Wave Particle Duality:

A particle means an object with a definite position in space and is identifiable by their distinct properties such as mass, momentum, kinetic energy, spin & electric charge. On the other hand, a wave means a periodically repeated pattern in space which is specified by its wavelength, frequency, amplitude of disturbances, intensity, energy and momentum.

The particle and wave properties of radiation can never be observed simultaneously. To study the path of a beam of monochromatic radiation, we use the wave theory, while to calculate the amount of energy transactions of the same beam, we have to recourse to the photon or particle theory. This strange & overwhelming ability of electromagnetic radiation to manifest itself as wave or as particle is now familiar as wave-particle dualism.

de-Broglie concept of Matter waves (1924)

According to de-Broglie's concept, a moving particle always has a wave associated with it and the motion of the particle is guided by that wave in a similar manner as photon is controlled by a wave.

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

Let us suppose a material particle, like electron or proton, is equivalent to a standing wave system in the regions of space occupied by the particle. The value of ψ at any instant, t at a point (x, y, z) may be expressed as

$$\psi = \psi_0 \sin \omega t \quad \text{or} \quad \psi = \psi_0 \sin 2\pi\nu t$$

If the particle is moving with a velocity v along positive x direction.

$$\psi = \psi_0 \sin\left[\frac{2\pi\nu\left(t' + \frac{vx'}{c^2}\right)}{\sqrt{1 - v^2/c^2}}\right]$$

The well known standard equation of wave motion is given by

$$\psi = \psi_0 \sin\left[2\pi\nu'\left(t' + \frac{x'}{u'}\right)\right]$$

Comparing $u' = \frac{c^2}{v}$ and $\nu' = \frac{\nu}{\sqrt{1 - v^2/c^2}}$

According to Einstein's mass-energy equation

$$E = mc^2 = h\nu' \quad \text{or} \quad \nu' = \frac{mc^2}{h}$$

$$\lambda = \frac{\text{velocity}}{\text{frequency}} = \frac{u'}{\nu'} = \frac{c^2/v}{mc^2/h} \quad \text{or} \quad \boxed{\lambda = \frac{h}{mv}}$$

de-Broglie wavelength of Photon

$$E = h\nu \quad \& \quad E = mc^2 \text{ (Einstein equivalence)}$$

$$h\nu = mc^2 \quad , \quad p = mc$$

$$h\nu = \cancel{mp}\ pc$$

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

For any particle of kinetic energy E

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

For neutrons

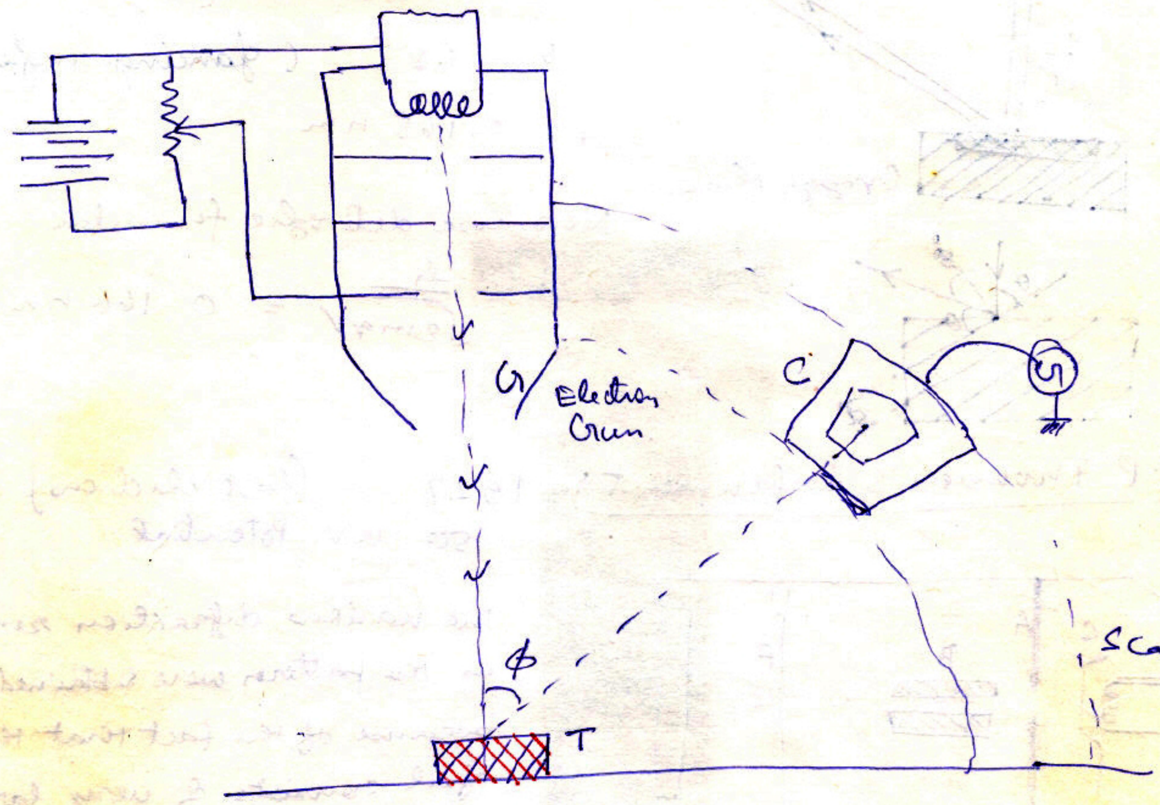
$$E = \frac{1}{2} m V_{rms}^2 = \frac{3}{2} KT$$

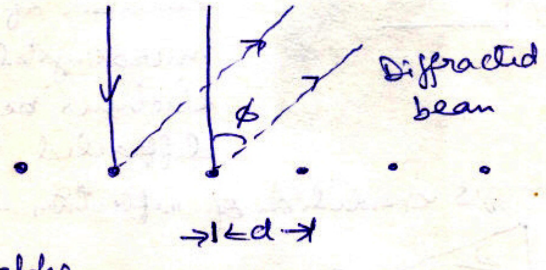
$$\lambda = \frac{h}{\sqrt{3mKT}}$$

For electron $\lambda = \frac{h}{\sqrt{2m_0eV}} = \frac{12.28}{\sqrt{V}}$ A°.

