Quantum Mechanics

Gravitational lensing proves mass energy equivalence.

→ Length contraction
→ ↑ in mass
→ Time dilation

Limitations of Classical Mechanics:

(i) Photoelectric effect:

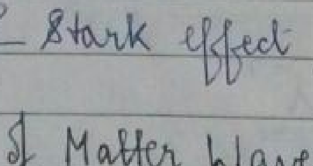
$$h\nu = W_0 + \frac{1}{2}mv^2$$

Acc to classical theory, Light imparts momentum greater the intensity, greater will be the velocity with which liberated e^- will travel

(ii) BlackBody Radiation:

Radiation ~~wavelength~~ emitted by black body depends only on temperature $\boxed{T \propto \lambda^4}$

(iii) Compton Effect:



$\nu > \nu'$

(iv) Size of atom:

(v) Zeeman & Stark effect.

★ Properties of Matter Waves:

→ Neither longitudinal, nor transverse It is a probability wave ⟨Theoretical wave⟩

★ wave group/wave packet can be described in terms of superposition of individual waves of different wavelengths. The interference of these waves gives variation in amplitude defining the shape of the wave group.

★ wave velocity or phase velocity, $\boxed{v_p = \frac{c^2}{v_{particle}} = \frac{\omega}{k}}$

$$y_1 = a \sin(\omega_1 t - k_1 x)$$
$$y_2 = a \sin(\omega_2 t - k_2 x)$$
$$y = y_1 + y_2$$
$$= 2a \sin\left\{\frac{\omega_1+\omega_2}{2}(t) - \frac{k_1+k_2}{2}(x)\right\} \cdot$$
$$\cos\left\{\frac{\omega_1-\omega_2}{2}(t) - \frac{(k_1-k_2)}{2}(x)\right\}$$

Group velocity: $v_g = \frac{d\omega}{dk}$

$$E = h\nu = \frac{h}{2\pi} 2\pi\nu = \hbar\omega \quad -(1)$$

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

$$p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k \quad -(2)$$

$$E = \frac{p^2}{2m}$$

$$\cancel{\hbar}\omega = \frac{\hbar^2 k^2}{2m}$$

$$\omega = \frac{\hbar k^2}{2m}$$

$$\frac{d\omega}{dk} = \frac{\hbar k}{m} = \frac{p}{m} = V_{particle}$$

★ Relation b/w group & phase velo

$$\boxed{V_g = V_p - \lambda\frac{dV_p}{d\lambda}}$$

Heisenberg Uncertainity Principle

You cannot make a measurement with 100% accuracy.

★ $\boxed{\Delta x \cdot \Delta p \geq h}$

~~Schrodinger's Wave Equation:~~

~~(i) Time Independent Wave Eqⁿ:~~

Wave Function (ψ):

The quantity whose periodic variations make up the matter wave is called wave function ψ.

The value of ψ at a particular point (x, y, z) in space at time 't' is related to the probability of finding the particle there at that time.

→ ψ should be <u>normalized</u> wave function so that <u>$|\psi|^2$ will</u> represent probability

→ ψ should be a <u>single valued</u> funcⁿ at every point in space as probability is also a single valued funcⁿ.

→ ψ must be <u>finite</u> at each & every point in space

→ ψ must be <u>continuous</u> in the region where it is defined.

→ The first order derivatives of ψ, i.e. $\frac{\partial \psi}{\partial x}$, $\frac{\partial \psi}{\partial y}$ & $\frac{\partial \psi}{\partial z}$ must be continuous in the region where ψ is defined.

ψ itself does not have any direct physical significance & is not an experimentally measurable quantity.

→ The probability of finding the particle described by the wave function ψ at a point (x, y, z) in space at time 't' is directly proportional to the value of $|\psi|^2$ at that point at time 't'.

* The probability of finding the particle in a certain volume element $dv = dx\, dy\, dz$ is $\boxed{|\psi|^2 dv}$ which is called the $\boxed{\text{probability density}}$ if $|\psi|^2$ represents probability.

* As the particle has to exist somewhere in space, <u>the total probability of finding the particle is 1</u>

$$\boxed{H\psi = E\psi}$$

$$\boxed{\int_{-\infty}^{\infty} |\psi|^2 dv = 1} \quad \text{--- (1)}$$

In Gen. the wave functions obtained as solutions of differential equations do not satisfy this.

