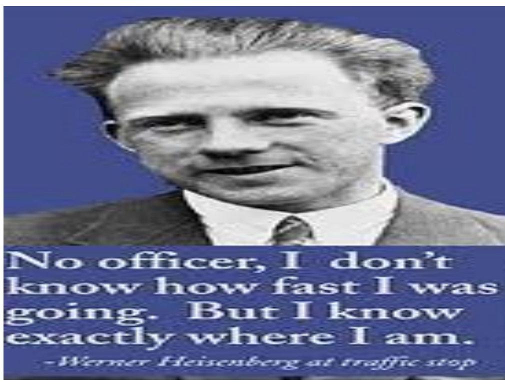
$$= \frac{\mathrm{v}_p}{2} = \frac{3 \times 10^8}{2} = \mathbf{1.5 \times 10^8}\ \boldsymbol{m/s}$$

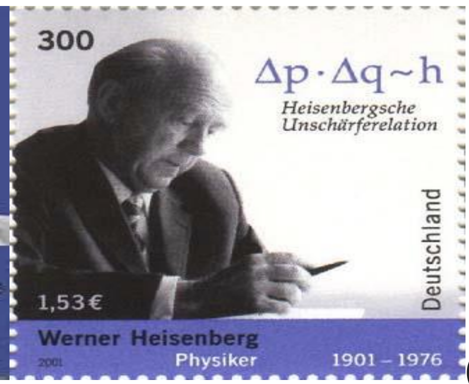
1.3 Heisenberg's uncertainty principle (or the principle of indeterminacy) –

Werner Karl Heisenberg [5th December, 1901 – 1st February, 1976]- Werner Karl Heisenberg was a German theoretical physicist and philosopher who **discovered (1925) a way** to formulate quantum mechanics in terms of matrices. In 1927 he published his uncertainty principle. He got **Nobel Prize** in Physics **1932** for this work.**(Curtsey of Google)**

In case of microscopic particles it is impossible to determine exactly the position $\left(\vec{r}\right)$ and momentum $\left(\vec{p}\right)$ of them simultaneously. Heisenberg's approach was to quantum mechanics as being matrix algebra. Similarly, some others canonical variables (e.g. energy (E) and time (t); angular momentum $\left(\vec{J}\right)$ and angular displacement (θ)) cannot be determined simultaneously. Heisenberg's uncertainty relations are: $\Delta p \, \Delta r \geq \frac{\hbar}{2}$**,** $\Delta E_k \, \Delta t \geq \frac{\hbar}{2}$ **&** $\Delta J \Delta \theta \geq \frac{\hbar}{2}$ where Δ denotes uncertainty

There is an interesting story of Heisenberg, when he was driving a vehicle very fast and suddenly the beaked his at red light, he is stopped by a policeman then his answer is quoted in fellow as:





(Curtsey of Google)

Applications of Heisenberg's uncertainty principle-

1. Electrons cannot exists inside a nucleus
2. Existence of protons and neutrons inside the nucleus of an atom
3. Radius of Bohr's first orbit
4. Binding energy of an electron in an atom
5. Zero point energy of a harmonic oscillator
6. Zero point energy of a particle in one dimensional box
7. Finite value for the natural width of a spectral line

1.4 Wave function and its Physical interpretation-

Max Born (11 December 1882 – 5 January 1970) was a German physicist and mathematician who developed quantum mechanics. He won the 1954 Nobel Prize in Physics for his "fundamental research in quantum mechanics, especially in the statistical interpretation of the wave function". **The term "quantum mechanics" is due to Born.** He also made contributions to solid-state physics and optics and supervised the work of a number of notable physicists in the 1920s and 1930s.**(Curtsey of Google)**

The height of the water surface (or level) fluctuates periodically in a water wave. The quantity that changes on a regular basis in a sound wave is the medium's pressure. Similar to this, a variable quantity in a matter wave is referred to as a wave function. Greek letter is used to indicate it. phi 'ψ'. The value of the wave function associated with a moving microscopic particle in particular position (x, y, z) and time 't' is concerned to the finding the probability there. Thus, displacement of a de Broglie wave is a wave function of space and time, i.e. $\psi(x, y, z, t)$. In general, a wave function $\psi(x, y, z, t)$ is a complex quantity (real and imaginary parts). Let ψ is represented as:

$$\psi\left(\vec{r}, t\right) = A + iB = \psi_0 e^{i\left(\vec{k}\cdot\vec{r} - \omega t\right)} \qquad \ldots\ldots (1.401)$$

where, A and B are real functions; ψ_0 is amplitude of the wave; $\vec{k}$ is wave vector; $\vec{r}\left(= x\hat{i} + y\hat{j} + z\hat{k}\right)$ is position vector. The complex conjugate of ψ is given as:

$$\psi^*\left(\vec{r}, t\right) = A - iB = \psi_0\, e^{-i\left(\vec{k}\cdot\vec{r} - \omega t\right)} \qquad \ldots\ldots.(1.402)$$

$$\therefore \quad \psi\left(\vec{r}, t\right)\psi^*\left(\vec{r}, t\right) = (A + iB)(A - iB) = A^2 + iAB - iAB + B^2 = A^2 + B^2 = (\psi_0)^2$$

It implies that probability is always real and positive quantity.