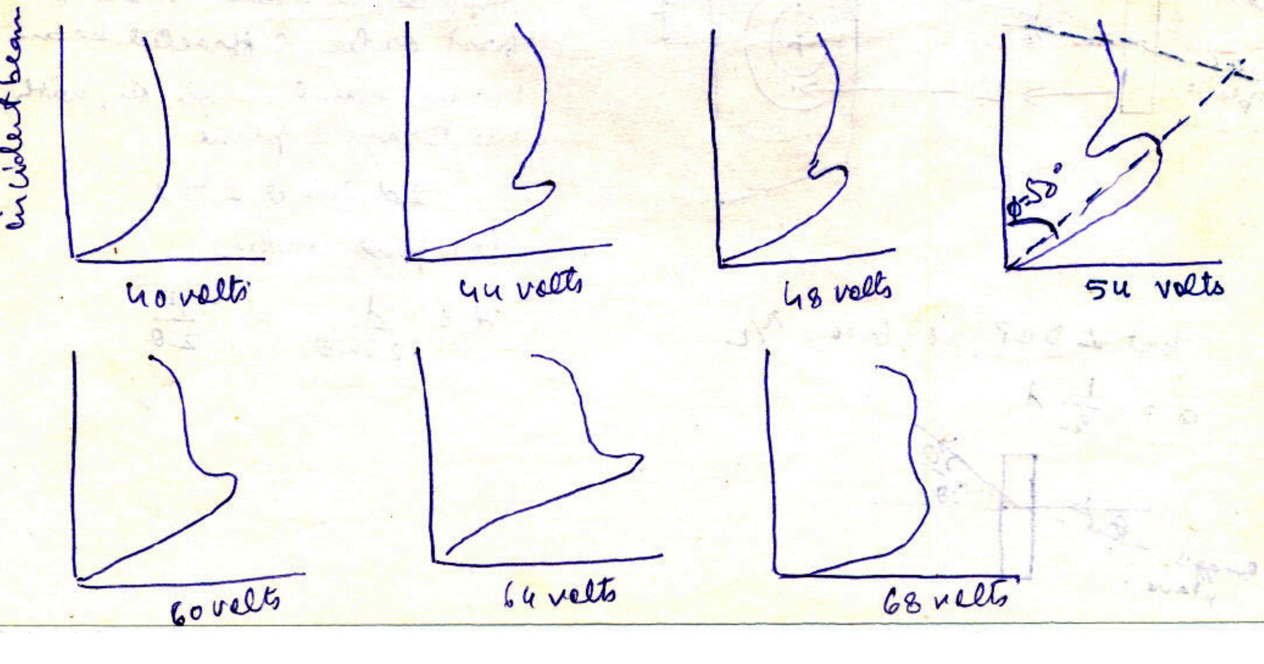
Davisson & Germer Experiment for the Existance of the Matter waves

(1927)

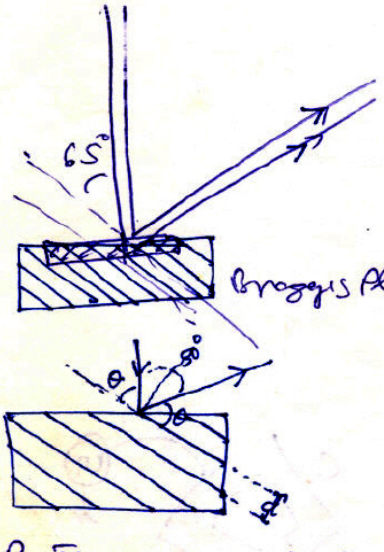




Observed Graphs



Calculation of wavelength (λ) As $\theta = \frac{180-50}{2} = 65^\circ$



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

$d = 0.091$ nm (For Nickel)

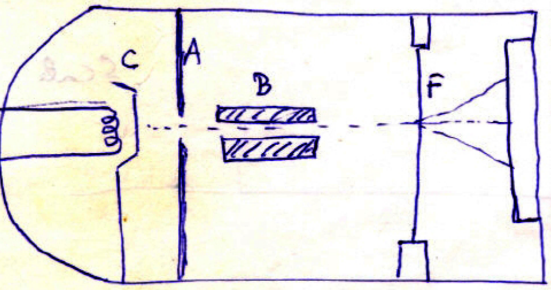
$\theta = 65^\circ$ (glancing angle)

$\lambda = 0.165$ nm

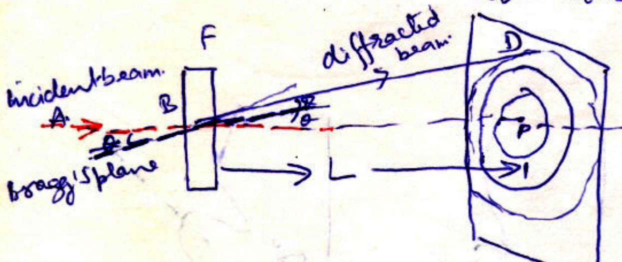
Now use deBroglie formulae.

$\lambda = \frac{h}{\sqrt{2mqV}} = 0.166$ nm.

G. P. Thomson's Experiment: 1927 (fast electrons) 50 KV Potential



The various diffraction rings in the pattern were obtained because of the fact that thin foil consists of very large number of randomly oriented microcrystals. The incident electrons beam is strongly diffracted by only those micro-crystals for which Bragg's condition of reflection is satisfied.



Suppose incident beam & first order diffracted beam make equal angle θ, with the Bragg's plane.

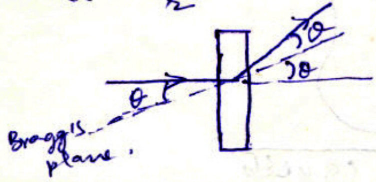
$2d\sin\theta = n\lambda$

for first order

$d = \frac{\lambda}{2\sin\theta} = \frac{\lambda}{2\theta}$

but ΔDBP, $2\theta = \tan 2\theta = R/L$

$d = \frac{L}{R}\lambda$



The de Broglie wavelength associated with a moving particle

$\lambda = \frac{h}{mv}$ as potential is very high 50 kV.