Instead $\boxed{\int_{-\infty}^{\infty} |\psi|^2 dv = N^2}$

Normalized wave func^n^ ψ_N is then constructed from ψ as:

$$\boxed{\psi_N = \frac{\psi}{N}}$$

The normalized wave function ψ_N satisfies (1) so that $|\psi_N|^2$ represents probability.

Schrodinger's time Independent Wave Equation

The general differential eq^n^ for a wave with wave function travelling with velocity 'u' in three dimensions is:

$$\frac{\partial^2 \psi}{\partial t^2} = u^2\left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}\right]$$

Laplace operator $\leftarrow \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

$$\rightarrow \boxed{\frac{\partial^2 \psi}{\partial t^2} = u^2 \nabla^2 \psi} \quad \text{--- (1')}$$

The general sol^n^ of (1) is of the form:

$$\boxed{\psi(x, y, z, t) = \psi_0 (x, y, z) e^{-i\omega t}}$$

$\psi_0 \rightarrow$ Amplitude of wave at pt. (x, y, z)

It can also be written as: $\boxed{\psi(\vec{r}, t) = \psi_0 (\vec{r}) e^{-i\omega t}}$

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$$

Differentiating this eq partially w.r.t. 't' twice:

$$\frac{\partial \psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \psi}{\partial t^2} = (-i\omega)(-i\omega)\,\psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi_0 e^{-i\omega t}$$

Now, $\psi = \psi_0 e^{-i\omega t}$

$$\rightarrow \boxed{\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi}$$

∴ Substituting in (1)

$$\boxed{-\omega^2 \psi = u^2 \nabla^2 \psi}$$

$$\nabla^2 \psi + \frac{\omega^2}{u^2}\psi = 0 \quad \text{— (2)}$$

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

$$\frac{\omega}{u} = \frac{2\pi}{\lambda}$$

$$\rightarrow \frac{\omega^2}{u^2} = \frac{4\pi^2}{\lambda^2}$$

From De Broglie Hypothesis for matter waves:

$$\lambda = \frac{h}{p} \rightarrow \lambda^2 = \frac{h^2}{p^2}$$

★ Total energy 'E' of a particle is sum of its kinetic energy ($\frac{1}{2}mv^2$) & potential energy $\langle V \rangle$

$$E = \frac{1}{2}mv^2 + V = \frac{m^2v^2}{2m} + V$$

$$\rightarrow E = \frac{p^2}{2m} + V$$

$$\rightarrow p^2 = 2m\langle E - V \rangle$$

$$\therefore \boxed{\lambda^2 = \frac{h^2}{2m\langle E - V \rangle}}$$

$$\rightarrow \frac{\omega^2}{u^2} = \frac{4\pi^2 \times 2m\langle E-V\rangle}{h^2}$$

$$\rightarrow \boxed{\frac{\omega^2}{u^2} = \frac{8\pi^2 m}{h^2}\langle E-V\rangle}$$

Substituting in (2), $\boxed{\nabla^2\psi + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0}$

Schrodinger's Time Independent Wave Eqⁿ

or $\frac{h}{2\pi} = \hbar$

$$\rightarrow \boxed{\nabla^2\psi + \frac{2m}{\hbar^2}\langle E-V\rangle\psi = 0}$$

Schrodinger's Time Dependent Wave Eqⁿ

The general differential eqⁿ for a wave with wave funcⁿ ψ, travelling with velocity 'u' in three dimensions is:

$$\frac{\partial^2\psi}{\partial t^2} = u^2\left[\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right]$$

$$\rightarrow \boxed{\frac{\partial^2\psi}{\partial t^2} = u^2\nabla^2\psi}$$

Gen. solⁿ of the differential eqⁿ is: $\psi(x,y,z,t) = \psi_0(x,y,z)e^{-i\omega t}$

$\psi_0 \rightarrow$ Amplitude of wave at (x,y,z)

$$\boxed{\psi(\vec{r},t) = \psi_0(\vec{r})e^{-i\omega t}}$$

↳ Differentiating partially w.r.t. 't':

$$\frac{\partial\psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t}$$

$$\psi = \psi_0 e^{-i\omega t}$$

$$\rightarrow \frac{\partial\psi}{\partial t} = -i\omega\psi$$

$$\rightarrow \omega = 2\pi\nu = 2\pi\frac{E}{h}$$

$$\rightarrow \frac{\partial\psi}{\partial t} = -i\frac{2\pi E}{h}\psi$$

$$E\psi = \frac{-h}{i2\pi}\frac{\partial\psi}{\partial t}$$

$$\rightarrow E\psi = \frac{ih}{2\pi}\frac{\partial\psi}{\partial t} \quad \text{--- (1)}$$

