Quantum Mechanics

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Content

- de Broglie’s hypothesis
- Heisenberg’s uncertainty principle
- Schrodinger’s time independent equation
- Particle in a rigid box
- Particle in a non-rigid box

Syllabus

Introduction, **importance of quantum mechanics in engineering and technology**, duality of radiation, failure of classical physics, De Broglie's hypothesis, Characteristics of De Broglie waves, De Broglie wavelength, applications of De Broglie's hypothesis (why electron microscope is better than optical microscope),
Concept of phase velocity and group velocity in brief , introduction to Heisenberg's uncertainty principle and its explanation using concept of wavegroups
Proving Heisenberg's uncertainty principle using electron diffraction experiment Wave function & its physical interpretation
Schrodinger's time independent equation
Particle in a rigid box (energy quantization and eigen functions) , particle in 3D box just to be mentioned
Particle in a non-rigid box (qualitative, without derivation), tunnel effect and list of it's applications

Introduction

- No one Had a aim to build quantum mechanics
- It built by itself
- Historical period of 1897 to 1940 where the ideas of quantum mechanics evolved and settled
- Niels Bohr, de Broglie, Werner Heisenberg, Erwin Schrödinger, Max Born, Wolfgang Pauli, Paul Dirac
- Quantum mechanics plays a decisive role when technology becomes delicate

Role of QM in Technology

- Invention of Transistor – Reduced size, cost, and power consumption of an electronic gadget
- High precession microscopes -SEM, TEM, STEM, AFM
- LASER
- SQUID
- Single electron transistor
- Photonics- Photon based electronics
- Spintronics-electron spin based electronics (Quantum Computers)
- Nanotechnology
- Molecular electronics

Failure of Classical Physics

- Newtonian classical theorams failed to explain behaviour of atoms, molecules or electronics
- In an atom negatively charged electrons revolving around positively charged nucleus
  - According to classical picture, there should be electrostatic force of attraction between them.thus they should come close to each other and collapse.
  - The electron move arround the nucleus, it will experiance a centripetal acceleration. WKT any accelerated charged particleradiates energy in the form of electromagnetic wave. Therefor the energy of of the electron should decrease continously and collapse
- This tells that atom is unstable.
- Here c**lassical mechanics fails** to explain stability of an atom

Wave Particle Duality

- James clerk Maxwell predicted that light is an electromagnetic wave.
- This prediction, gave birth to several optical instruments from microscopes to telescope, Interferometers to difractometer
- The experimentally observed black body Spectrum was not being completely explained using wave theory. The
- formele developed using wave theory could explain limited part of the experimentally observed black body spectrum. But Max Planck came with an idea that the black body could emit and absorb the radiation not continously and not in the form of waves but in a quantized manner or particle like manner
- The quanta (Packets of Energy) absorbed/ emitted by a black body have on Energy $E=h\nu$
- This explained phenomenon such as Photo electric effect, Compton effect, emission and absorption of radiation, etc.

- Hence one conclude that the electromagnetic radiation has dual characters
- In certain situations it exhibits wave properties andin other behaves like particle
- These properties can never be observed simaltaneously
- To study the path of a beam of monochromatic radiation, We use wave theory,
- while calculating energy transaction of the same beam we use particle theory (Photon)
- It is difficult to separate wave and particle aspects of electromagnetic radiation
- This ability of electromagnetic radiation to manifest itself as wave or particle is known as **wave particle dualism**

De-Broglie Hypothesis

- A mooving particle always has a wave associated with it and the motion of a particle is guided by wave in a similar manner as photon

  i.e. materials also have wave like properties called de-Broglie waves or matter waves

  for photon energy (E)

$$E = h\nu = hc/\lambda$$

For Particle

$$E = mc^2 = pc$$

$$hc/\lambda = pc$$

$$\lambda = h/p$$

Wavelength of the de-Broglie wave

WKT Kinetic Energy (K.E.)

$$K.E. = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

$$P = \sqrt{2mK}$$

$$\lambda = \frac{h}{\sqrt{2mK}}$$

If a charged particle of charge **q** and mass m is accelerated with a potential difference **V**, then the electrostatic work done on the charged particle is converted in to its kinetic energy

- is given by

$$\frac{1}{2}mv^2 = qV$$

$$\lambda = \frac{h}{\sqrt{2mqV}} \qquad \lambda = \frac{12.26}{\sqrt{V}} A^o$$

m --- mass of charged particle

charged particles --- proton, deuteron, and alpha particle

$$P = \sqrt{2mK}$$

$$\lambda = \frac{h}{\sqrt{2mK}}$$

- The wave associated with moving particle are called as matter waves or de-broglie waves
- From the above relation,
- The mass of the body increases, its wavelength tends to zero

  the wavelength of macroscopic bodies is insignificant incomparision to the size of the bodies themselves even at very low velocities
- Among the electromagnetic radiations, low energy radiation is like radio waves (1eV) have higher wavelengths and high energy radiations like gamma rays (1Mev) have considerly smaller wavelengths
- i.e as we move from energy lower to higher, the wave nature reduces partical nature increases

The subatomic world is restless

- Ground state energy of any sub atomic particle can not be zero

$$\lambda = h / p$$

- if P $\longrightarrow$ 0 then λ $\longrightarrow \infty$

  ie any sub atomic particle which exist in finite regions such as atoms, molecules de-Broglie wavelength cannot be infinite

  ie can not be greater than size of an object in which it exists

- Therefor sub atomic particle is restless
- **Extreemly small value of Planck’s constant allow us to take rest**

- if we consider a cricket ball of 500gm flying with velocity of 50km/hr.

  Then its wavelength

  $\lambda = (6.62 \text{ X } 10^{-34}) / (0.5 \text{ X } 13.9) = 10^{-34} \text{ m} = 10^{-24}$ Å

- Which insignificant in comparision to size of the ball

  ie wave process does not affect the interaction between macroscopic bodies

- The waves associated with particles are not real 3-D waves like sound waves

- **They are probability waves**

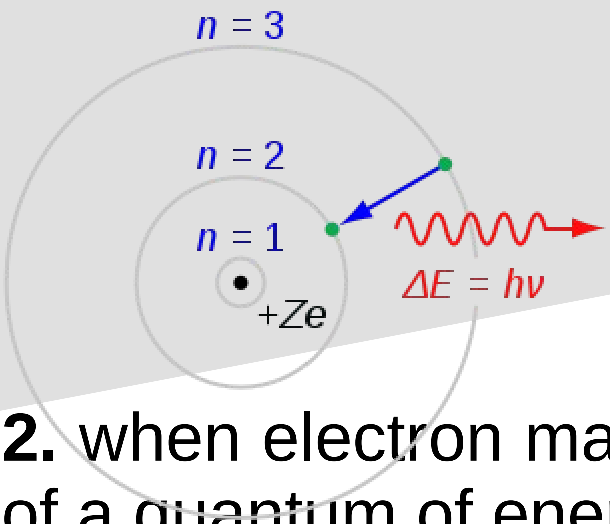
- Probability of finding the particles in various places and with various properties

de-Broglie Hypothesis and Bohr Model

de-Broglie’s Hypothesis is consistent with quantization of Bohr orbits

- **Bohr Postulates**
- The orbits of electrons in the atom are quantized. Only those orbits are possible where the angular momentum (L), radius (r) and energy (E) is given by

$$L = n\frac{h}{2\pi} = n\hbar \qquad r = 0.511 n^2 A^o \qquad E_n = -\frac{13.6}{n^2}\,\text{eV}$$



2. when electron makes transition from upper to lower orbit, Emission of a quantum of energy (photon) takes palce, .

orbits of electrons are quantized

Explains the observed **spectrum of the hydrogen atom**,

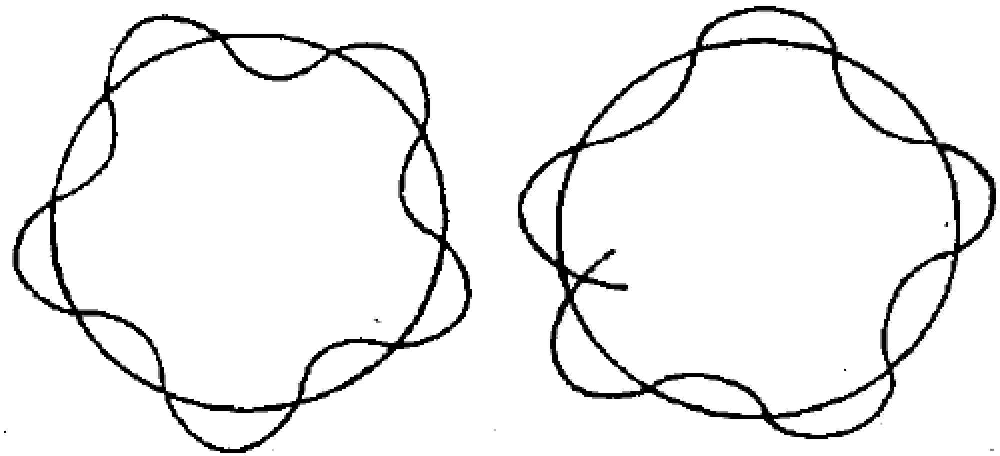
No explanation to the why electron rotates only certain allowed orbits

No explaination why electron does not emit radiation in stationery-allowed orbit.

Bohr's model supported from de Broglie's hypothesis, which treats electrons as waves

If electron, as a wave is to be smoothly fitted in the orbit, then following relation must be satisfied

$$\textit{Total length of the orbit} = \textit{circumference} = \qquad 2\pi r = n\lambda$$



$$2\pi r = n\frac{h}{p}$$

$$rp = n\frac{h}{2\pi}$$

$$\text{angular momentum } L = n\hbar$$

This gives the condition for existence of Bohr's allowed orbits

This confirms that the idea of quantization which was first applied to radiation, extends to matter

This confirms de Broglie's hypothesis

An Experimental Proof To de-Broglie's Hypothesis

Electrons can be diffracted and their wavelength can be measured

Davisson and Germer and G.P Thomson- **electron diffraction experiments**

Davisson and Germer diffracted the electrons thorough nickel crystal and found that electrons, after scattering through Bragg planes of the **Nickel crystal**, produced well defined diffraction patterns.

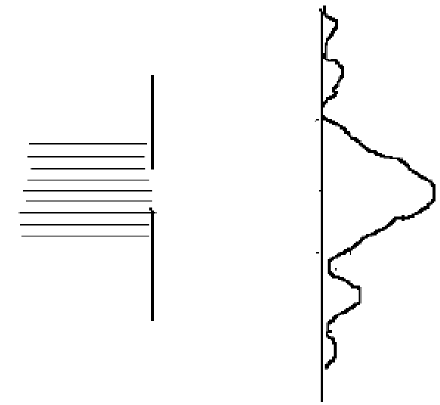
By measuring angle of diffraction (θ) and substituting it in the Bragg's relation

$$2d\sin\theta = n\lambda$$

they found that this **wavelength was 1.67Å**
it correctly matched with the wavelength calculated from **de-Broglie relation**

In Thomson's experiments also electrons exhibited well defined diffraction patterns after passing through the **Gold foil**.