Although it is hard to pinpoint a minuscule particle's location, it is possible to determine the odds of seeing it in any given location. The quantity $|\psi|^2 \left(= \psi^* \psi\right)$, the square of the absolute value of ψ, shows the intensity of matter wave. **Probability density** represents probability of finding the particle in a given unit volume at a given instant of time. Wave function ψ itself is not a measurable quantity but its probability density $|\psi|^2$ is measurable. **Note-**The displacement of any matter wave may be positive, negative or zero at any time but its **probability can never negative**.

The complex nature of the wave function ψ is no concern to us. Here, we are interested only in a single dimension (say x- axis) along the observing direction and for a given time.

Max Born interpretation of wave function ψ -The probability that a particle will be found in the infinitesimal interval dx about the point x, denoted by $p(x)dx$ is

$$P(x)\,dx = \psi^*(x,t)\,\psi(x,t)\,dx \qquad \text{......(1.403)}$$

where $\psi^*(x,t)$ is complex conjugate of $\psi(x,t)$.

The probability that a particle be in a particular space and time must lie between 0 (i.e. the particle is not there) and 1 (i.e. the particle is there). Let us consider an intermediate probability is 0.3, i.e. there is 30% chance of finding the particle in the given space and time. The probability that the particle will be found in a certain region $(x_1 - x_2)$ is the integral of the probability density over the region is given by:

$$\boxed{P_{x_1,\,x_2} = \int_{x_1}^{x_2} |\psi|^2\, dx}$$

For a microscopic object, if the probability of finding the object over all space is finite then it is somewhere, i.e.

$$\int_{x_1,y_1,z_1=-\infty_1}^{x_2,y_2,z_2=\infty_2} |\psi|^2\, dx = 1 \quad \Rightarrow \text{Normalization condition of a wave function}$$

Besides being nonmalleable of the wave function ψ , it must be single valued, since the probability density has only one particular value at a certain place and time and continuous. Every wave function can be normalized by multiplying it by a proper constant.

$$\int_{x_1,y_1,z_1=-\infty_1}^{x_2,y_2,z_2=\infty_2} |\psi|^2\, dx = K \neq 0$$ $\Rightarrow$ ψ is not normalized. It can be normalized if ψ is divided by the square root of the constant K, i.e. $\sqrt{K}$.

$$\int_{x_1,y_1,z_1=-\infty_1}^{x_2,y_2,z_2=\infty_2} |\psi|^2\, dx = 0 \quad \Rightarrow \text{Orthogonality condition for the wave function.}$$

This shows that the particle does not exist there.

• A wave function must meet the following requirements in order to be considered acceptable across a certain interval:

(1) ψ Must be continuous and single valued everywhere.

(2) Its partial derivatives i.e. $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}$ *and* $\frac{\partial\psi}{\partial z}$ must be continuous and single valued everywhere.

(3) ψ Must be nonmalleable i.e. it must has a finite value 1.

(4) ψ Must be a solution of Schrödinger's wave equation.

Physical significance of a wave function $\psi\left(\vec{r}, t\right)$- A wave function describes how a particle behaves at a specific place (r) and time (t). Where there is a high likelihood of discovering the particle, the wave function has a big magnitude, and the opposite is also true. As a result, a wave function calculates the likelihood of a particle being in a specific location.

Applications of wave functions-

(i) To determine probability of finding a particle in a given space.

(ii) To determine average or expectation value of a physical observable quantity f is given as:

$$< f > = \frac{\int_{-\infty}^{\infty} \psi^*(\mathrm{r,t}) f_{op} \psi(\mathrm{r,t})\, \mathrm{d}\tau}{\int_{-\infty}^{\infty} \psi^*(\mathrm{r,t}) \psi(\mathrm{r,t})\, \mathrm{d}\tau} \quad \cdots\cdots (1.404\ ii) \text{where} \mathrm{d}\tau = \mathrm{dx\ dydz}$$

In case of normalized wave function $\int_{-\infty}^{\infty} \psi^*(\mathrm{r,t}) \psi(\mathrm{r,t})\, \mathrm{d}\tau = 1$ the denominator of the above expression becomes unity, then

$$< f > = \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t})\ f_{op} \psi(\mathrm{r,t})\, \mathrm{d}\tau$$

Examples: (i) Expectation value of position vector $\boldsymbol{r}$**:**

$$< r > = \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t})\ \mathrm{r}\ \psi(\mathrm{r,t})\, \mathrm{d}\tau == \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t})\ (\mathrm{x}\hat{\imath} + \mathrm{y}\hat{\jmath} + \mathrm{z}\hat{k})\ \ \psi(\mathrm{r,t})\, \mathrm{d}\tau$$