Schrodinger's time independent wave eqⁿ: $\nabla^2\psi + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$

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

$$\rightarrow \boxed{\frac{-h^2}{8\pi^2 m}\nabla^2\psi + V\psi = E\psi}$$

Substituting in (1),

$$\boxed{\frac{-h^2}{8\pi^2 m}\nabla^2\psi + V\psi = \frac{ih}{2\pi}\frac{\partial\psi}{\partial t}}$$

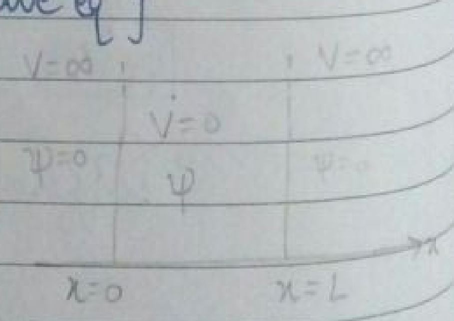
Schrodinger's time dependent wave eqⁿ

Particle in a Rigid Box (Infinite Potential Well)

{Applⁿ of Schrodinger's wave eqⁿ}

Taking potential energy of the particle to be infinite at & beyond the walls:

★ $V = \infty$ for $x \leq 0$ & $x \geq L$



The potential energy of the particle is constant inside the box which can be taken to be zero.

→ Energy & Wave func^n are obtained

★ $V=0$ for ~~...~~ $0<x<L$

★ It is as if the particle is inside an <u>infinite potential well</u> As the particle does not exist at the walls & beyond them:

$$\psi = 0 \quad \text{for} \quad x \le 0 \ \& \ x \ge L$$

The wave func^n exists only for $0<x<L$

Schrodinger's time independent wave eq^n:

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

As it is a problem in one dimension along x-axis.

★ $\nabla^2\psi$ can be replaced by $\frac{\partial^2\psi}{\partial x^2}$

Also substituting $V=0$ for $0<x<L$

$$\rightarrow \frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}E\psi = 0$$

★ Let $\boxed{K^2 = \frac{8\pi^2 mE}{h^2}}$

$$\rightarrow \frac{\partial^2\psi}{\partial x^2} + K^2\psi = 0$$

General sol^n of the eq^n is:

★ $\boxed{\psi = A\sin Kx + B\cos Kx}$

A & B → arbitrary constants → ~~can~~ to be determined using boundary conditions.

First Boundary Condition: $\psi = 0$ at $x=0$

$$\rightarrow 0 = A\sin 0 + B\cos 0$$

$$\rightarrow \boxed{B=0}$$

★ $\therefore \boxed{\psi = A\sin Kx}$

Second Boundary Condition: $\psi = 0$ at $x=L$

$$\rightarrow 0 = A\sin KL$$

★★ <u>$A\neq 0$</u> as for $A=0$, $\psi=0$ for all values of x which will mean particle does not exist inside the box.

★ Classically, the probability of finding a particle ... box is ... at every point in the box whereas quantum mechanically, probability of finding the particle will depend on the energy of the particle.

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$\rightarrow \sin KL = 0$

$\rightarrow \boxed{KL = n\pi}$

$\rightarrow K = \frac{n\pi}{L}$

$\rightarrow \frac{8\pi^2 m}{h^2} E = \frac{n^2\pi^2}{L^2}$

$\rightarrow \boxed{E_n = \frac{n^2 h^2}{8mL^2}}$

Smallest possible value of Energy, $E = \frac{h^2}{8mL^2}$ which is non-zero

★ → This contradicts classical mechanics according to which particle can have zero energy.

★ → The energy values are discrete, not continuous as expected from classical mechanics.