Characteristics of de-Broglie Waves



1. de Broglie waves are the probability waves

For light,

E$^2 \rightarrow$ probability density of photons $\rightarrow$ probability of finding the photons per unit volume

For electrons,

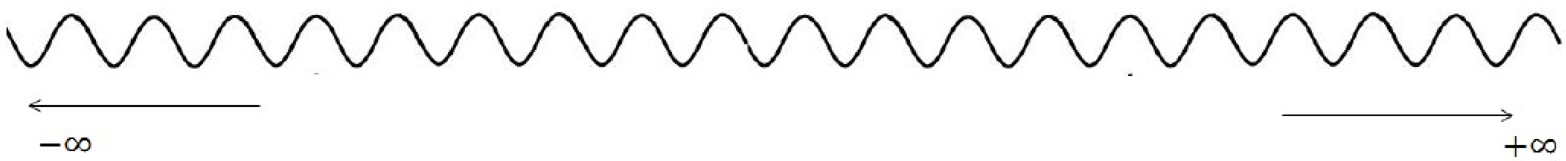
$|\Psi|^2 \rightarrow$ probability density of electrons $\rightarrow$ probability of finding the electrons per unit volume

2. Sub atomic particles are restless
3. The energy of the de-Broglie waves associated with the confined particle is quantized
4. de-Broglie waves associated with confined particles are wave groups

Two Types of particles
Absolutely free particle and Confined Particle in a definite space
Absolutely free particle is entirely **an idealization**.
Almost all the subatomic particles or the objects that we encounter in day to day life are confined to a fixed region.
electron is confined to atom, atom is confined to a molecule, a proton is confined to a nucleus and a cricket ball is confined to a box in which it is kept

The free particle can exist anywhere in space and probability of finding such particle is same in the entire infinite space.

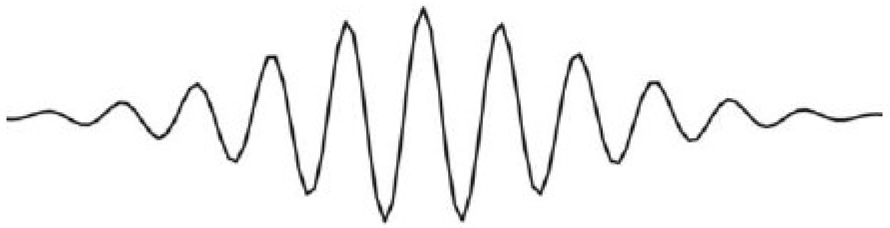
The de Broglie wave associated with such particle is a single progressive wave accompanying the entire infinite space.
The amplitude of this wave is same everywhere, as the probability of finding the corresponding particle is same everywhere. This infinitely long wave **does not have to satisfy any boundary condition and therefore it is not quantized**

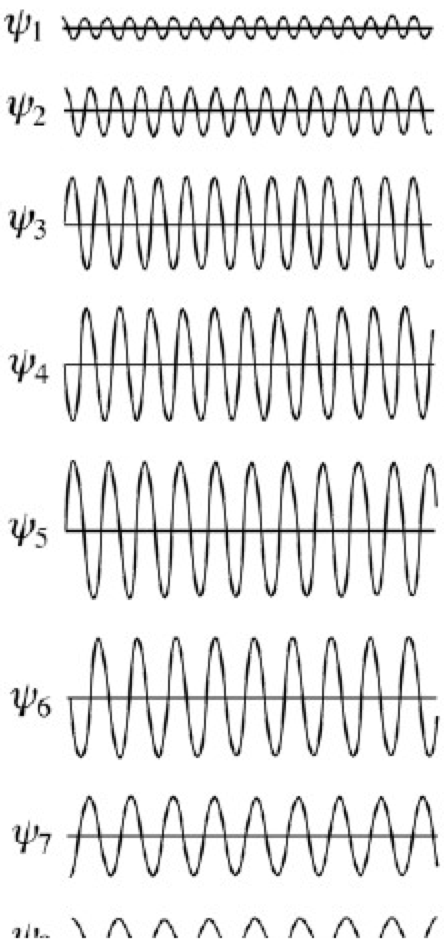


Confined Particles

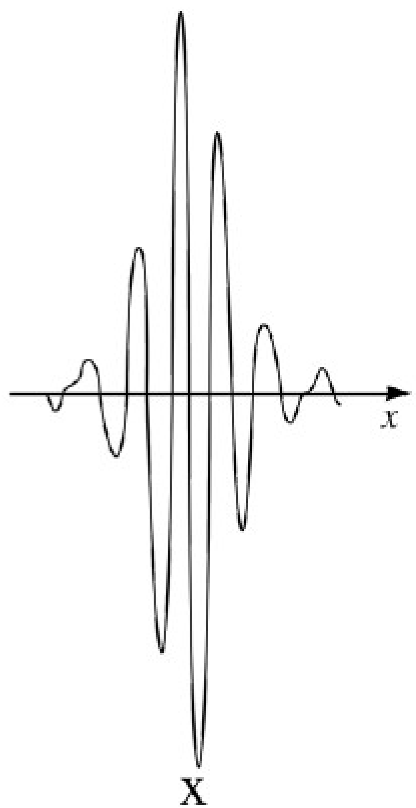
waves limited to the size of the region in which their particle exists.
For ex. the de Broglie wave associated with the electron in the atom can be maximally as long as atom itself.
Such waves of limited length are not progressive waves but they are wave-groups.

A **wave-group** is obtained by **superimposing different progressive waves of different wavelengths.**

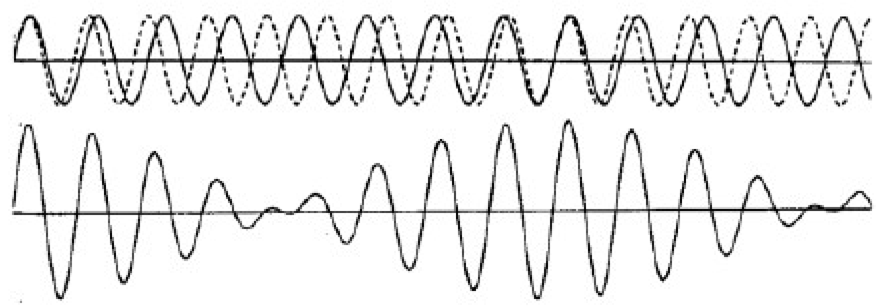




ψ_1
ψ_2
ψ_3
ψ_4
ψ_5
ψ_6
ψ_7



x
X



The Velocity of de-Broglie Waves

De Broglie waves have **two velocities**, the **phase velocity** and the **group velocity**

Let us consider a free progressive and sinusoidal wave associated with an absolutely free particle.

A simple progressive wave is represented by

$$\psi = \psi_o \sin(\omega t - kx)$$

$$\text{Where } \omega = \text{angular velocity} = 2\pi\nu \text{ and } k = \text{wavenumber} = \frac{2\pi}{\lambda}$$

The **phase velocity** is defined as

$$u = \frac{\omega}{k}$$

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

$$u = \lambda\nu$$

We have

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

electron being a wave-particle (***wavicle***), both equations of energy are valid

E = mc^2

E = hν

$$E = mc^2 = h\nu$$

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

Substituting λ and ν

$$u = \lambda \nu$$

$$u = \frac{h}{p} \times \frac{mc^2}{h}$$

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

$$u = \frac{h}{mv} \times \frac{mc^2}{h}$$

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

Now according to **special theory of relativity v, the velocity of any particle/object cannot exceed c** (*v* **< c**). Thus

$$u > c$$

$$u > c$$

Does this mean that De Broglie waves travel faster than light?

WKT an infinitely long sinusoidal progressive wave is associated with an absolutely free particle.

Such situation (u>c) and therefore such De Broglie waves never exist.

All objects/particles in the nature are confined and therefore the De Broglie waves associated with them are not infinitely long single and sinusoidal waves (which would move faster than light), but they are the **wave-groups** which are limited in space.

Group veolciy (V_g) = *velocity of particle* ($V_{particle}$)

Phase velocity of the individual waves which make up the wave- group is still greater than the velocity of light

The ultimate velocity of the wave-group which comes in to existence after the superposition of individual waves is exactly equal to the velocity of the particle.

Thus the wave-group exactly follows the motion of the particle with which it is associated.

Thus **de Broglie's hypothesis does not violate the theory of relativity**

Phase Velocity	Group Velocity
The average velocity of the advancement of individual monochromatic wave in the medium with which a wave packet is constructed	The velocity with which a wave group moves in a medium
$u=\omega/k$	$V_g=d\omega/dk$
$u>c$	$V_g<c$

Heisenberg’s Uncertainty Principle

In classical Physics one can determine Position, momentum, energy and time of moving object by using below formula

$$F = ma$$

$$v = \int \frac{F}{m} dt$$

$$a = \frac{F}{m}$$

$$p = mv$$

$$\frac{dv}{dt} = \frac{F}{m}$$

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

$$x = \int v\,dt$$

Measurements are accurate
with absolute precision with the help of sophisticated instruments

Can similar approach be followed for subatomic particles?

behave like waves
probability waves, and they are described Ψ.

Similar approach can not be used for subatomic particle due to wave nature

$$\psi = \psi_o \sin(wt - kx)$$

$$\psi = \psi_o \sin\left(2\pi\nu t - \frac{2\pi}{\lambda}x\right)$$

$$\psi = \psi_o \sin\left(\frac{2\pi}{h}h\nu t - \frac{2\pi}{h}\frac{h}{\lambda}x\right)$$

$$\psi = \psi_o \sin\frac{1}{\frac{h}{2\pi}}(Et - px)$$

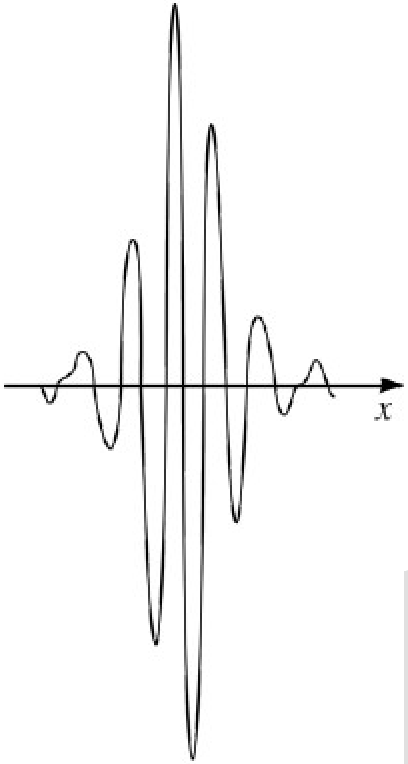
$$\psi = \psi_o \sin\frac{1}{\hbar}(Et - px)$$

A wave-group (ψ) provides every information required for describing the motion of subatomic particle.