$m = \frac{m_0}{\sqrt{1-v^2/c^2}}$ $\therefore$ $\lambda = \frac{h}{m_0 v/\sqrt{1-v^2/c^2}}$

Relativistic equation

K.E = Total energy − rest mass energy

$K.E = \frac{m_0c^2}{\sqrt{1-v^2/c^2}} - m_0c^2$ or $K.E = m_0c^2\{(1-v^2/c^2)^{-1/2} - 1\}$

If the electron or any material particle of charge q are accelerated from rest to a potential of V volts, then

$m_0c^2\left[\left(1-\frac{v^2}{c^2}\right)^{-1/2} - 1\right] = qV$ or $\left(1-\frac{v^2}{c^2}\right)^{-1/2} = 1 + \frac{qV}{m_0c^2}$

or $1 - \frac{v^2}{c^2} = \left(1+\frac{qV}{m_0c^2}\right)^{-2}$ or $\frac{v^2}{c^2} = 1 - \left(1+\frac{qV}{m_0c^2}\right)^{-2}$

$$v = c\left[1 - \left(1+\frac{qV}{m_0c^2}\right)^{-2}\right]^{1/2}$$

therefore $\frac{v}{\sqrt{1-v^2/c^2}} = c\left(1+\frac{qV}{m_0c^2}\right)\left[1-\left(1+\frac{qV}{m_0c^2}\right)^{-2}\right]^{1/2}$

$$= c\left[\left(1+\frac{qV}{m_0c^2}\right)^2 - 1\right]^{1/2}$$

$$= c\left[1 + \left(\frac{qV}{m_0c^2}\right)^2 + \frac{2qV}{m_0c^2} - 1\right]^{1/2}$$

$$= c\left[\frac{2qV}{m_0c^2} + \left(\frac{qV}{m_0c^2}\right)^2\right]^{1/2}$$

or $\frac{v}{\sqrt{1-v^2/c^2}} = c\left[\frac{2qV}{m_0c^2}\left(1+\frac{qV}{2m_0c^2}\right)\right]^{1/2}$

$$\frac{m_0 v}{\sqrt{1-v^2/c^2}} = \left\{2m_0qV\left[1+\frac{qV}{2m_0c^2}\right]\right\}^{1/2}$$

$\therefore$ $\boxed{\lambda = \frac{h}{\left\{2m_0qV\left[1+\frac{qV}{2m_0c^2}\right]\right\}^{1/2}}}$ Now substituting λ in expression of d..

$$d = \frac{L}{2}\frac{h}{\sqrt{2m_0eV}}\left(1+\frac{qV}{2m_0c^2}\right)^{-1/2}$$

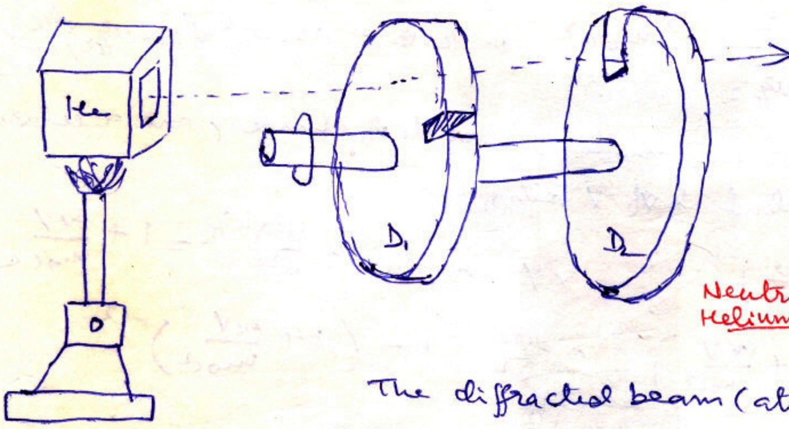
Observed by this technique for gold foil $d = 4.08\,A^0$

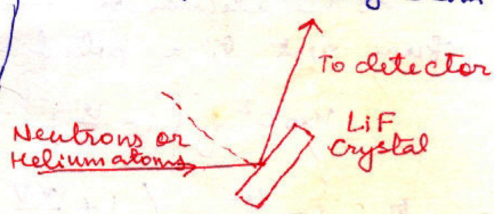
observed by x-rays technique $d = 4.06\,A^0$. Hence de-Broglie concept of matter waves was verified.

Bragg reflection of Helium Beam (Neutral Particles)

Wave nature of moving He atoms was experimentally demonstrated by Estermann, Frisch and Stern in 1930.

The beam of helium atoms is obtained by heating helium gas in an enclosure to 400 K. In order to secure a beam of uniform velocity a velocity selector was used.





The diffracted beam (atoms) in a given direction are collected in a small evacuated enclosure. The resulting pressure of helium gas in the enclosure was measured by means of hot wire gauge.

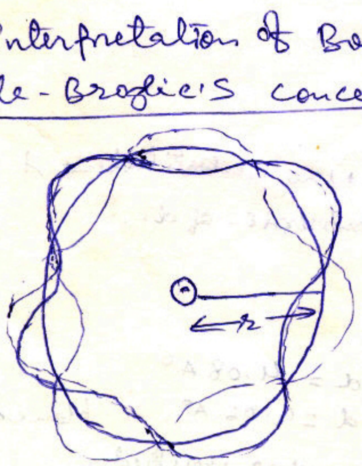
$$2d\sin\theta = n\lambda$$

The wavelength of He atom was calculated.