These discrete energy values are known as Energy Eigen values

$\because \boxed{K = \frac{n\pi}{L}}$

we have, $\boxed{\psi = A \sin\left(\frac{n\pi x}{L}\right)}$

The complex conjugate of ψ is: $\psi^* = A \sin\left(\frac{n\pi x}{L}\right)$

To normalize the wave function, we find: $\int_0^L \psi\psi^* dx$

$$\rightarrow \int_0^L \psi\psi^* dx = \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx$$

$$= A^2 \int_0^L \left\{\frac{1 - \cos 2\left(\frac{n\pi x}{L}\right)}{2}\right\} dx$$

$$= \frac{A^2}{2}\left[x - \frac{\sin\left(\frac{2n\pi x}{L}\right)}{\left(\frac{2n\pi}{L}\right)}\right]_0^L$$

$\hbar \gg$

Quantum Mechanics (discrete) — Classical Mechanics (continuous)

$$\rightarrow \boxed{\int_0^L \psi\psi^* \, dx = \frac{A^2 L}{2}}$$

Let RHS be N^2

$$\rightarrow N^2 = \frac{A^2 L}{2}$$

$$\rightarrow \boxed{N = A\sqrt{\frac{L}{2}}}$$

Normalized wave function, $\psi_N = \frac{\psi}{N}$

$$\rightarrow \boxed{\psi_N = \frac{A \sin\left(\frac{n\pi x}{L}\right)}{A\sqrt{\frac{L}{2}}}}$$

$$\rightarrow \boxed{\psi_N = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}} \rightarrow \text{wave func}^n$$

These normalized wave functions are called Eigen functi

Probability function is: $P(x) = |\psi_N|^2 = \psi_N \psi_N^* = \boxed{\frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right)}$

→ {Probability func^n & wave func^n graphs}

Particle in a Non-Rigid Box
{Finite Potential Well}

Particle of mass 'm' is confined to a non-rigid box of length 'L'

As the walls are not rigid, the potential energy of the particle would be finite → V_0

Inside the box, potential energy is constant, taken to be zero.

★ We consider the case where $E < V_0$ i.e, particle energy is less th the energy required to overcome barrier represented by the walls

Schrodinger's time independent wave equation in one dimension is:

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

In region I, $V = V_0$ & $\psi = \psi_I$

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

As $E < V_0 \rightarrow E - V_0 < 0$

$\therefore$ let $\frac{8\pi^2 m}{h^2}(E-V_0) = -(K')^2$

$$\rightarrow \boxed{\frac{\partial^2 \psi_I}{\partial x^2} - K'^2 \psi_I = 0}$$

The general solⁿ of this eqⁿ is:

$$\boxed{\psi_I = Ae^{K'x} + Be^{-K'x}}$$

$\psi_I \rightarrow 0$ as $x \rightarrow -\infty$

$\rightarrow B = 0$

$$\rightarrow \boxed{\psi_I = Ae^{K'x}}$$

In region II, $V = 0$ & $\psi = \psi_{II}$

$$\rightarrow \frac{\partial^2 \psi_{II}}{\partial x^2} + \frac{8\pi^2 m}{h^2} E \psi_{II} = 0$$

let $K^2 = \frac{8\pi^2 m E}{h^2}$

$$\rightarrow \frac{\partial^2 \psi_{II}}{\partial x^2} + K^2 \psi_{II} = 0$$

Gen solⁿ of this eqⁿ is:

$$\boxed{\psi_{II} = Ce^{iKx} + De^{-iKx}}$$

In region III, $V = V_0$ & $\psi = \psi_{III}$

$$\rightarrow \frac{\partial^2 \psi_{III}}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V_0)\psi_{III} = 0$$

$$\rightarrow \frac{\partial^2 \psi_{III}}{\partial x^2} - (K')^2 \psi_{III} = 0$$

Gen sol^n of this eq^n is : $\boxed{\psi_{III} = Fe^{K'x} + Ge^{-K'x}}$

$\psi_{III} \to 0$ as $x \to \infty$

$\rightarrow \boxed{F = 0}$

★ $\boxed{\psi_{III} = Ge^{-K'x}}$

★ Boundary Conditions to be imposed on the wave func^n are :

(i) Continuity of wave function at $x=0$:

$$[\psi_I]_{x=0} = [\psi_{II}]_{x=0}$$

(ii) Continuity of wave func^n at $x=L$:

$$[\psi_{II}]_{x=L} = [\psi_{III}]_{x=L}$$

(iii) Continuity of first order derivative of wave func^n at $x=0$:

$$\left[\frac{d\psi_I}{dx}\right]_{x=0} = \left[\frac{d\psi_{II}}{dx}\right]_{x=0}$$

(iv) Continuity of first order derivative of wave func^n at $x=L$:

$$\left[\frac{d\psi_{II}}{dx}\right]_{x=L} = \left[\frac{d\psi_{III}}{dx}\right]_{x=L}$$

Using these four boundary conditions, the four arbitrary constants A, C, D & G can be evaluated to obtain solution for ψ_I, ψ_{II} & ψ_{III}.