The highest peak specifies the most probable position, the distance between consecutive peaks gives λ.

P **= h/λ gives momentum.**

E **= $p^2/2m$ gives energy.**

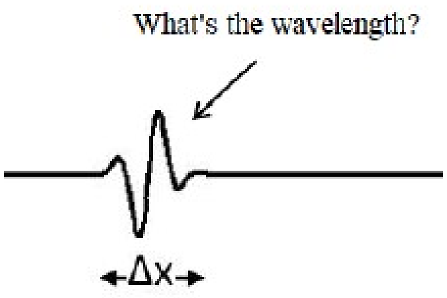


Thus deterministic description of p requires deterministic description of λ;

and a glance at the de-Broglie wave-group undoubtedly indicates that it does not have a precise wavelength.

The distance between various neighboring peaks varies from peak to peak.
This means that the association of De Broglie wave with a particle also imposes an unavoidable uncertainty in describing its wavelength and hence the momentum.

Is uncertainty in position and uncertainty in momentum can be minimized ?



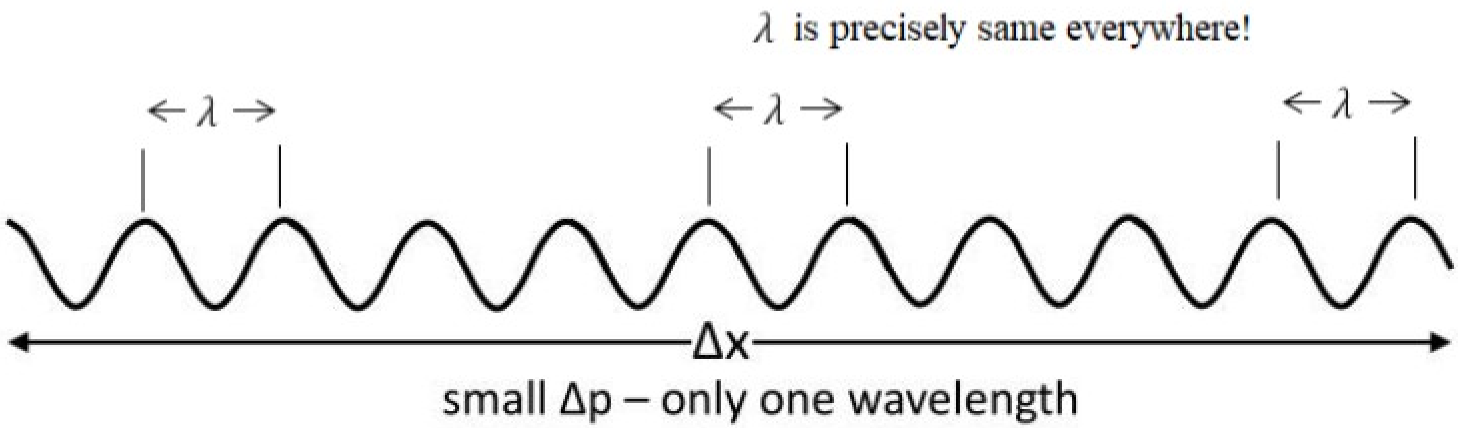
If the number of interfering waves, each having different wavelengths is infinity, then the size of resultant wave-group will become zero

the wave-group is so compact that it is extremely difficult to measure it's wavelength

wavelength becomes uncertain, the momentum becomes uncertain
tiny wave-group has been formed by the interference of many waves, each having large variation in wavelength.
Thus when Δx becomes smaller and smaller, Δp becomes larger, and larger.
Simultaneous accuracy in position (x) and momentum (p) is not possible in this case

In case of wave-group of the medium size, both Δx and $\Delta\lambda$, and hence Δp are fairly moderate, but none of them tends to zero.

Thus simultaneous accuracy in x and p is not possible in this case also.



We will start widening the wave-group, it will decrease the number of interfering waves. widened wave-group, easily find out the wavelength.

But widening opens the the particle which is supposed to have one definite position at a given instant has many probable positions spread in the widened wave-packet.
The conclusion is that Δx has increased.

An extreme end, The number of interfering waves has reduced to one.

The wavelength being same everywhere, the $\Delta\lambda=0$, $\Delta x = \infty$
Our attempts to achieve simultaneous accuracy in x and p have once again failed!

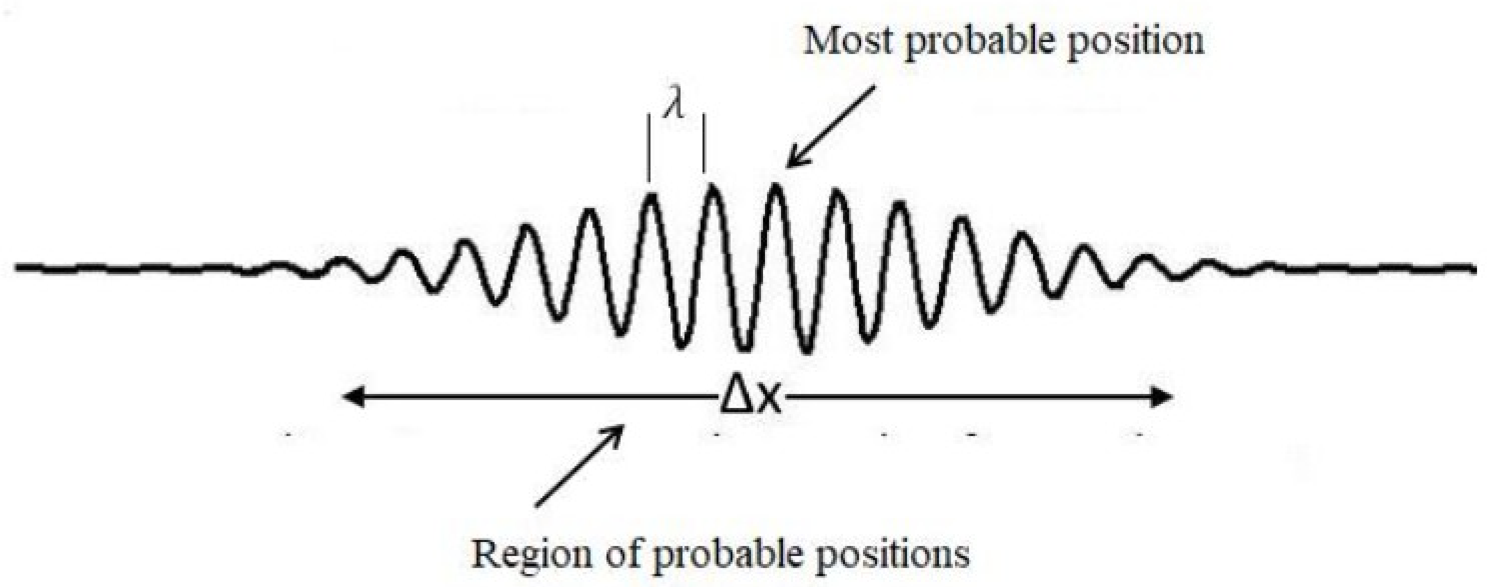
“ it is not possible to construct a wave-group of any size or shape, which gives us simultaneous accuracy in x and p”

Heisenberg’s Uncertainty Principle

Wave like properties of subatomic particles lead to an unavoidable uncertainty in determining their motion

“It is not possible to make simaltaneous measurements of the position and momentum of a particle to an unlimited accuracy”

$$\Delta x \Delta p \geq h/4\pi$$



Δx --- uncertainty in position

Δp --- uncertainty in momentum

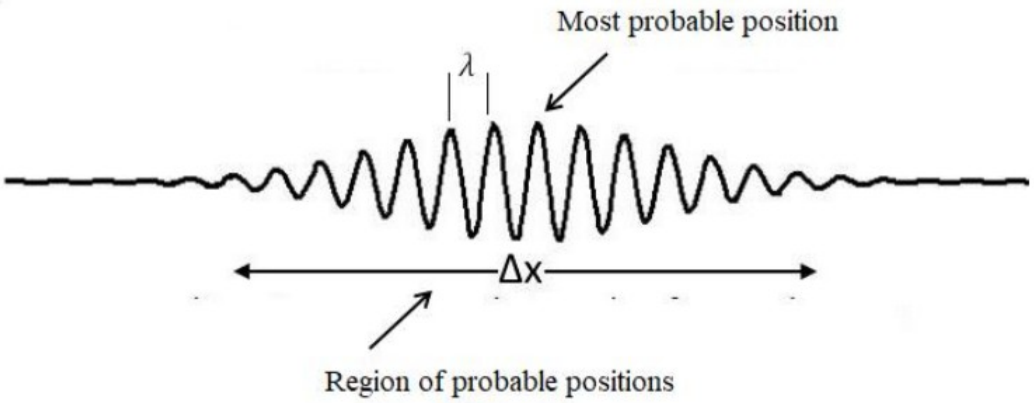
ΔxΔp≥h

For accurate momentum (P) require accurate value of λ, but wave group does not posses accurate λ, because peak to peak distance between neighboring waves varies

So it imposes an unavoidable uncertainity in momentum

Size of the de-Broglie wave represents region of uncertainity in position (Δx)

It is difficult to reduce uncertainity in x and P



If x reduces P increases and vice varsa

Size of the wave group is given by

$$\Delta x = \frac{\lambda_{av}^2}{\Delta\lambda}$$

We Know That

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

$$P = h\lambda^{-1}$$

$$\Delta p = -h\lambda^{-2}\Delta\lambda$$

If Δp is considered as an error in p, then

$$\Delta p = \left| -h\lambda^{-2}\Delta\lambda \right|$$

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

Taking the product of Δx and Δp

$$\Delta x \Delta p = h$$

Thus the minimum value of the product of Δx and Δp is h.
The product cannot be made less than h.
Further, as error has no upper limit