(ii) Expectation value of momentum or velocity $\boldsymbol{p}$ **or v:**

$$< p > = \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t}) \boldsymbol{p}_{op} \psi(\mathrm{r,t}) \mathrm{d}\tau = \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t})(-i\hbar\nabla) \psi(\mathrm{r,t}) \mathrm{d}\tau$$

$$= -i\hbar \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t}) \left(\frac{\partial}{\partial x}\hat{\imath} + \frac{\partial}{\partial y}\hat{\jmath} + \frac{\partial}{\partial z}\hat{k}\right) \psi(\mathrm{r,t})\, \mathrm{d\tau}$$

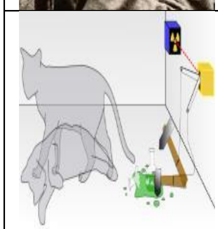
(iii) Expectation value of total energy E:

$$< E > = \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t})\ E_{op}\psi(\mathrm{r,t})\, \mathrm{d\tau} = \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t}) \left(i\hbar\frac{\partial}{\partial t}\right) \psi(\mathrm{r,t})\mathrm{d\tau}$$

$$= i\hbar \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t}) \left(\frac{\partial}{\partial t}\right) \psi(\mathrm{r,t})\, \mathrm{d\tau}$$

(iv) Expectation value of potential V: $< V > = \int_{-\infty}^{\infty} \psi^*(\mathrm{r,t})\ \mathrm{V(r)}\ \psi(\mathrm{r,t})\, \mathrm{d\tau}$

1.5Time-dependent Schrödinger wave equation-

	**Erwin Rudolf Josef Alexander Schrödinger** [12 August 1887 – 4 January 1961, Austrian theoretical Physicist]- Schrödinger, along with Paul Dirac, won the Nobel Prize in Physics in 1933 for his work on quantum mechanics. He is most known for his "Schrödinger's cat or Quantum Cat" thought experiment. He is known as father of wave function and cosmologist.**(Curtsey of Google)**
	**Schrödinger's cat or Quantum Cat-** It is not a reality but a paradox that after consuming the poison by the cat there is certain probability of the live or alive. This concept is used in case of probability of finding a particle: across a barrier, outside the finitely deep potential well etc. which is impossible in real sense. (**Curtsey of Google)**

According to de- Broglie concept a matter wave is associated to a moving particle. The wavelength of the matter wave is given as:

$$\lambda = \frac{h}{p}\ or, p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k \ \ ......(1.501)$$

Where p is momentum of the particle, h is Planck's constant, $k\left(=\frac{2\pi}{\lambda}\right)$ wave number and $\hbar\left(=\frac{h}{2\pi}\right)$.

According to Planck- Einstein energy relation total energy (E) of the particle is given by:

$E = h\nu = \frac{h}{2\pi}\ 2\pi\nu = \ \hbar\omega\ \ ......(1.502)$ where $\omega\left(=2\pi\nu\right)$ is angular frequency of the wave.

Motion of the particle along positive x-axis is given as:

$$\Psi(\vec{x},t) = \Psi_0 e^{i(\overrightarrow{k_x}\cdot\,\vec{x} - \omega t)} \ldots\ldots (i)$$

Putting the value of k and ω from equation (1.501) and equation (1502) in equation(i), we get.

$$\Psi(\vec{x},t) = \Psi_0 e^{\frac{i}{\hbar}(\overrightarrow{p_x}\cdot\vec{x}-Et)} \text{......}(1.503)$$

where $\psi(\vec{x},t)$ is **wave function** which is a complex and measurable quantity taken in quantum mechanics, ψ_0 is initial amplitude of the wave and i = √-1

On partially differentiating equation (1.0703) w.r.t. 'x', we get.

$$\frac{\partial\psi(\vec{x},t)}{\partial x} = \psi_0 \frac{ip_x}{\hbar} e^{\frac{i}{\hbar}(\vec{p}_x\cdot\vec{x}-Et)} = \frac{ip_x}{\hbar}\psi(\vec{x},t)$$

On multiplying by 'i' on both sides in above equation and arrange it, we have.

$$i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial x} = -p_x\Psi(\vec{x},t) \text{......}(1.504) \Rightarrow \boxed{(p_x)_{op} = -i\hbar\frac{\partial}{\partial x}}$$ Operator form of momentum

On partially differentiating equation (1.0803) w.r.t. 't', we get:

$$\frac{\partial\Psi(\vec{x},t)}{\partial t} = \Psi_0\left(-\frac{i}{\hbar}E\right)e^{\frac{i}{\hbar}(\overrightarrow{p_x}\cdot\vec{x}-Et)} = -\frac{i}{\hbar}E\,\Psi(\vec{x},t)\cdots\cdots(1.505)$$

On multiplying by 'i' on both sides in above equation and arrange it, we have:

$$i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial x} = E\,\Psi(\vec{x},t)\text{......}(1.506) \Rightarrow \boxed{E_{op} = i\hbar\frac{\partial}{\partial t}}$$ Operator form of energy

In <u>non-relativistic case</u> total energy of the particle is the sum of kinetic energy (K.E.) plus potential energy (P.E. or U) given as:

$E = K.E. + P.E. = \frac{p^2}{2m} + U\,(x,t)\cdots(ii)$ where m is the mass of the particle.