The wavelength of helium atoms obtained by this experimental technique was found in good agreement with those obtained theoritically by using the expression.

$$\lambda = \frac{h}{\sqrt{3mKT}}.$$

Interpretation of Bohr's Quantization rule on the basis of de-Broglie's concept of Matter wave



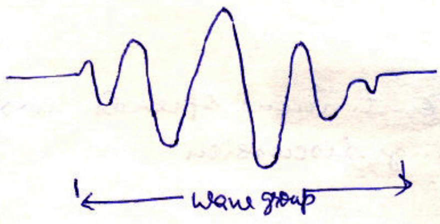
$$2\pi r = n\lambda$$

$$2\pi r = \frac{nh}{mv}$$

$$\boxed{mvr = \frac{nh}{2\pi}}$$

Phase & Group Velocities :

The amplitude of the de Broglie waves that correspond to a moving body reflects the probability that it will be found at a particular place at a particular time. Therefore, we expect the wave representation of a moving body to correspond to a wave packet or wave group, whose waves have amplitudes upon which the likelihood of detecting the body depends.



Let us assume that wave group arises from the combination of two waves that have the same amplitude A but differ by an amount $\Delta\omega$ in angular frequency and an amount Δk in wave number. We may represent original waves by the formulas

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

The resultant displacement y at any time t and any position x is the sum of y_1 and y_2. With the help of the identity

$$\cos\alpha + \cos\beta = 2\cos\tfrac{1}{2}(\alpha+\beta)\cos\tfrac{1}{2}(\alpha-\beta)$$

and $\cos(-\theta) = \cos\theta$

we find that

$$y = y_1 + y_2$$
$$= 2A\cos\tfrac{1}{2}[(2\omega+\Delta\omega)t - (2k+\Delta k)x]\cos\tfrac{1}{2}(\Delta\omega t - \Delta k x)$$

Since $\Delta\omega$ and Δk are small compared with ω and k respectively,

$$2\omega + \Delta\omega \simeq 2\omega$$
$$2k + \Delta k \simeq 2k$$

and so

$$y = 2A\cos(\omega t - kx)\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)$$

This equation represents a wave of angular frequency ω and wave number k that has superimposed upon it a modulation of angular frequency $\frac{1}{2}\Delta\omega$ and of wave number $\frac{1}{2}\Delta k$.

The effect of modulation is thus to produce successive wave groups. The phase velocity v_p is

Phase velocity $\quad v_p = \frac{\omega}{k}$

and the velocity v_g of the wave group is

Group velocity $v_g = \frac{\Delta\omega}{\Delta k}$

When ω and k have continuous spreads instead of the two values in the preceding discussion

$$v_g = \frac{d\omega}{dk}$$

for de Broglie waves

$$\omega = 2\pi\nu = \frac{2\pi mc^2}{h} = \frac{2\pi m_0 c^2}{h\sqrt{1-v^2/c^2}}$$

& $$k = \frac{2\pi}{\lambda} = \frac{2\pi m_0 v}{h\sqrt{1-v^2/c^2}}$$

The group velocity

$$v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv}$$

Now $\frac{d\omega}{dv} = \frac{2\pi m_0 v}{h(1-v^2/c^2)^{3/2}}$, $\frac{dk}{dv} = \frac{2\pi m_0}{h(1-v^2/c^2)^{3/2}}$

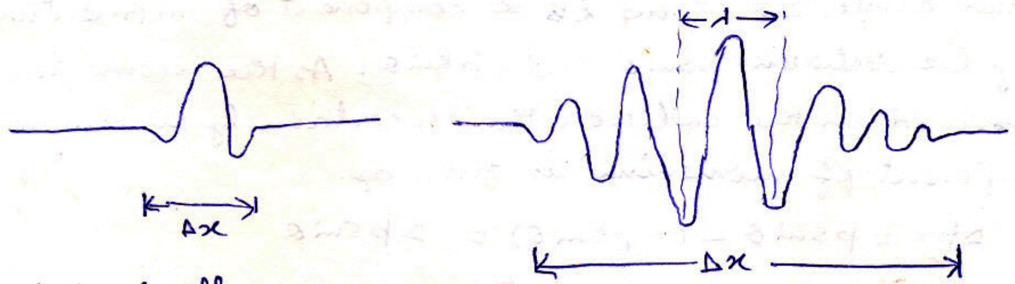
So the group velocity turns out to be

$$\boxed{v_g = v}$$

The phase velocity $\boxed{v_p = \frac{\omega}{k} = \frac{c^2}{v}}$

Here $v_p > c$. But phase velocity has no physical significance because it is the motion of the wave group, not the motion of the individual waves that make up the group. $v_g < c$ as it should be. The fact that $v_p > c$ for de Broglie waves therefore does not violet special relativity.

Heisenberg's Uncertainity Principle:



Δx small
Δp large

Δp small
Δx large

It is impossible to measure precisely and simultaneously both the members of pairs of certain canonically conjugate variables that describe the behaviour of an atomic system.

Quantitatively, the uncertainity principle states that the order of magnitude of the product of uncertainities in the simultaneous measurements of the two canonically conjugate variables must be at least of the order of Planck's constant $h/2\pi$.

$$\Delta p_x \cdot \Delta x \geq \hbar$$

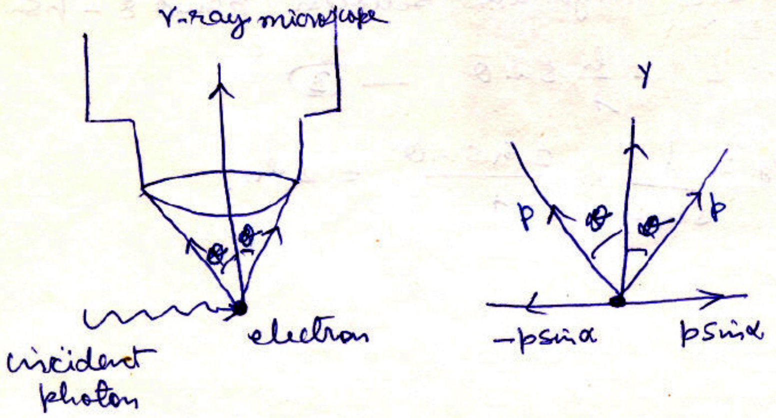
$$\Delta J \cdot \Delta \phi \geq \hbar$$

$$\Delta T \cdot \Delta t \geq \hbar$$

$\Delta T \rightarrow$ uncertainity in measurement of kinetic energy.