$$\Delta x \Delta p \geq h \qquad \Delta x \Delta p \geq \frac{\hbar}{2}$$

Heisenberg’s uncertainty principle in terms of energy and time

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

$$\Delta E = \frac{1}{2} m 2 v \Delta v$$

$$\Delta E = (m \Delta v) v$$

$$\Delta E = \Delta p \frac{\Delta x}{\Delta t}$$

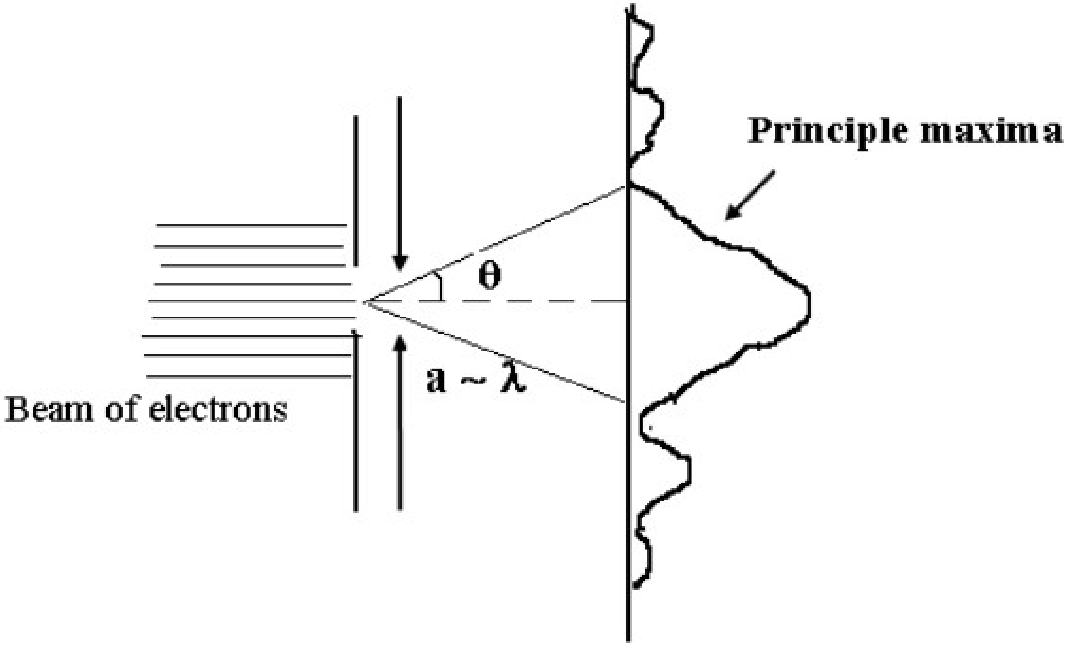
$$\Delta E \Delta t = \Delta p \Delta x \geq h$$

$$\Delta E \Delta t \geq h$$

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Experimental Proof of Uncertainty Principle

SINGLE SLIT ELECTRON DIFFRACTION



Beam of electrons passing through a slit having width comparable with the wavelength of electrons.
Electrons, get diffracted through the slit and form a diffraction pattern on the slit

Though several electrons, after passing through the slit, produce a well defined diffraction pattern

predicting the exact position of one electron when it passed through the slit is extremely difficult as it can pass through any part of the slit.

Thus uncertainty involved in determining the position of the electron while it is passing through the slit is

$$\Delta y = a$$

a is the width of the slit

From the theory of single slit diffraction, the minima is

$$a\sin\theta = n\lambda$$

$$\Delta y\sin\theta = n\lambda$$

n = 1, as the principle image of slit is mainly reflected in the principle (central) maxima and the minima associated with the central maxima is the first minima .
Secondary maxima are too weak to be considered.

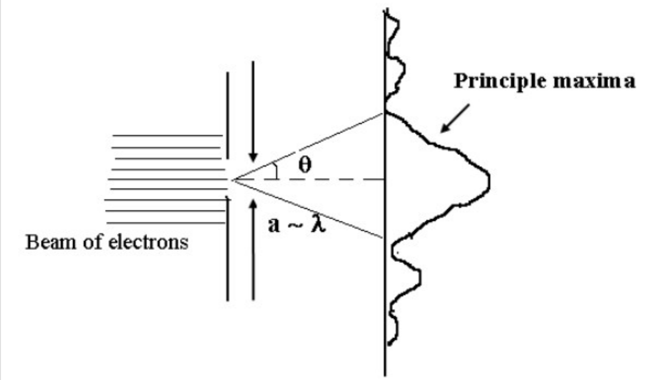
Thus

$$\Delta y= \lambda / \sin\theta$$

The electron doesn’t possess momentum in y direction before passing through the slit, its entire momentum is in x direction.

According to De Broglie’s hypothesis

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



While passing through the slit, electronundergoes diffraction .

electron acquires y component of momentum after getting diffracted.

Note that the well-defined principle maximum is the result of diffraction of several electrons.
Out of such several electrons, the y component of a single electron is almost unpredictable.

After diffraction, a single electron posses **x** (**$h/(\lambda\sin\theta)$**) as well as **y** (**$\pm h/(\lambda\cos\theta)$**) components of momentum,

As the electron while approaching towards the principle maxima has a freedom to proceed at any angle within a ‘cone having angle 2θ,

it may acquire y component of momentum which may have any value from **$+h/(\lambda\sin\theta)$ to $-h/(\lambda\sin\theta)$**

where θ is the angle of diffraction of the first minimum.
The secondary maxima are too weak to be considered.

Thus, uncertainty in y momentum is

$$\Delta p_y = 2\frac{h}{\lambda}\sin\theta$$

Taking the product of Δy and Δp$_y$, we get

$$\Delta y\,\Delta p_y = 2h$$

Due to extremely small value of Planck's constant, h and 2h are almost equally small. The minimum value of the product is

$$\Delta y\,\Delta p_y = h$$

And as error has no upper limit,

$$\Delta y \Delta p_y \geq h$$

$$\Delta y \Delta p_y \geq h$$

This indicates that as Δy increases Δp_y decreases, and vice versa.

Simultaneous accuracy in position and momentum is thus not possible.

It can also be observed that a smaller slit will yield less uncertainty in position, but then, as diffraction takes place more strongly for a tiny slit, the θ will be large, leading to higher uncertainty in momentum.

wide silt will increase the uncertainty in position, but will decrease the uncertainty in momentum,

as for wider slit, the less diffraction and hence θ will be small.

There doesn't exist a slit which can give simultaneous and minimum accuracy in position and momentum at the same time.

This itself is the bottom line of Heisenberg's uncertainty principle.

WAVE FUNCTION

Wave- propogation of disturbance in a medium

Charecterised - Some quantity varies with position and time

light waves – electromagnetic field variations
Sound waves – Pressure variations

But de-Broglie wave associated with electron can't be specifiedby similar way

Because of its dual nature (particle and wave)

To characterise the de-Broglie wave associated with a material particle, we need a quantity that varies in space and time called wave function (Ψ)

Ψ(x, y, z, t)- position of a particle in space at time t.

It is not possible to locate a particle precisely at position (x, y, z), but there is only probability of the particle being at that specific position

Ψ- Mathematically describes motion of an electron

Ψ- complex as well exponential quantity

Ψ- Has no direct physical significance as it is not an observable quantity

WKT displacement of a wave can either positive or negative

i.e. Ψ can have either positive or negative values

According to uncertainity principle, we have only probability of finding particle at (x, y, z) at time t

as probability can not be negative
∴ Ψ can not be a direct measure of the presence of the particle as itrepresents the wave associated with the particle motion

de Broglie waves is represented as

$$\psi = \psi_o \sin(\omega t - kx)$$

$$\psi = \psi_o \sin [(1/\hbar)(Et - px)]$$

Where $k = 2\pi/\lambda$, $p = h/\lambda$, $\omega = 2\pi\nu$, $E = h\nu$

Instead of sine function, we may choose cosine function, or even a combination of both sine and cosine, i.e. exponential function.

$$\psi = \psi_o e^{-\left(\frac{i}{\hbar}\right)(Et-px)}$$

i- inhibits the realistic and direct interpretation of ψ
∴ de Broglie waves are probability waves,
$|\psi|^2$ represents the probability density

$|\psi|^2$ represents the probability density

$|\psi|^2 \rightarrow$ probability of finding the particle/unit length (1-D de Broglie wave) or per unit volume (3-D de Broglie wave)

Thus

$|\psi|^2\, dx \rightarrow$ Probability of finding the particle in a region having length dx

$\int_{-x_1}^{+x_2} |\psi|^2 dx$ → Probability of finding the particle in a region in the de Broglie wave between $-x_1$ and x_2

$\int_{-\infty}^{+\infty} |\psi|^2 dx$ =1 =Total probability of finding the particle in the entire space = normalisation condtion

$$\int_{-\infty}^{+\infty} |\psi|^2 dx \neq 0 \qquad \int_{-\infty}^{+\infty} |\psi|^2 dx \neq \infty$$

An acceptable (well behaved) wavefunction must be normalized or at least normalizable

As $|\psi|^2$ represents probability, ψ must satisfy below conditions

1. ψ must be finite for all values of x

Ψ can never be infinite

Ex: $\psi = \psi_o$ tanx cannot be an acceptable – x=90^o → tanx=∞

$\psi = \psi_o$ sin(1/x) is also not an acceptable wavefunction – x=0 → sin (1/x)=∞

2. ψ must be single valued

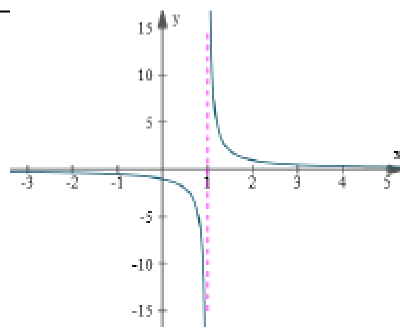
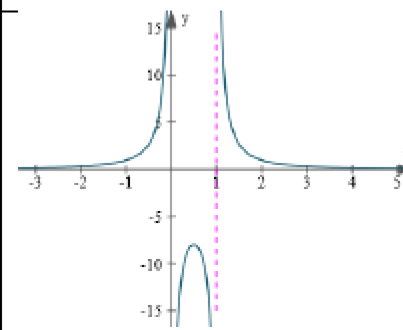
→ there is no multiple probabilities of finding the particle at the same point

Ex: $\psi = \psi_o$ sin√x- not an acceptable wavefunction (for given x, √x has (±) two values)

3. ψ should be continuous

i.e. probability of finding particle at all the points in the region of intrest can be specific

Examples of discontinous ψ

Formula	Graph	Formula	Graph
$\psi(x) = \frac{1}{x-1}$		$\psi(x) = \frac{2}{x^2 - x} = \frac{2}{x(x-1)}$	

4. derivatives of ψ such as δψ/δx, δψ/δy, δψ/δz must be finite, single valued and continous

$$\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}, and\ \frac{\partial\psi}{\partial z}$$

SCHRÖDINGER'S EQUATION

Schrodingers time independent (Staedy state) equation

It is an universal equation, obeyed by all de-broglie waves under motion.

Wave equation is given by

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{u^2}\frac{\partial^2 f}{\partial t^2} \qquad \text{----- 1}$$

Above is a progressive wave equation, which describes all waves such as light, sound etc

f--- function describes electric and magnetic field for light wave and pressure for sound wave
u --- Speed of light or sound respectively

In 3-Dimensions above equation can be written as

$$\nabla^2 f = \frac{1}{u^2}\frac{\partial^2 f}{\partial t^2} \qquad \text{----- 2}$$

Where

$$\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$ **= Laplacian operator**

In order to apply equation [2] to de-Broglie wave, f will be replaced by Ψ and u represents phase velocity de-Broglie wave

[2] becomes

$$\nabla^2 \psi = \frac{1}{u^2}\frac{\partial^2 \psi}{\partial t^2}$$ **----- [3]**

It is one form of Schrodinger equation, where u represents wave properties.