Multiplying on both sides in above equation, we have:

$$E\Psi(\vec{x},t) = \frac{p^2}{2m}\Psi(\vec{x},t) + U\,\Psi(\vec{x},t) \quad \cdots\cdots(1.507)$$

Now, putting the value of E and p in operator form in above equation we have:

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

It is Schrödinger's time dependent equation in one dimensional motion of the particle. It can be given in three-dimensional motion of the particle by replacing $\frac{\partial}{\partial x} \rightarrow \nabla \left(= \frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial x}\hat{j} + \frac{\partial}{\partial x}\hat{k} \right)$ and $\vec{x} \rightarrow \vec{r}$ then above equation becomes as:

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi(\vec{r},t) + U(\vec{r},t)\psi(\vec{r},t)$$ **It is 3-D time dependent Schrödinger Wave Equation**

Time-independent Schrödinger wave equation-

If the potential energy is a function of position only, i.e. $U(r)$, then the time dependent SWE is separable. Thus, a plane monochromatic wave can be written as:

$$\psi\left(\vec{r}, t\right) = = \psi_0\, e^{\frac{i}{\hbar}\left(\vec{p}\cdot\vec{r} - Et\right)} = \psi_0\, e^{\frac{i}{\hbar}\left(\vec{p}\cdot\vec{r}\right)}\; e^{\frac{i}{\hbar}(-Et)} = R(r)T\;(t) \quad ...... \quad (1.508)$$

where, $R(r) = \psi_0\; e^{\frac{i}{\hbar}\left(\vec{p}\cdot\vec{r}\right)}$ and $T\;(t) = e^{\frac{i}{\hbar}(-Et)}$

Using eq. (1.508) in3-D time dependent Schrödinger Wave Equation, we get:

$$i\hbar \frac{\partial R(r)T(t)}{\partial t} = \left[\frac{-\hbar^2}{2m}\nabla^2 + U(r)\right]R(r)T(t)$$

Or, $i\hbar R(r)\frac{\partial\, T(t)}{\partial t} = \frac{-\hbar^2}{2m}T(t)\,\nabla^2 R(r) + U(r)R(r)T(t)$

On dividing in above equation by $\psi\left(\vec{r}, t\right) = R(r)T\;(t)$, we get:

$$i\hbar \frac{R(r)}{R(r)T(t)}\frac{\partial\, e^{\frac{i}{\hbar}(-Et)}}{\partial t} = \frac{-\hbar^2}{2m}\frac{T(t)}{R(r)T(t)}\;\nabla^2 R(r) + U(r)$$

or, $i\hbar \frac{1}{T(t)}\left(\frac{-iE}{\hbar}\right)T(t) = \frac{-\hbar^2}{2m}\frac{1}{R(r)}\;\nabla^2 R(r) + U(r)$

$$E\,R(r) = \frac{-\hbar^2}{2m}\nabla^2 R(r) + U(r)R(r) = H\,R(r)$$

Applications of Time independent

1. Motion of a particle in one dimensional infinitely deep potential well-

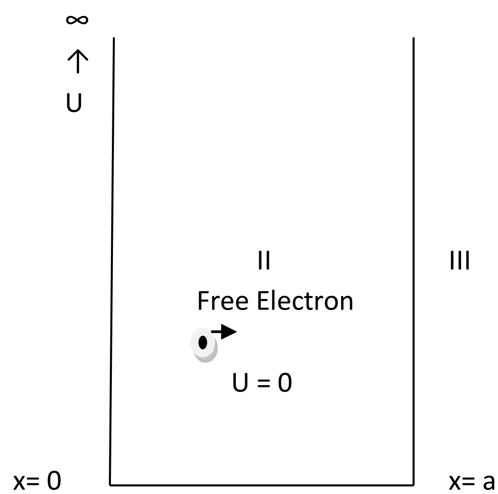
A particle is restricted to one dimensional motion between the barriers of length $'a'$. The height of the potential barriers goes to infinity. The one dimensional region $-\infty \langle x \langle \infty$ can be divided into three parts (I, II and III) (Fig. 1.5 a). To solve this problem we use initial and boundary conditions.