Exprimental Illustration of Uncertainity Principle:

(1) Determination of the position of a particle by microscope:



$\alpha = \theta$

Resolving power of microscope

$$\Delta x = \frac{\lambda}{2\sin\theta} \quad -(1)$$

When a photon of initial momentum $p = \frac{h}{\lambda}$, after scattering enters the field of view of microscope, it may be anywhere within angle 2θ. Thus its x component of momentum i.e p_x may lie between $p\sin\theta$ and $-p\sin\theta$. As the momentum is conserved in the collision, the uncertainity in the x component of momentum is given by.

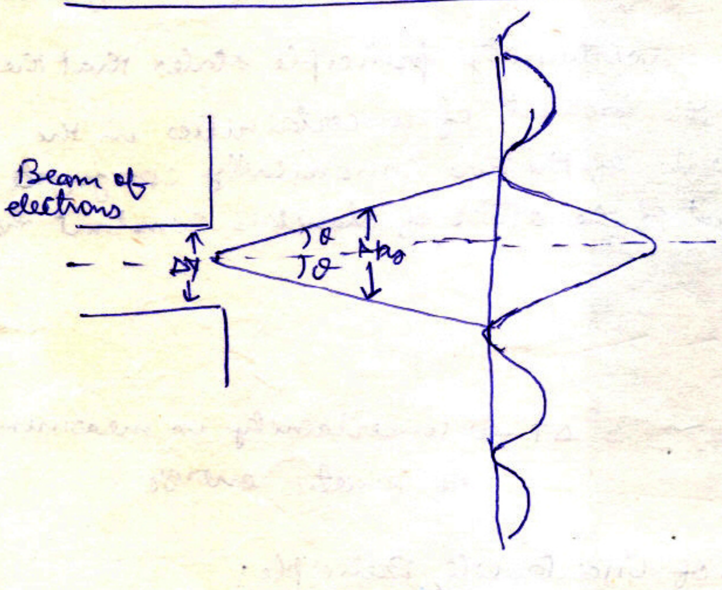
$$\Delta p_x = p\sin\theta - (-p\sin\theta) = 2p\sin\theta$$

$$= 2\frac{h}{\lambda}\sin\theta \quad \text{— (2)}$$

from eqn (1) & (2)

$$\Delta x \cdot \Delta p_x = \frac{\lambda}{2\sin\theta} \times \frac{2h}{\lambda}\sin\theta \quad \text{i.e} \quad \boxed{\Delta x \cdot \Delta p_x \simeq h.}$$

2) Diffraction by a single slit:



The first minimum of the pattern is obtained by $n=1$.

$$\Delta y \sin\theta = \lambda \quad \text{— (1)}$$

$$\Delta y = \frac{\lambda}{\sin\theta} \quad \text{— (2)}$$

Initially electrons are moving the x-axis and hence they have no component of momentum along y-axis. After diffraction at the slit, they are deviated from their initial path to form the pattern and have a component $p\sin\theta$. y component lie anywhere between $p\sin\theta$ & $-p\sin\theta$.

$$\Delta p_y = 2p\sin\theta = 2\frac{h}{\lambda}\sin\theta \quad \text{— (3)}$$

Hence $$\Delta y \cdot \Delta p_y = \frac{\lambda}{\sin\theta} \times \frac{2h\sin\theta}{\lambda} = 2h.$$

Applications of Uncertainity Principle:

1. Non existance of electron in the nucleus

The radius of nucleus is $\approx 10^{-14}$ m. For the electron to be part of nucleus the uncertainity Δx must not be greater than 2.0×10^{-14} m.

$$\Delta x\,\Delta p \geq \hbar$$

$$\text{or} \quad \Delta p = \frac{\hbar}{\Delta x} = \frac{6.625\times10^{-34}}{2\times10^{-14}} = 3.31\times10^{-20}\ \text{kg-m/sec} \quad \text{—(1)}$$

electron momentum must be atleast must be of order of uncertainity, that is $p \approx 3.31\times10^{-20}$ kg-m/sec.

$$E^2 = p^2c^2 + m_0^2c^4$$

$$pc = 3.31\times10^{-20}\times3\times10^{8} = 9.91\times10^{-12}\ \text{Joules}$$

$$= \frac{9.91\times10^{-12}}{1.6\times10^{-19}} \approx 62\ \text{MeV}$$

Thus, if the electron is the constituent of the nucleus, it should have an energy of the order of 62 MeV. However, it is observed that β particles (electron) ejected from the nucleus during β decay have energies of about 3 MeV, which is quite different from the calculated value. Moreover, experimental observations show that no electron in the atom possesses energy greater than 4 MeV. Therefore, it is confirmed that electrons do not reside inside the nucleus.

2) Radius Of Bohr's First Orbit

$$\Delta x\,\Delta p \geq \hbar \quad \text{or} \quad \Delta p \geq \frac{\hbar}{\Delta x} \quad \text{—(1)}$$

The total energy of the electron

$$E = \text{kinetic energy} + \text{potential energy} = T + V$$

$$\Delta E = \Delta T + \Delta V \quad \text{—(2)}$$

$$T = \frac{1}{2}mv^2 \qquad \Delta T = \frac{1}{2}m(\Delta v)^2$$

$$\text{or} \quad \Delta T = \frac{(m\Delta v)^2}{2m} = \frac{1}{2}\frac{(\Delta p)^2}{m}$$

$$\text{or} \quad \Delta T = \frac{1}{2}\frac{\hbar^2}{(\Delta x)^2 m} = \frac{\hbar^2}{2m(\Delta x)^2} \quad \text{—(3)}$$

$$V = -\frac{Ze^2}{x} \quad \text{and} \quad \Delta V = -\frac{Ze^2}{\Delta x} \quad \text{— (4)}$$