∴ we need to incorporate particle property also

Simplest wave equation is given by

$$\psi = \psi_o \sin(\omega t - kx) \qquad \text{-----[4]}$$

The [4] can be expressed interms of exponential function

i.e $$\psi = \psi_o e^{-i(\omega t - kx)} \qquad \text{----[5]}$$

Now separate space dependent and time dependent parts

$$\psi = \psi_o e^{+ikx} e^{-i\omega t}$$

Now replace space dependent term ($\psi_o e^{+ikx}$) by ψ_o'
ψ_o' represents time independent part of wavefunction
Now [5] becomes

$$\psi = \psi_o' e^{-i\omega t} \qquad \text{----[6]}$$

Diffrentiating [6], i.e. Ψ w.r.to time (t)

$$\frac{\partial \psi}{\partial t} = (-i\omega)\psi_o' e^{-i\omega t}$$

Diffrentiating again

$$\frac{\partial^2 \psi}{\partial t^2} = (-i\omega)(-i\omega)\psi_o' e^{-i\omega t} = -\omega^2 \psi \qquad \text{----[7]}$$

Substituting [7] in [3]

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

Now using identities ω = 2πν and u = λν, we get

$$\nabla^2 \psi = -\frac{(2\pi\nu)^2}{(\lambda\nu)^2}\psi$$

$$\Rightarrow \nabla^2 \psi = -\left(\frac{2\pi}{\lambda}\right)^2 \psi \qquad \text{----[8]}$$

∴ for de-Broglie wave $\lambda = h/p$

Now [8] becomes

$$\nabla^2\psi = -\left(\frac{2\pi}{\frac{h}{p}}\right)^2 \psi$$

$$\Rightarrow \quad \nabla^2\psi = -\left(\frac{p}{\frac{h}{2\pi}}\right)^2 \psi$$

$$\Rightarrow \nabla^2\psi = -\frac{p^2}{\hbar^2}\psi \qquad \text{----[9]}$$

[3], [8], [9] are various forms of Schrodinger's equation in terms of u, ω, λ and p

For a particle in motion, the total energy (E) is conserved

i.e. E= Kinetic energy + Pottential energy

$$\therefore \quad E = \frac{1}{2}mv^2 + V(x,t)$$

$$\Rightarrow E = \frac{p^2}{2m} + V(x,t)$$

$$\Rightarrow p^2 = 2m\{E - V(x,t)\} \qquad \text{----[10]}$$

Substitute [10] in [9]

$$\nabla^2\psi = -\frac{2m\{E - V(x,t)\}}{\hbar^2}\psi$$

Rearranging

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + V(x,t)\psi = E\psi} \qquad \text{----[11]}$$

This is the Schrodingers time independent (Staedy state) equation

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(x,t)\right\}\psi = E\psi$$

$$H\psi = E\psi$$

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

H--- Hermitian operator

E--- energy oprator

Schrodinger's Time dependent equation

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

Here, the term V(x, t) represents the potential energy.
Potential energy signifies the ‘boundedness’ of the particle.
In fact, a particle, whose motion is restricted, is always acted upon by some force.

Force and potential energy are related by following expressions

$$V = \int F dx \qquad\qquad F = \frac{dV}{dx}$$

We have also see that, potential energy in eqn is a function of x as well as t .

However in some situations the potential energy may be a function of only position and independent of time.

For ex. the potential energy of an electron in an atom and harmonic oscillator is given by

$$V = -\frac{1}{4\pi\epsilon_o}\frac{Ze^2}{r} \qquad\qquad V = \frac{1}{2}kx^2$$

In both the cases potential energies are only space dependent and time independent

Now consider the motion of an electron in an atom placed in a time dependent electric or magnetic field.
consider the motion of a harmonic oscillator, where the spring is held in a furnace. The elastic constant of the spring and consequently the potential energy will then change with time.

Such motions are attempted with Schrödinger’s time dependent equation.

Particle in a rigid box

All motions in the nature are in way that they are moving in a boxes

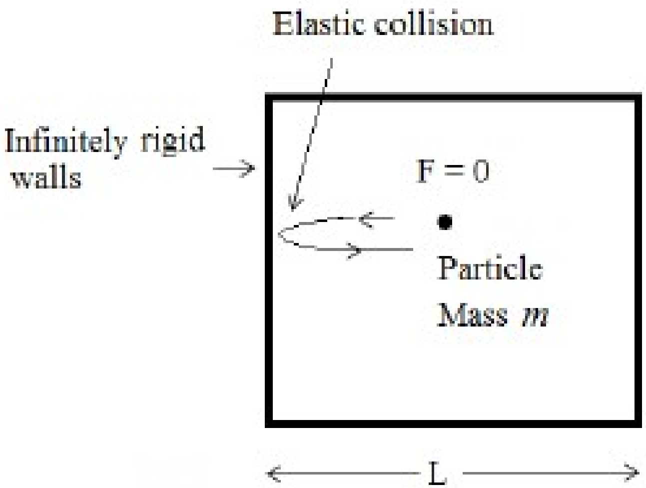
For Ex:

Electron in an atom
Nucleon in a Nucleus
Atom in a Molecule
Cricket ball in the ground

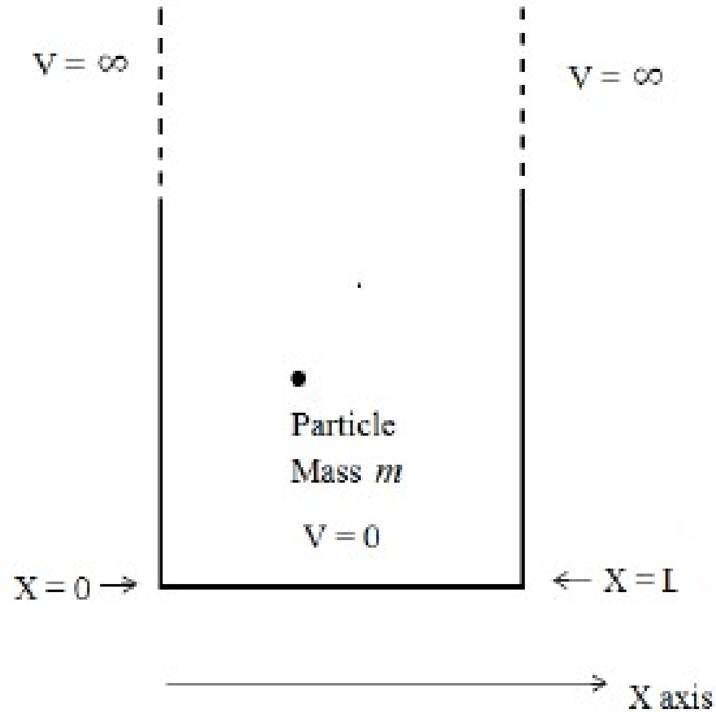
The energy of a particle trapped in a box is quantized and the ground state energy of such particles cannot be brought down to absolute zero

In order to solve Schrodinger equation for such motion requires some assumptions such as

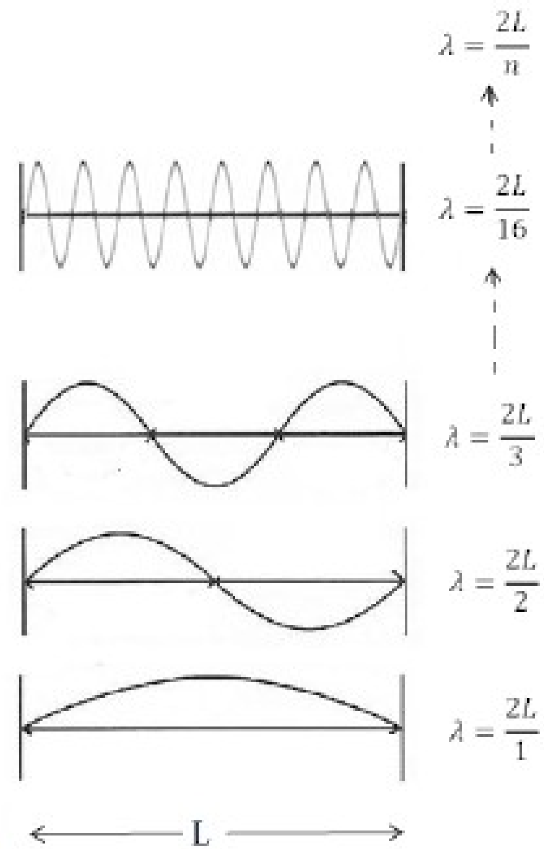
Infinitely rigid walls
One dimensional motion
Zero pottential energy



Particle in a rigid box



Pottential Well



Wave functions

Here we have to analyze motion of a particle in an infinitely rigid box (Infinitely deep rigid box)

The pottential energy (V) of the particle at x=0 and x=L is ∞

While inside the box (0<x<L) is Zero

Such pottential well does not change with time

Schrodinger time independent (Steady State) equation is given by

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

As the motion is one dimensional, ∇ reduces to $\partial^2/\partial x^2$ and becomes d^2/dx^2

Further pottential energy inside the box is zero
Thus,

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

$$\frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2}\right)\psi = 0$$ **---[1]**

Collision of the particle with walls are elastic, therefor E is constant
Thus

$$\left(\frac{2mE}{\hbar^2}\right) = constant = k^2$$ **---[2]**

[1] --->

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$ **---[3]**

One of the standard solution for [3] is

$$\psi = \psi_o sin(kx + B) \quad \text{---[4]}$$

Here Ψ is finite, continous and single valued wave function

Let us test Ψ for the boundary conditions of the problem

Now first boundary condition

Ψ=0 at x=0

[4]---> $$0 = \psi_o sin(k \times 0 + B)$$

$$\Rightarrow 0 = \psi_o sinB \Rightarrow either\ \psi_o = 0\ or\ sinB = 0$$

However Ψ_o can not be zero as then the Ψ disappears for all x

Now SinB=0 requires either B=0, ±π, ±2π, ±3π, ...

If B=0,

$$\psi = \psi_o sinkx \quad \text{---[5]}$$

Now second boundary condition is Ψ=0 at x=L

$$0 = \psi_o sinkL \Rightarrow either\ \psi_o = 0\ or\ sinkL = 0$$

Once again ψ_o cannot be taken zero due to reason explained above,
Thus

$$sinkL = 0 \Rightarrow kL = n\pi \Rightarrow k = \frac{n\pi}{L}$$ **---[6]**

n= ±1, ±2, ±3....= integer
n=0 is not possible ∵ if n=0 ---> Ψ=0
The values of n is only restricted to integers called Quantum Numbers
k is quantised

Substitute **k=nπ/L in [5]**

$$\psi = \psi_o sin \frac{n\pi}{L} x$$

---[7]

Wkt Ψ satisfies boundary conditions, but it should satisfy normalisation condition also

$$\int_{-\infty}^{+\infty} \psi^2 dx = \int_0^L \psi^2 dx = 1$$ **---[8]**

Substituting Ψ

$$\int_0^L \left(\psi_o sin\frac{n\pi}{L}x\right)^2 dx = 1$$

$$\Rightarrow \psi_o{}^2 \int_0^L \left(sin\frac{n\pi}{L}x\right)^2 dx = 1$$

$$\psi_o{}^2 \times \frac{L}{2} = 1$$

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

$$\psi_o = \sqrt{\frac{2}{L}}$$

Substitute Ψo value in [7]

$$\psi_n = \sqrt{\frac{2}{L}} sin\frac{n\pi}{L}x$$

---[9]

[9] gives complete wavefunction of the particle trapped in a rigid box

Ψ_n is called as general solution because all the constants Ψ_o, k and B are unknown

From [6] k is quantised due to boundary conditions Ψ=0 at x=L

Equating [2] and [6]

$$k^2 = \left(\frac{2mE}{\hbar^2}\right) = \left(\frac{n\pi}{L}\right)^2$$

$$E_n = \frac{n^2h^2}{8mL^2} \qquad \text{---[10]}$$

By substituting n=1, 2, 3....