Initial conditions- $U(x)=\infty \quad \text{for } x \langle 0 \text{ and } x \rangle a \quad .....(i)$

$U(x)=0 \quad \text{for } 0 \langle x \langle a \quad ....(ii)$

Boundary conditions- $\psi(x)=0 \quad at\ x=0 \quad .....(iii)$

$\psi(x)=0 \quad at\ x=a \qquad (iv)$



- In regions I and III the **time independent** SWE is given as:

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}(E-\infty)\psi(x)=0 \quad ......(1.501)$$

Fig. 1.5 a- Motion of a free electron in infinitely deep potential well

As $U(x)\rightarrow\infty$ at the boundaries of the potential well then $\psi(x)\rightarrow 0$. Therefore, LHS also becomes zero so the above equation is ignored because its both sides become zero.

In region II the time independent SWE is given as:

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

$$Let \quad k^2=\frac{2mE}{\hbar^2} \quad ....(v)$$

or, $$\frac{d^2\psi(x)}{dx^2}+k^2\,\psi(x)=0 \quad ....(1.502)$$

Here, it is convenient to write the solution of eq. (1.602) as a sum of sine and cosine than as a sum of exponential terms, i.e.

$$\psi(x)=A\cos kx+B\sin kx \quad ....(vi)$$

On applying boundary condition (eq. iii) in the wave function, we have:

$\psi(0) = A\cos k0 + B\sin k0$, or $0 = A$

$\therefore \quad \psi(x) = B\sin kx \qquad (1.503)$

On applying boundary condition (eq. iv) in the wave function, we have:

$\psi(a) = B\sin ka$

or, $0 = B\sin ka \quad \Rightarrow B \neq 0$ Otherwise wave function will be zero.

$\therefore \quad \sin ka = 0 = \sin n\pi$

or, $k = \dfrac{n\pi}{a}$ ......(1.504), where, $n = 1, 2, 3\ldots \quad but\ n \neq 0$

Substituting the value of k from eq. (1.504) in eq. (1.503), we have:

$$\psi(x) = B\sin\frac{n\pi}{a}x \quad ......(1.504)$$

Substituting the value of k from eq. (2.604) in eq. (v), we have:

$$E = \frac{\left(\frac{n\pi}{a}\right)^2 \hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad ....(1.505) \Rightarrow \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

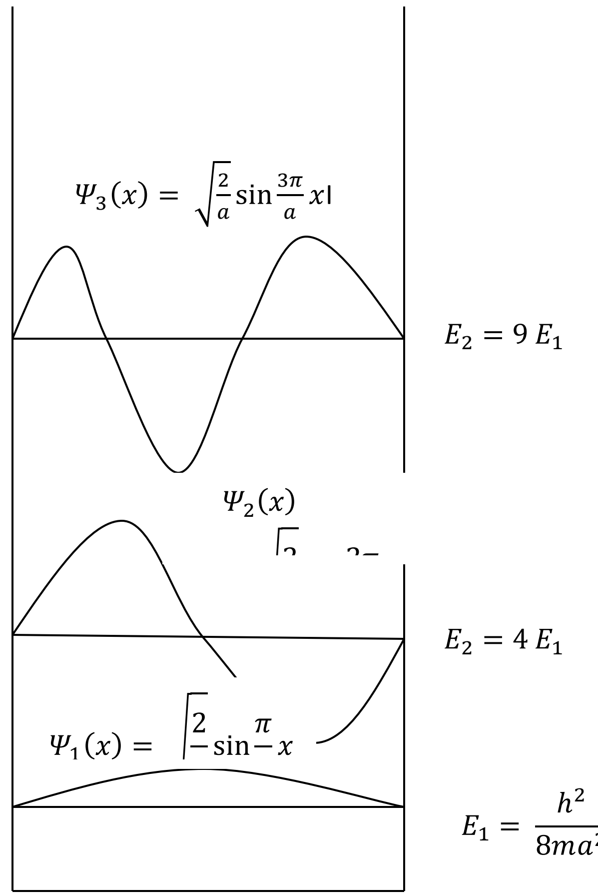


Fig.1.6 b Eigen functions & Eigen values in infinitely deep potential well

To calculate the wave function, we must normalize the wave function, i.e.

$$\int_0^a \psi^*(x)\,\psi(x)\,dx = 1$$

$$\text{or, } 1 = \int_0^a B^2\sin^2\frac{n\pi}{a}x\,dx = \frac{B^2}{2}\int_0^a\left(1 - \cos\frac{2n\pi}{a}x\right)dx = \frac{B^2}{2}\left[x - \frac{a}{2n\pi}\sin\frac{2n\pi}{a}x\right]_0^a$$

$$= \frac{B^2}{2}\left[(a-0) - \frac{a}{2n\pi}(\sin 0 - \sin 2n\pi)\right] = \frac{B^2}{2}a \text{ or, } \quad B = \sqrt{\frac{2}{a}} \quad ......(1.506)$$

Substituting the value of B from eq. (1.606) in eq. (1.604), we get:

$$\psi(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x \quad ....(1.507) \quad \Rightarrow \quad \boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x}$$

Wave or Eigen function corresponding to n[th] energy level is given by:

2. Motion of a particle in three dimensional infinitely deep potential wells-

It is the application of time independent SWE. Here, the wave function must be a function of three spatial coordinates, i.e. $\psi(x, y, z)$ only. Thus, the SWE is given as:

$$E\psi\,(x,y,z)=\frac{-\hbar^2}{2m}\nabla^2\psi\,(x,y,z)+U(r)\psi\,(x,y,z) \quad ....(1.508)$$

Here, we assume that a particle can only move in three dimensions between obstacles of length, and along the x, y, and z axes, respectively, or it can move freely inside a box with the dimensions (a, b, and c). We utilize the same method as when we used a one-dimensional infinitely deep potential well to solve this problem (identify wave functions and energy levels). The wave functions must be 0 at the walls and beyond because the box's closed walls are infinite potential barriers. So, with U = 0, we resolve the SWE inside the box. Inside the box, the particle is unconfined. As a result, the wave functions' x, y, and z dependent portions must be independent of one another. The result of the equation above is:

$$E\psi\,(x,y,z)=\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi\,(x,y,z) \quad ....(1.508\ a)$$

Its solution is given as:

$$\psi\,(x,y,z)=A\sin(k_1\,x)\sin(k_2\,y)\,\sin(k_3\,z) \quad ....(1.509)$$

where A is a normalization constant. The quantities $k_i\ (i=1,2,3)$ are determined by applying boundary conditions.

$\psi = 0$ at $x = a$, $y = b$ and $z = c$, we have:

$$k_1=\frac{n_1\,\pi}{a},\ k_2=\frac{n_2\,\pi}{b} \text{ and } k_3=\frac{n_3\,\pi}{c}$$

where n_1, n_2 and n_3 are integers whose values varies 1,2,3 ……

Thus, we have

$$\psi\,(x,y,z)=A\sin\left(\frac{n_1\,\pi}{a}x\right)\sin\left(\frac{n_2\,\pi}{b}y\right)\,\sin\left(\frac{n_3\,\pi}{c}z\right) \quad ....(1.510)$$

On partially differentiating eq. (1.509) w.r.t. x, we get:

$$\frac{\partial \psi}{\partial x} = A k_1 \cos(k_1 x) \sin(k_2 y) \sin(k_3 z)$$

and $\frac{\partial^2 \psi}{\partial x^2} = -A(k_1)^2 \sin(k_1 x) \sin(k_2 y) \sin(k_3 z) = -(k_1)^2 \psi$ ....$(1.511a)$

Similarly we get:

$$\frac{\partial^2 \psi}{\partial y^2} = -(k_2)^2 \psi \quad ....(1.511b)$$

$$E\psi(x,y,z) = \frac{-\hbar^2}{2m}\left[-\left\{(k_1)^2 + (k_2)^2 + (k_3)^2\right\}\right]\psi = \frac{\hbar^2}{2m}\left\{\left(\frac{n_1 \pi}{a}\right)^2 + \left(\frac{n_2 \pi}{b}\right)^2 + \left(\frac{n_3 \pi}{c}\right)^2\right\}\psi$$

$$\boxed{E_{n_1,n_2,n_3} = \frac{\hbar^2 \pi^2}{2m}\left\{\left(\frac{n_1}{a}\right)^2 + \left(\frac{n_2}{b}\right)^2 + \left(\frac{n_3}{c}\right)^2\right\} \quad ....(1.512)}$$

For cubical box $a = b = c$ we have $E_{n_1,n_2,n_3} = \frac{\hbar^2 \pi^2}{2ma^2}\left\{(n_1)^2 + (n_2)^2 + (n_3)^2\right\}$ and

$$\psi(x,y,z) = A \sin\left(\frac{n_1 \pi}{a} x\right) \sin\left(\frac{n_2 \pi}{a} y\right) \sin\left(\frac{n_3 \pi}{a} z\right).$$

For ground state $n_1 = 1 = n_2 = n_3$ we have: $E_{1,1,1} = \frac{3\hbar^2 \pi^2}{2ma^2}$ and

$$\psi_{1,1,1}(x,y,z) = A \sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{\pi}{a} y\right) \sin\left(\frac{\pi}{a} z\right).$$

For first excited state $n_1 = 2,\ n_2 = 1\ and\ n_3 = 1;\ n_1 = 1,\ n_2 = 2\ and\ n_3 = 1$ or $n_1 = 1,\ n_2 = 1\ and\ n_3 = 2$ we have $E_{2,1,1} = E_{1,2,1} = E_{1,1,2} = \frac{3\hbar^2 \pi^2}{ma^2}$ and

$$\psi_{2,1,1}(x,y,z) = A \sin\left(\frac{2\pi}{a} x\right) \sin\left(\frac{\pi}{a} y\right) \sin\left(\frac{\pi}{a} z\right)$$

$$\psi_{1,1,1}(x,y,z) = A \sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{\pi}{a} y\right) \sin\left(\frac{\pi}{a} z\right)$$

$$\psi_{1,1,2}\,(x,y,z) = A\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{\pi}{a}y\right)\sin\left(\frac{2\pi}{a}z\right)$$