Substituting values

$$\Delta E = \frac{\hbar^2}{2m(\Delta x)^2} - \frac{Ze^2}{\Delta x} \quad \text{— (5)}$$

the uncertainity in the energy would be minimum if

$\frac{d(\Delta E)}{d(\Delta x)} = 0$ and $\frac{d^2(\Delta E)}{d(\Delta x)^2}$ is positive

differentiating eqn (5) w.r.t. Δx, we get

$$\frac{d(\Delta E)}{d(\Delta x)} = -\frac{\hbar^2}{m(\Delta x)^3} + \frac{Ze^2}{(\Delta x)^2}$$

for minimum value of E

$$\frac{d(\Delta E)}{d(\Delta x)} = 0 = -\frac{\hbar^2}{m(\Delta x)^3} + \frac{Ze^2}{(\Delta x)^2} \quad \text{or} \quad \Delta x = \frac{\hbar^2}{mZe^2} \quad \text{— (6)}$$

Further differentiating eqn (5)

$$\frac{d^2(\Delta E)}{d(\Delta x)^2} = \frac{3\hbar^2}{m(\hbar^2/mZ^2)(\Delta x)^3} - \frac{2Ze^2}{(\Delta x)^3} = \frac{3Ze^2}{(\Delta x)^3} - \frac{2Ze^2}{(\Delta x)^3} \text{ and is +ve.}$$

Hence Δx is minimum.

$$r = \Delta x = \frac{\hbar^2}{mZe^2} = \frac{h^2}{4\pi^2 mZe^2}$$

$$\boxed{r = \frac{h^2}{4\pi^2 mZe^2}}$$ This is the expression for the Bohr's first orbit.

B) Minimum energy of a harmonic Oscillator:

$$\Delta p = \frac{\hbar}{2\Delta x}$$

$$E = T + V = \frac{(\Delta p)^2}{2m} + \frac{1}{2}k(\Delta x)^2 = \left(\frac{\hbar}{2\Delta x}\right)^2 \cdot \frac{1}{2m} + \frac{1}{2}k(\Delta x)^2$$

$$= \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2}k(\Delta x)^2$$

Minimising this energy with respect to Δx, i.e., $\frac{\partial E}{\partial(\Delta x)} = 0$ we get

$$-\frac{\hbar^2}{4m(\Delta x)^3} + k\Delta x = 0 \quad \text{or} \quad \Delta x = \left(\frac{\hbar^2}{4mk}\right)^{1/4}$$

$$E_{min} = \frac{\hbar^2}{8m}\left(\frac{4mk}{\hbar^2}\right)^{1/2} + \frac{1}{2}k\left(\frac{\hbar^2}{4mk}\right)^{1/2} = \frac{\hbar}{2}\left(\frac{k}{m}\right)^{1/2}$$

$$\boxed{E_{min} = \frac{1}{2}\hbar\omega}$$

Schrodinger wave equation:

1. Schrodinger time independent wave eqn or steady-state schrodinger equation: (1926)

According to classical wave optics, the differential equation of a wave motion is given by

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = \frac{1}{c^2}\frac{\partial^2 \phi}{\partial t^2}$$

In analogy with optics, the differential equation of a wave motion of particle can be written as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{v^2}\frac{\partial^2 \psi}{\partial t^2} \quad -(1)$$

the wave fn $\psi(x,y,z,t)$ of the particle can be separated into space dependent (x,y,z) and time dependent (t) functions as

$$\psi(x,y,z,t) = \psi(x,y,z)\, f(t) \quad -(2)$$ for a wave $f(t)$ must be periodic

$$\psi(x,y,z,t) = \psi(x,y,z)\, e^{i\omega t} \quad -(3)$$

differentiating eqn (3) partially twice with respect to x, we get

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial^2 \psi}{\partial x^2} e^{i\omega t} \quad -(4)$$

Similarly

$$\frac{\partial^2 \psi}{\partial y^2} = \frac{\partial^2 \psi}{\partial y^2} e^{i\omega t} \quad \text{and} \quad \frac{\partial^2 \psi}{\partial z^2} = \frac{\partial^2 \psi}{\partial z^2} e^{i\omega t}$$

differentiating eqn (3) with respect to t,

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

substituting values in equation (1), we have

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = -\frac{\omega^2}{v^2}\psi$$

or $$\nabla^2\psi + \frac{\omega^2}{v^2}\psi = 0$$

but $\omega = 2\pi\nu$, $\nu = \frac{v}{\lambda}$ & $\lambda = \frac{h}{p}$

$$\frac{\omega^2}{v^2} = \frac{(2\pi v/\lambda)^2}{v^2} = \frac{4\pi^2}{\lambda^2} \quad \text{or} \quad \frac{\omega^2}{v^2} = \frac{4\pi^2 p^2}{h^2}$$

But $T = E - V$

$T = \frac{p^2}{2m}$ or $p^2 = \frac{\cancel{2mT}}{2mT} = 2m(E-V)$

Substituting this value of p^2

$$\frac{w^2}{u^2} = \frac{8\pi^2 m(E-V)}{h^2} = \frac{2m}{\hbar^2}(E-V)$$

So the equation becomes

$$\boxed{\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0}$$

Time independent schrodinger wave eqn. Potential (force) acting on the particle is independent of time.

Schrodinger time-dependent wave equation. (1926)

When potential is time dependent. The energy is a function of time. The differential equation representing a one-dimensional wave motion is

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{u^2}\frac{\partial^2 y}{\partial t^2}$$

The general solution of the equation is of the form

$$y = Ae^{-i(\omega t - kx)}$$

The monochromatic wave equivalent to a free particle moving along positive x-direction may be expressed by a corresponding equation as

$$\psi(x,t) = Ae^{-i(\omega t - kx)}$$

$$\psi(x,t) = Ae^{-\frac{i2\pi}{h}(Et - px)}$$

Wave representing moving particle with total energy E and momentum p.

$$\frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}Ae^{-i/\hbar(Et-px)}$$

$$i\hbar\frac{\partial\psi}{\partial t} = E\psi \quad —(1)$$

&

$$\frac{\partial\psi}{\partial x} = \frac{ip}{\hbar}\psi$$

$$\frac{\partial^2\psi}{\partial x^2} = \left(\frac{ip}{\hbar}\right)\left(\frac{ip}{\hbar}\right)\psi$$

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi \Rightarrow p^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2}$$

In non relativistic limit, the total energy of the particle is the sum of its kinetic energy & potential energy.

$$E = \frac{p^2}{2m} + V \quad \text{— (3)}$$

or $$E\psi = \frac{p^2\psi}{2m} + V\psi \quad \text{— (4)}$$

Now substituting value for $E\psi$ & $p^2\psi$.