Discrete energy levels of a particle in a rigid box
Energy also Quantised

$$E_4 = \frac{16h^2}{8mL^2}$$

$$E_3 = \frac{9h^2}{8mL^2}$$

$$E_2 = \frac{4h^2}{8mL^2}$$

$$E_1 = \frac{h^2}{8mL^2}$$

WKT

Total Energy E= Kinetic Energy + Pottential Energy

$$E = \frac{1}{2}mv^2 + V(x,t)$$

In our case V(x,t)=0

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

$$\Rightarrow p = \sqrt{2mE}$$

Substitute value of E from [10]

$$p = \sqrt{2m\left(\frac{n^2h^2}{8mL^2}\right)}$$

$$\Rightarrow p_n = \pm\frac{nh}{2L} \quad \text{---[11]}$$

Thus along with energy, momentum is also quantised
The ± sign indicates that momentum has direction

We have λ=h/p

From [11]

$$\lambda = \frac{h}{\left(\frac{nh}{2L}\right)} = \frac{2L}{n} \qquad \text{---[12]}$$

The wavelength also quantised

The boundary condition Ψ=0 at x=L, KE, p and λ is quantised which indicates that a sort of restriction on the motion always leads to quantisation

The boundary condition signifies restriction on the motion

According to Schrodinger

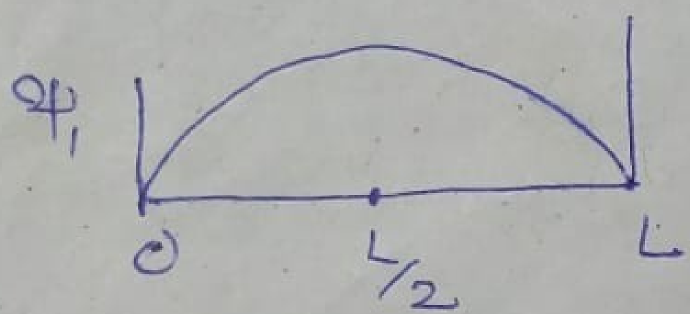
A free particle can access any energy but the energy of a bounded particle is always quantised

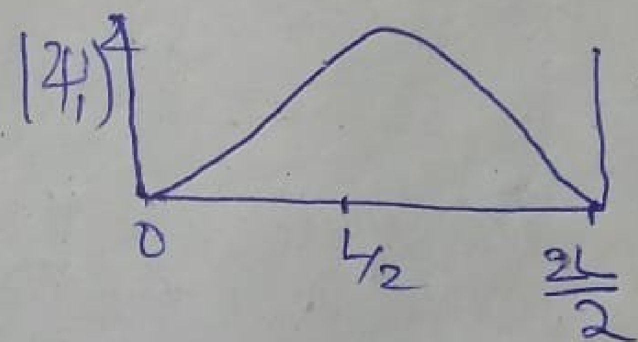
Stationary states of the particle in a box:

For n=1,2, 3,... Ψ_n and $|\Psi_n|^2$ can be calculated and represented graphically

for n=1 ground state

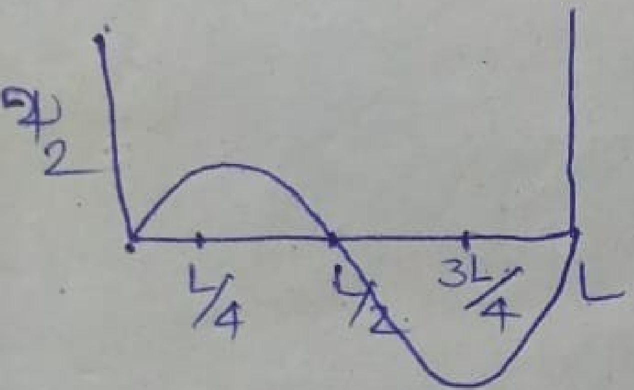
$E_1 = \frac{h^2}{8mL^2}$, $P_1 = \pm \frac{h}{2L}$, $\lambda_1 = 2L$ & $\psi_1 = \sqrt{\frac{2}{L}} \sin \frac{\pi}{L} x$

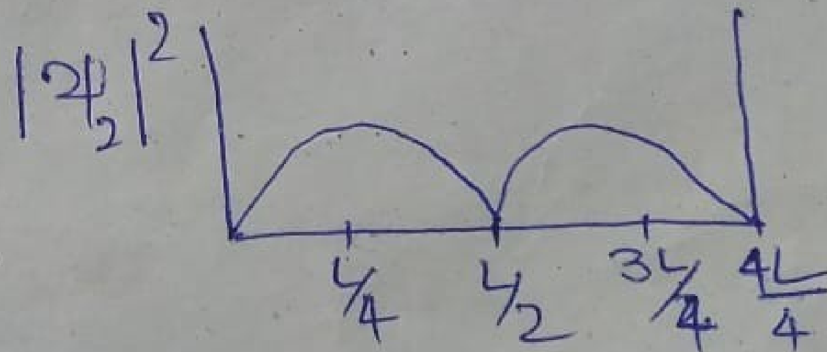




for n=2 (first excited state)

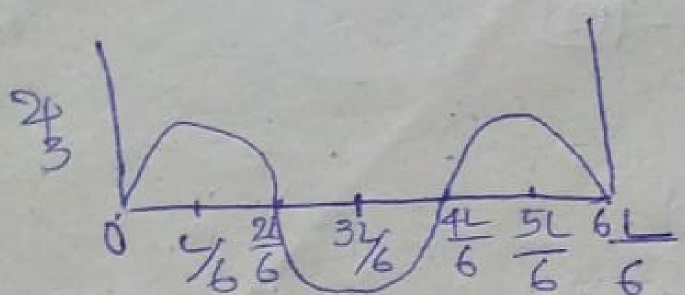
$E_2 = \frac{4h^2}{8mL^2}$, $P_2 = \pm \frac{2h}{2L}$, $\lambda_2 = \frac{2L}{2}$ & $\psi_2 = \sqrt{\frac{2}{L}} \sin\frac{2\pi}{L}x$

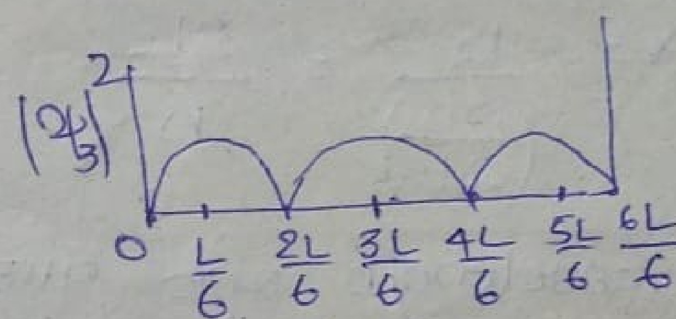




n=3 (second excitation state

$E_3 = \frac{9h^2}{8mL^2}$, $P_3 = \pm \frac{3h}{2L}$, $\lambda_3 = \frac{3L}{2}$ & $\psi_3 = \sqrt{\frac{2}{L}} \sin\frac{3\pi}{L}x$





Here n represents number of peaks

For n is extreemly large, number of peaks wiil extreemly large

Practically all position becomes equally probable

Classical mechanics also proposes same thing

ie for extreemly large values of n, quantum mechanics approaches classical mechanics

Now particle in a rigid box having large n, then pottential energy =0

It posses only kinetic energy and it is quantised

Now

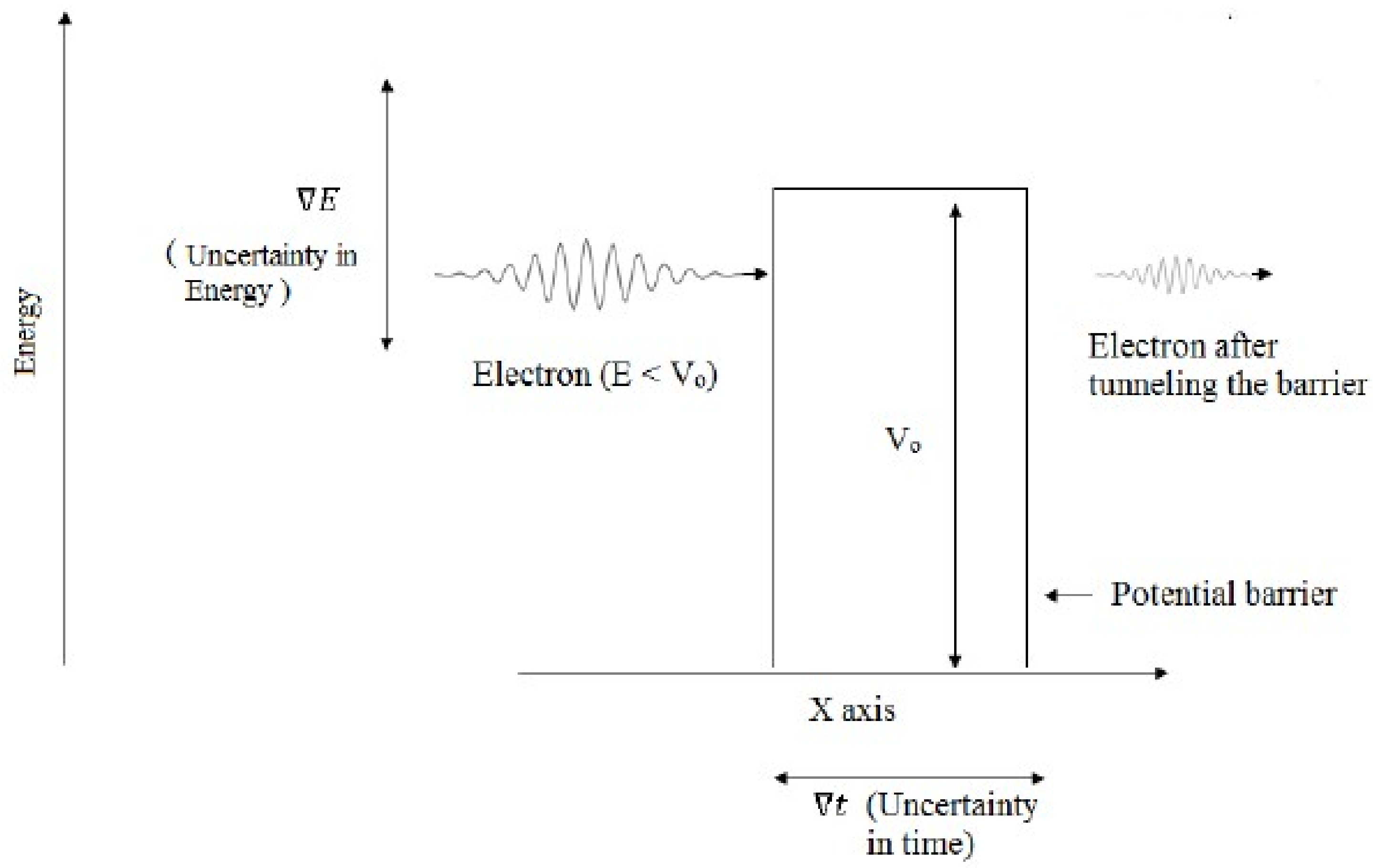
$$E_n = \frac{n^2h^2}{8mL^2} = \frac{1}{2}mv^2$$

$$n = \frac{2mvL}{h}$$

PARTICLE IN A NON-RIGID BOX (FINITE POTENTIAL WELL)

Barrier penetration (tunnel effect) explained using Heisenberg's uncertainity principle

An electron is incident on a pottential barrier



The energy of an electron (E) is less than barrier height (V_o)

Classically we expect the electron to bounce back as its energy is insufficient to cross the barrier.