As a result, the first excited state, which is a threefold degenerate state, corresponds to three wave functions. When there are several wave functions for a given energy, an energy state or level is said to be degenerate. The symmetry of the cube in this instance is what causes the degeneracy. Degeneracy is caused by specific features of the potential energy function. '$U\left(\vec{r}\right)$' which explain the system. The degeneracy can be eliminated by a perturbation of potential energy. Degeneracy can also be eliminated by adding external magnetic (Zeeman effect) or electric (Stark effect) fields. If the box had three unequal sides, such as a cuboids', the degeneracy would also be eliminated because the three quantum numbers (211, 121, and 112) would produce three distinct energies. Degeneracy can also be found in classical systems, such as planetary motion, where orbits with varying eccentricities may have the same energy.

Qualitative analysis of finite potential well-

Finite potential wells are potential wells with a finite depth. A one-dimensional finite square well potential is comparable to an infinite one, except in this case we allow the potential to be finite in regions I and III while remaining zero in regions II. The time independent SWE for regions I and III is given as:

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

or, $\frac{d^2\psi\,(x)}{d\,x^2} = \frac{2m}{\hbar^2}\{U - E\}\psi\,(x) = \alpha^2\,\psi\,(x)$......(1.513) where $\alpha^2 = \frac{2m}{\hbar^2}\{U - E\}$ is a constant. It (α^2) is positive because $U \rangle E$. The solution of eq. (1.513) has exponential forms $e^{\alpha x}$ and $e^{-\alpha x}$. The positive exponential must be rejected in region III where $x \rangle a$ to keep $\psi_{III}\,(x)$ finite as $x \to \infty$; similarly the negative exponential must be rejected in region I where $x \langle 0$ to keep $\psi_I\,(x)$ finite as $x \to -\infty$. Thus we have $\psi_I\,(x) = A\,e^{\alpha x}$ and $\psi_{III}\,(x) = B\,e^{-\alpha x}$. The coefficients A and B are determined by matching these wave functions smoothly onto the wave function in the interior of the well. We require $\psi\,(x)$ and its first derivative $\frac{d\,\psi\,(x)}{d\,x}$ to be continuous at $x = 0$ and $x = a$. This can be done only for certain value of E which corresponds to allowed energies for the bound particles. The wave functions join smoothly at the boundaries of the potential well. Figure 2.7 b shows the wave functions and probability densities corresponding to three lowest allowed particle energies. Wave function $\psi\,(x)$ is nonzero at the walls increases the de Broglie wave outside the well.

In the region II, time independent SWE is given as:

$$\frac{d^2\psi_{II}(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi_{II}(x) = -k^2\psi_{II}(x) ....(1.514)$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$

Instead of sinusoidal solution of solution of eq. (2.702), we write it in term of exponential as:

$$\psi_{II} = C\,e^{ikx} + D\,e^{-ikx} \qquad (i)$$

On applying boundary conditions, i.e. $\psi(x) = 0 \quad at\ x = 0\ and\ x = a$ we get quantized energy values E_n and particular wave functions $\psi_n(x)$. The particle has a finite probability of being outside the well. Here, the wave functions join smoothly at the edge of the well and approach zero exponentially outside the well. The occurrence of the particle outside the well is prohibited classically, but it occurs in quantum mechanics. Because of the exponentially decrease of the wave functions $\psi_I(x)$ and $\psi_{III}(x)$. The probability of the particle penetrates a distance greater than $\delta \approx \frac{1}{\alpha}$ being to decrease remarkably. The distance δ is known as **penetration depth**.

$$\delta \approx \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m\{U - E\}}} \quad \Rightarrow \delta \propto \frac{1}{\sqrt{U-E}}$$

If $U = \infty$ then $\delta = 0$, i.e. the wave function will not come out in case of infinitely deep potential well. For first energy state E_1, $U - E_1$ is very large therefore δ_1 is small. For second energy state E_2, $U - E_2$ is smaller than $U - E_1$ therefore δ_2 is larger than δ_1.