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

This is the time dependent schrodinger equation for a particle of mass m and potential energy V moving along x axis.

If the particle is moving in three - dimensional space, then the equation becomes

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

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}}$$

Physical Interpretation of wave fn ψ:

Schrodinger interpretation in terms of charge density. Applicable to directional distribution of photo electrons, intensity distribution in compton scattering, the stable states of Bohr atom, the emission of spectral lines etc. Difficulty arises when we wish to follow flight of single particle.

Probalistic interpretation by Max-Born in 1926 and then developed by Bohr, Dirac & Heisenberg.

" $\psi\psi^* = |\psi|^2$ respresents the probability density of the particle in the state ψ.

$$P(r)\,d\tau = |\psi(r,t)|^2 d\tau \qquad \text{in volume element } d\tau.$$

Since particle is certainely somewhere

$\int_{-\infty}^{\infty} |\psi|^2 d\tau = 1$, wave fn ψ is normalised.

- Every acceptable wave fn must be normalised.
- It must be finite everywhere.
- It must be single valued
- It must be continuous and have a continuous first derivative everywhere

NORMALISED & ORTHOGONAL WAVE FUNCTIONS

If ψ_i & ψ_j are two different wave functions,

if. $\int \psi_i \psi_i^* d\tau = 1$ & $\int \psi_j \psi_j^* d\tau = 1$ both fns are normalised.

if. $\int \psi_i^* \psi_j d\tau = 0$ or $\int \psi_j^* \psi_i d\tau = 0$, $i \neq j$ wave fns are said to be mutually orthogonal.

If satisfies both, Orthonormal

$$\int \psi_i^* \psi_j \, d\tau = \delta_{ij} = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases}$$

OPERATORS ASSOCIATED WITH DIFFERENT OBSERVABLES;

An operator is a rule by means of which a given fn is changed into another fn.

The measurable quantities like energy, momentum, position etc. are called observables. Each observable has a definite operator associated with each.

Expectation values of Dynamical quantities :

The average or expectation value of a dynamical quantity is the mathematical expectation for the result of a single measurement.

OR

It may be defined as the average of the result of a large number of measurements on independent systems.

$$\langle f \rangle = \frac{\int \psi^*(r,t)\, f_{op}\, \psi(r,t)\, d\tau}{\int \psi^* \psi\, d\tau}$$

if wave fn is normalised.

$$\langle f \rangle = \int \psi^*(r,t)\, f_{op}\, \psi(r,t)\, d\tau$$

where f_{op} is operator associated with observable f

Energy operator:

$$H\psi = E\psi \quad , \quad E_{op} = H = -\frac{\hbar^2}{2m}\nabla^2 + V$$

& $E_{op} = H = i\hbar\frac{\partial}{\partial t}$.

Momentum operator:

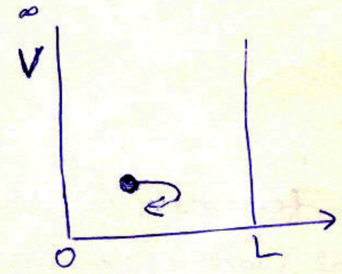
$$H = K.E + P.E = \frac{p^2}{2m} + V$$

$$-\frac{\hbar^2}{2m}\nabla^2 + V = \frac{p^2}{2m} + V.$$

$$p^2 = -\hbar^2\nabla^2 \quad , \quad P_{op}^2 = \frac{\hbar^2}{i^2}\nabla^2 \quad , \quad P_{op} = \frac{\hbar}{i}\nabla$$

Observable	Associated Operator Symbol	operator
energy	E_{op} or H	$-\frac{\hbar^2}{2m}\nabla^2 + V$ or $i\hbar\frac{\partial}{\partial t}$
kinetic energy	T_{op}	$-\frac{\hbar^2}{2m}\nabla^2$
Potential energy	V_{op}	V
Momentum	p_{op}	$\frac{\hbar}{i}\nabla$
	$(p_x)_{op}$	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
	$(p_y)_{op}$	$\hbar/i\,\frac{\partial}{\partial y}$
	$(p_z)_{op}$	$\frac{\hbar}{i}\frac{\partial}{\partial z}$
velocity	v_{op}	$\frac{\hbar}{im}\nabla$
	$(v_x)_{op}$	$\frac{\hbar}{im}\frac{\partial}{\partial x}$
	$(v_y)_{op}$	$\frac{\hbar}{im}\frac{\partial}{\partial y}$
	$(v_z)_{op}$	$\frac{\hbar}{im}\frac{\partial}{\partial z}$
Position	r_{op}	r
	x_{op}	x
	y_{op}	y
	z_{op}	z

Particle in a box : One Dimensional



$\psi = 0$ at $x \le 0$ & $x \ge L$

Within the box the schrodinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0 \qquad \text{since } V = 0$$

Soln. $\psi = A \sin \frac{\sqrt{2mE}}{\hbar} x + B \cos \frac{\sqrt{2mE}}{\hbar} x$

Since $\cos 0 = 1$, second term can not describe the particle, so $B = 0$.