But in subatomic world the electron unexpectedly tunnels through the barrier. This can be explained by Heisenberg's uncertainity principle

Assume that the electron has energy E and correspondingly a speed v and L be the width of the barrier

Thus electron, if it were allowed to cross the barrier, it would take time $t=L/v$

Now according to Heisenberg's uncertainity principle E and t can never be measured accurately

We have

$$\Delta E \Delta t \approx h$$

Uncertain energy of an electron is given by
$$\Delta E = h/\Delta t$$

At the atomic scales the bariers are sufficiently narrow therefore can be crossed in lesser time

Thus t and Δt are small enough, correspondingly greater value of ΔE allows electron to posses an energy higher than the barrier height in time interval t.

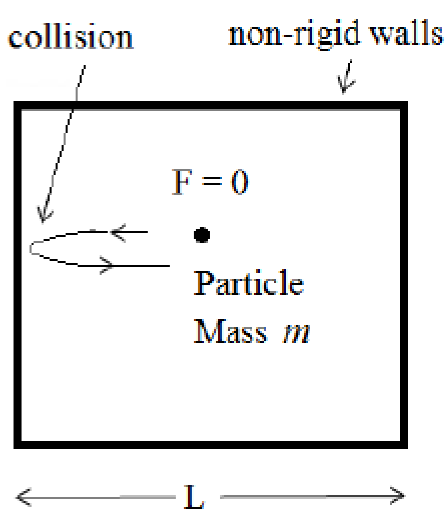
Thus the electron tunnels through the barrier.

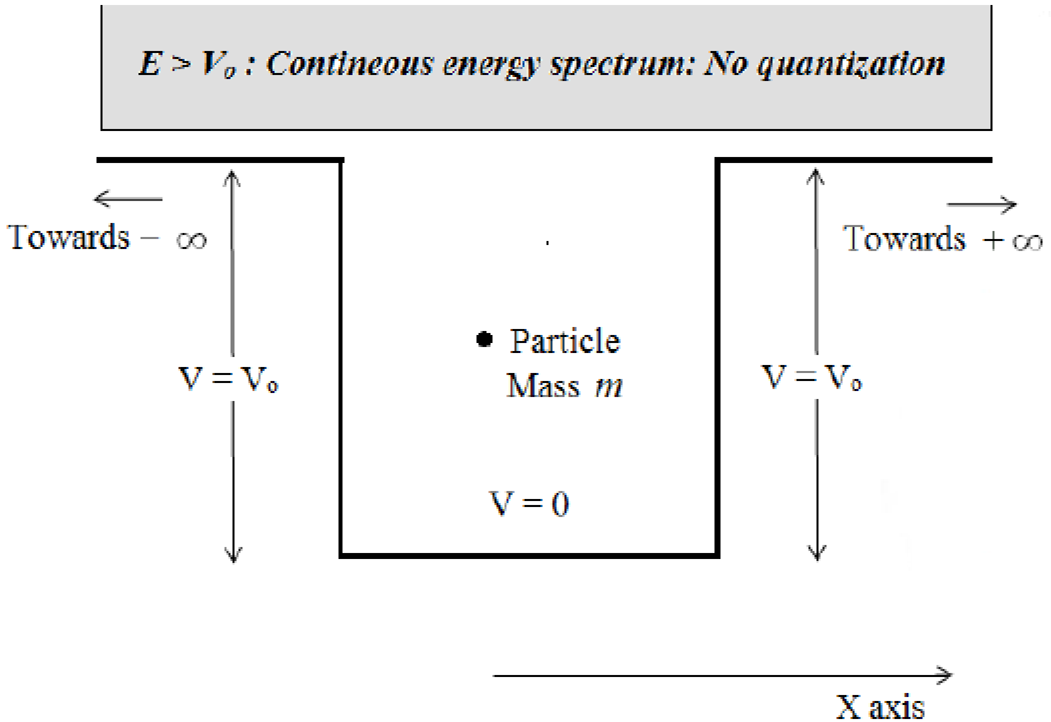
Before and after tunneling, the electron moves in an empty space, wide enough to demand extreemly large time interval t to cover the space

Thus before and after the barrier, Δt is extreemly large and thus in these regions the electrons energy E is well defined and quite certain

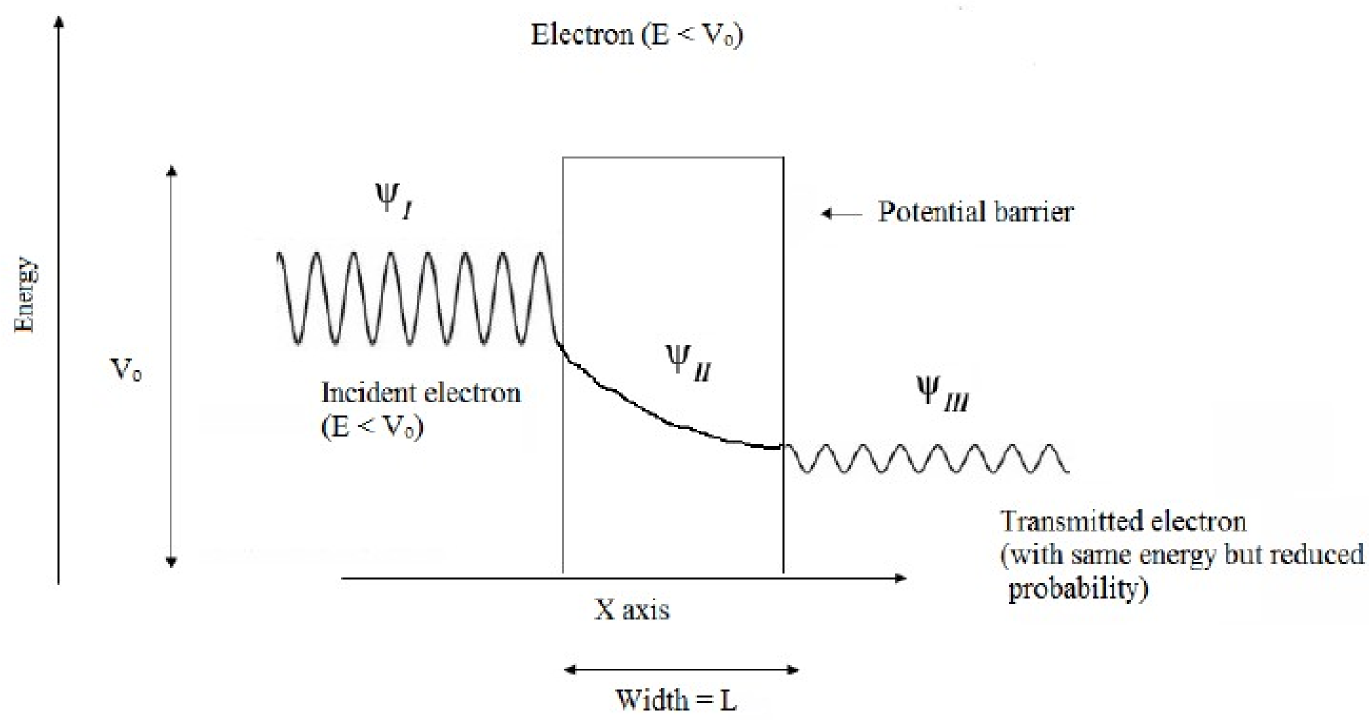
When electron hits the barrier, it borrows an extra energy to cross the barrier in time t and returns it after tunneling through the barrier

The ability of a sub atomic particle to tunnel through a barrier without having sufficient energy is called as tunnel effect or barrier penetration





Tunnel Effect



Instead of pottential well, a thin pottential barrier of height V_o and Length L

The pottential energy is Zero for x<0 and x>L

If an electron of energy E<V hits the barrier, it has finite chance to leak to the other side of the barrier

i.e. electron tunneled through the pottential barrier-- Tunneling

The region arround the barrier can be divided in to 3 regions as in figure

1. Region I : where $-\infty < x < 0$ and $V = V_o$
2. Region II : where $0 < x < L$ and $V = 0$
3. Region III : where $L < x < +\infty$ and $V = V_o$

in this problem barrier height Vo is finite, the particle can have energy E<Vo or E>Vo

if E>Vo, then particle can easily cross the barrier and therfore it is a free particle