∵ Wall is not rigid, wave func^n will not end at the wall. It extends slightly behind the wall.

★ Probability of finding the particle is non-zero at the walls of the box.

★ Energy of the particle is less than that of the barrier but it can still come out, not by breaking the barrier. This phenomena is known as **Tunneling**

Thinner the potential barrier, greater will be the probability of the particle breaking out,

Thicker the potential barrier, lesser will be the probability of the particle breaking out

ex. $\boxed{\alpha\text{-decay}}$ & $\boxed{\beta\text{-decay}}$

The particle can touch the wall in this case so there is probability of it existing in the neighbourhood of the wall & then there is a probability that it can come outside the box

Probability of escape is 1 in 10^{56} (low but finite)

Tunnel Diode

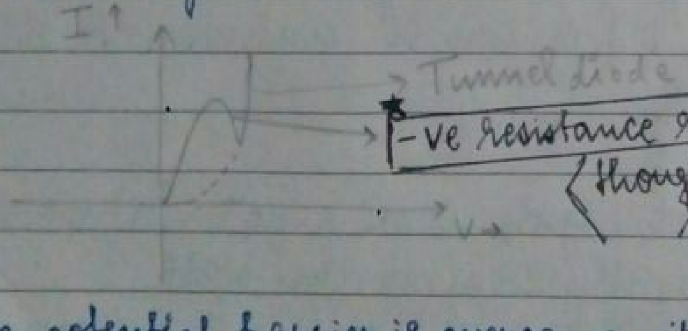
The energy of the particle is less than the barrier but it still manages to get through. It does not break the barrier instead tunnels through it.

In tunnel diode, this tunneling effect is increased by increasing the doping.

Normal diode → 1 in 10^6 base atoms

Tunnel diode → 1 in 10^3 base atoms

On ↑ doping, barrier ↑ but width of depletion region ↓ so particles can tunnel through.



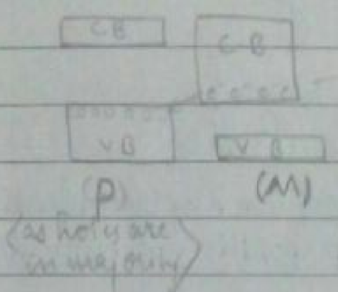
$\boxed{\text{-ve resistance region}}$ (though the voltage is ↑, current still ↓)

Once the potential barrier is overcome, it behaves like a normal diode.

They are used for $\boxed{\text{high frequency operation}}$ (as it is a quantum phenomena, it takes place very quickly)

★ Because of negative resistance region, it can be used a $\boxed{\text{Switch}}$

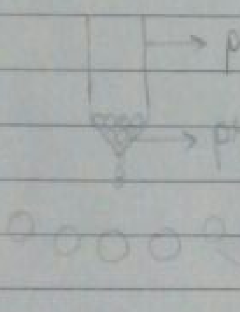
★ They are not affected by radiations so they find applications in Space Technology.



★★ { These e⁻ keep combining with the holes & current keeps ↑
Once all the holes are neutralised, current starts ↓
& -ve resistance region is obtained }

★ Scanning Tunneling Electron Microscope

Based on Tunneling effect



→ piezoelectric stylus

→ probe (very very fine) at the bottom, it is just one atom thick

[piezoelectric effect: when pressure is applied, charges are produced. Converse is true: the applying charges, surface can be under stress]

→ The stylus is moved on the surface of molecules.

From the probe, the e⁻ tunnel onto the surface. The space b/w the probe & surface behaves like a $\boxed{\text{potential barrier}}$.

★ More e⁻ will be tunneled when the gap is less & more current passes through.

★ As current ↑, the stylus contracts & pulls the probe upwards. The stylus has been designed for a constant value of current. As the dist ↑, current ↓ so in order to maintain constant current, the stylus pushes the probe downwards.

Scanning is done line by line {line by line tracing}

[Perception of height is also obtained due to this & 3D image is obtained]

Non conductors have to be coated with conductors to be observed under STM eg, gold.

Quantum Computing

Have 3 bits → 0, 1, anything b/w 0 & 1

So they are known as Qubits

D wave computers are based on superconductivity.

★ Quantum computing involves superposition & entanglement of Qu...

★ In STM, some charge is given to the lower surface as well in order to have the e⁻ tunnel to it

★ The energy in ~~non~~ $\boxed{\text{rigid box}}$ will be $\boxed{\text{greater}}$ than non rigid box