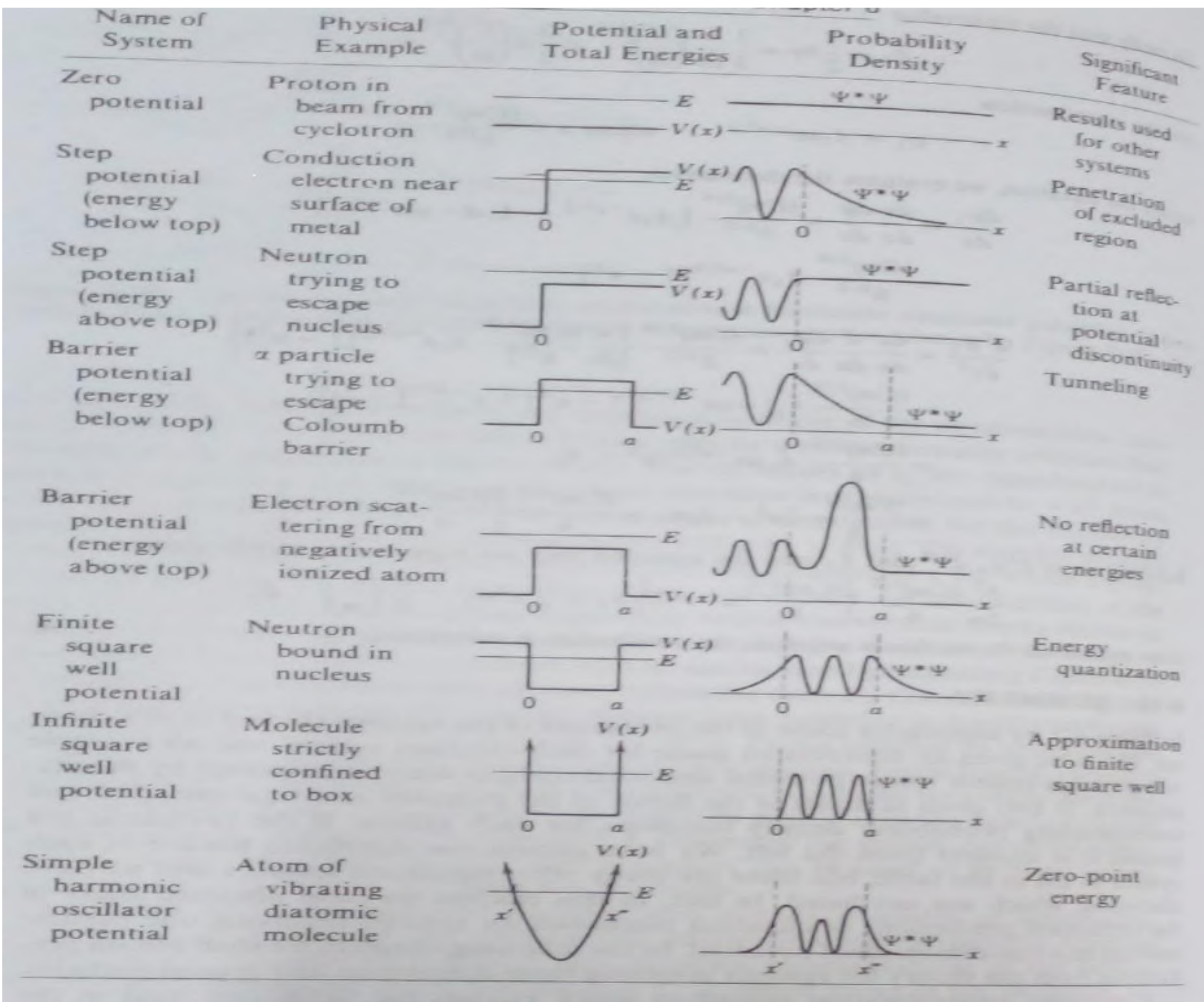
It is clear from above equation that the penetration length is proportional to Planck's constant h which violets the concept of classical physics. This result is also consistent (or favorable) with the uncertainty principle because in order for the particle to be in the well, the uncertainty ΔE of the energy must be very large. This can occur only for very short period of time Δt according to Heisenberg's uncertainty relation (i.e. $\Delta E \Delta t \geq \hbar/2$). At a distance δ beyond the well, the amplitude of the wave function has fallen to $1/e$ of its value at the boundaries and approaches zero exponentially in the regions I and III. Thus, the exterior wave is necessarily zero beyond penetration depth on either side of the potential well. In case of electrons tunneling through semiconductors and nuclear alpha decay the value of penetration depth is $10/\alpha$ and $20/\alpha$.

Here, the allowed energies are given by the expression of energy by replacing $a \rightarrow a + 2\,\delta$, i.e.

$$E_n = \frac{n^2\,\pi^2\,\hbar^2}{2\,m\left(a + 2\,\delta\right)^2} \qquad n = 1,\ 2,\ 3, \ldots$$

It is clear from eq. (2.703) and eq. (2.704) δ is energy dependent and smaller than length a of the well. The approximation is best for the lower- lying states and breaks down completely as E approaches U, where δ becomes infinite. Thus, the particles with energies $E \rangle U$ are not bound to the well, i.e. they may be found with comparable probability in the exterior regions I and III.

Eigen Functions and Eigen values in various cases are shown in below figure-



(From Quantum Physics of Atom, Molecules, Solids, Nuclei & Particles **Robert Eisberg& Robert Resnick)**

References:

1. Quantum Physics of Atom, Molecules, Solids, Nuclei & Particles-by **Robert Eisberg& Robert Resnick**; Wiley

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3. Modern Physics by **Raymond A. Sevey, Clement Moses and Curl Moyer,**Tomson Brooks/ Cole, Cengage Learning

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