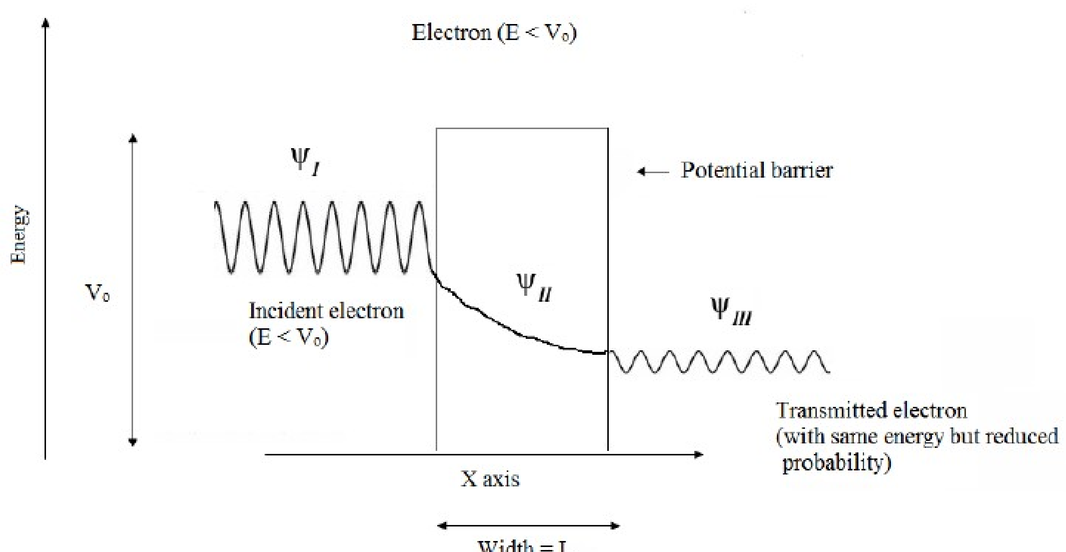
if E<Vo is a bounded particle, is of quantum mechanical importance

this problem consists of 3 regions I, II and III
Even though it is a single particle moving in all 3 regions
Therefor Schrodinger equation to be solved for all 3 regions is represented by $\Psi_I, \Psi_{II}, \Psi_{III}$
And represented as

$$\frac{d^2\psi_I}{dx^2} + \frac{2m}{\hbar^2}\{E - V_o\}\psi_I = 0$$

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2mE}{\hbar^2}\psi_{II} = 0$$

$$\frac{d^2\psi_{III}}{dx^2} + \frac{2m}{\hbar^2}\{E - V_o\}\psi_{III} = 0$$



These wave functions need to satisfy following boundary conditions

i.e

$\psi_I = \psi_{II}$ at $X = 0$

$\partial\psi_I/\partial x = \partial\psi_{II}/\partial x$ at $X = 0$

$\psi_{II} = \psi_{III}$ at $X = L$

$\partial\psi_{II}/\partial x = \partial\psi_{III}/\partial x$ at $X = L$

The probability of finding the particle having finite energy at $X = \pm\infty$ needs to be zero, two more boundary conditions, as given below, need to be satisfied

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

$\psi_{II} \rightarrow 0$ as $X \rightarrow +\infty$

when we apply such boundary conditions to the wavefunctions, the energy is quantized. six boundary conditions only for specific values of the energies, cannot be satisfied for any arbitrary energy of the particle.

Thus the energy levels for which boundary conditions are satisfied are the 'allowed' ones and those where the boundary conditions are not satisfied are 'forbidden'.

ΨI corresponds to free electron with momentum $P=\sqrt{(2mE)}$

ΨII is not zero in region I has a probability of being found in region III

ΨIII represents wave transmitted through the barrier and the free electron in region III with the same momentum as in I

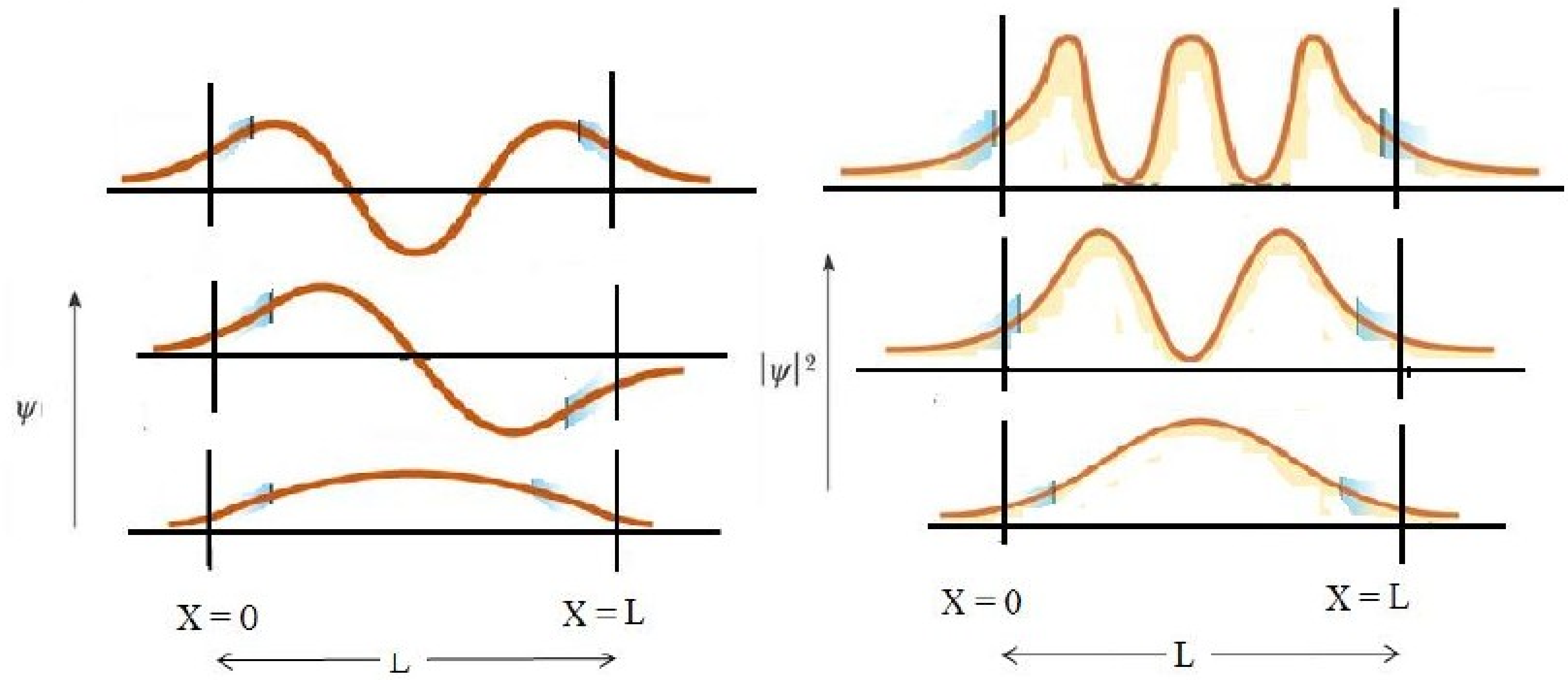
Thus it ispossible for a particle penetrate through the pottential barrier even if its energy is less than that of height of the barrier

The probability that the particle gets through the barrier is called transmission coefficient (T)

i.e Transmission probability(or transmission coefficient) = $T \approx e^{-2k'L}$

$$k'^2 = \frac{2m}{\hbar^2}(V_o - E) \Rightarrow \mathrm{k}' = \sqrt{\frac{2m}{\hbar^2}(V_o - E)}$$

ψ and ψ^2 for finite potential well meant for first three quantum states



Practical Aspects of Tunnel effect

1. Alpha decay from radioactive nuclides:

Heavy nuclides such as U^{238}, $_{92}Th^{232}$ emit α-rays in order to get stability

In nucleus there is a strong attractive force which keep nucleon together

In above nuclides, the pottential barrier formed due to attractive force is about 25MeV

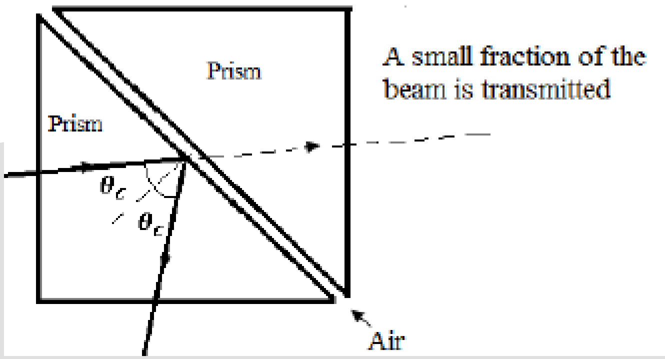
But α particle has energy of 4-9MeV

Eventhough α-particle emitted out from the nucleus

In U_{238}, an α-particle hits the barrier 10^{38} times, then the possibility of tunnel through the barrier is 1

2. Nuclear Fusion in SUN and other stars

Nuclear fusion is responsible for emission of light through stars.
For fusion of proton has to overcome pottential barrier of 1MeV due to Coulombic repulsion between protons
Incase of Sun, has temperature 10^7K, energy corresponding to this temperature is 1KeV. Still sun is shining due to Tunnel Effect



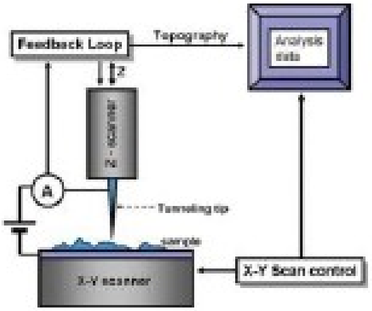
3. Conduction of electrons through copper wire
4. Frustrated total internal reflection

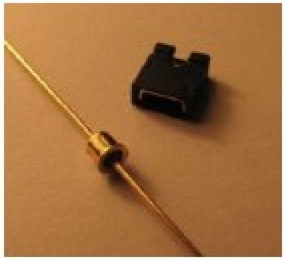
Applications of Tunnel Effect

1. Scanning Tunneling Microscope (STM):

If tip of only one atom wide brought extreemly close to surface and a small potential diffrence is applied

A thin airgap is formed between tip and surface, still electrons tunnel through this air gap and enter into the tip and gives tunnel current.





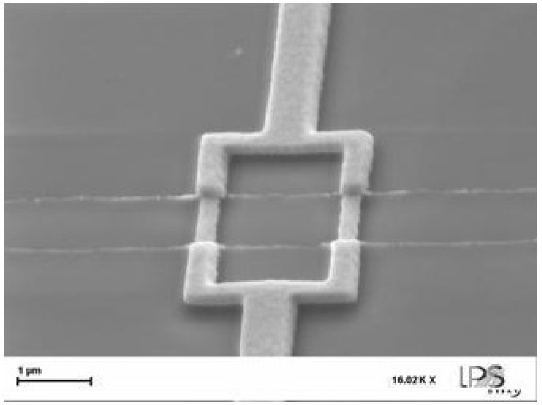
Tunnel current decreases if tip moves ahead
From this data one can analyse atom easily

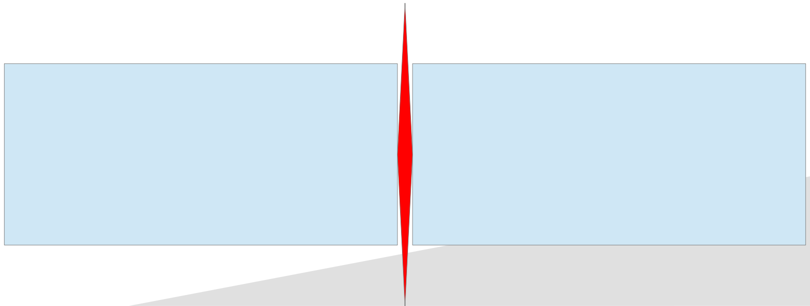
2.Tunnel Diode

Heavily doped P-N junction diode, in which majority charge carriers can tunnel through the barier called depletion layer
---> Oscillators, Fast switches used in computers

3. Josephson Junction

Used in Super Conducting Quantum Interfacing Devices (SQUID)





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