Now $x = L$, $\psi = 0$

$$\frac{\sqrt{2mE}}{\hbar} L = n\pi \qquad n = 1, 2, 3 \ldots$$

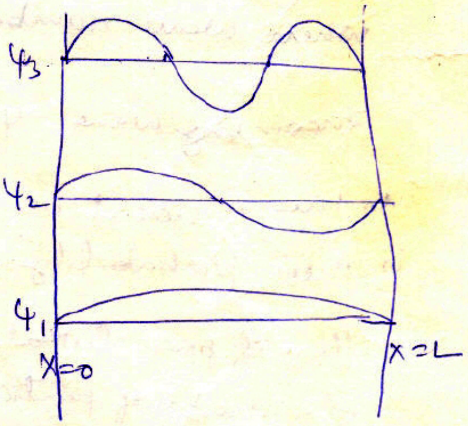
$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2h^2}{8mL^2}$$

Wave fns of particle in a box

$$\psi_n = A \sin \frac{\sqrt{2mE_n}}{\hbar} x$$

Substituting

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

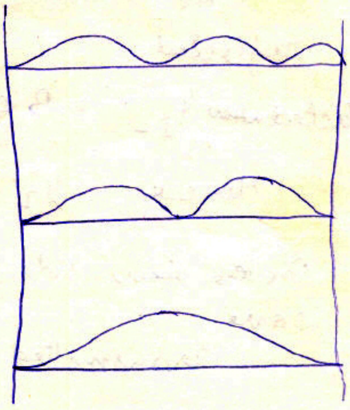


Normalise

$$\int_{-\infty}^{\infty} |\psi_n|^2 dx = \int_0^L |\psi_n|^2 dx = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx$$

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

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

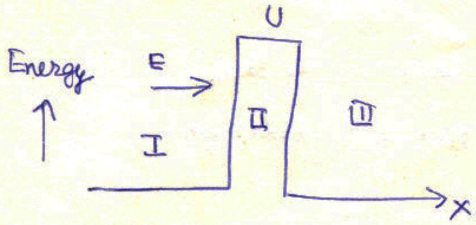


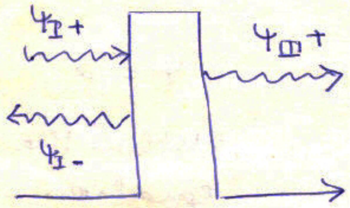
but $\int_{-\infty}^{\infty} |\psi_n|^2 dx = 1$

$$A^2\frac{L}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

$$\boxed{\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}} \qquad n = 1, 2, 3 \ldots$$

Potential Barrier :





An alpha particle whose energy is only a few mev is able to escape from a nucleus whose potential wall is perhaps 25 Mev high.

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

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

The solutions of these equations that are appropriate

$$\psi_I = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_{III} = Fe^{ik_1x} + Ge^{-ik_1x}$$

where wave number outside barrier $k_1 = \frac{\sqrt{2mE}}{\hbar}$

Incoming wave $\psi_{I+} = Ae^{ik_1x}$ This beam corresponds to the incident beam of particles in the sense that $|\psi_{I+}|^2$ is their probability density.

flux of particles that arrive at the barrier $S = |\psi_{I+}|^2 v_{I+}$
($S \Rightarrow$ number of particles per square meter per second).

At $x=0$ incident beam strikes the barrier & partially reflected

Reflected wave $\psi_{I-} = Be^{-ik_1x}$

Hence $\psi_I = \psi_{I+} + \psi_{I-}$

On the far side of the barrier $(x > L)$ there can only be a wave

Transmitted wave $\psi_{III+} = Fe^{ik_1x}$ travelling in the $+x$ direction. Hence $G=0$.

(22)

$\psi_{III} = \psi_{III+} = Fe^{ik_1x}$

The transmission probability T for a particle to pass through the barrier is the ratio.

Transmission Probability $$T = \frac{|\psi_{III+}|^2 v_{III+}}{|\psi_{I+}|^2 v_{I+}} = \frac{FF^* v_{III+}}{AA^* v_{I+}}$$

T is the fraction of incident particles that succeed in tunneling through the barrier. Classically T=0 because a particle with E<U can not exist inside the barrier. Now use quantum mechanics

In region II schrodinger's equation for the particle is

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2}(E-U)\psi_{II} = \frac{d^2\psi_{II}}{dx^2} - \frac{2m}{\hbar^2}(U-E)\psi_{II} = 0$$

Since U > E the solution is

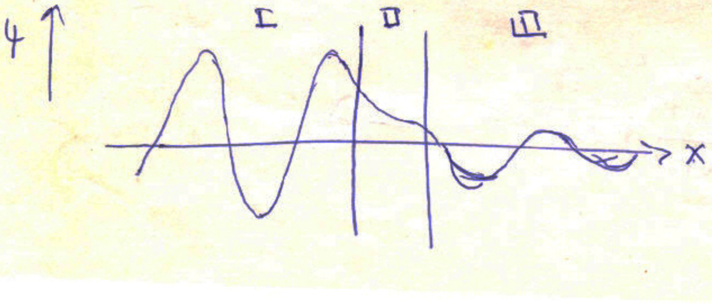
wave function inside barrier $\psi_{II} = Ce^{-k_2x} + De^{k_2x}$

Where the wave number inside the barrier is

$$k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$$

Since the exponents are real quantities, ψ_{II} does not oscillate and therefore does not represent a moving particle. However, the probability density $|\psi_{II}|^2$ is not zero, so there is a finite probability of finding a particle within the barrier. Such a particle may emerge into region III or it may return to region I.

Applying the boundary conditions:



boundary condition that wave fn & its derivative must be continuous

at $x=0$ $\qquad \psi_{I} = \psi_{II}$

$$\frac{d\psi_{I}}{dx} = \frac{d\psi_{II}}{dx}$$

at right hand side

$$\left.\begin{aligned} \psi_{II} &= \psi_{III} \\ \frac{d\psi_{II}}{dx} &= \frac{d\psi_{III}}{dx} \end{aligned}\right\} x=L$$

Which yields

$$A+B = C+D \quad \text{——(1)}$$

$$ik_1 A - ik_1 B = -k_2 C + k_2 D \quad \text{——(2)}$$

$$Ce^{-k_2 L} + De^{k_2 L} = Fe^{ik_1 L} \quad \text{——(3)}$$

$$-k_2 C e^{-k_2 L} + k_2 D e^{k_2 L} = ik_1 F e^{ik_1 L} \quad \text{——(4)}$$

eqn (1) & (4) may be solved for (A/F).

$$\frac{A}{F} = \left[\frac{1}{2} + \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right] e^{(ik_1+k_2)L} + \left[\frac{1}{2} - \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right] e^{(ik_1-k_2)L} \quad \text{——(5)}$$

Let us assume that the potential barrier U is high relative to the energy E of the incident particle. If this is the case $\frac{k_2}{k_1} > k_1/k_2$ and $\frac{k_2}{k_1} - \frac{k_1}{k_2}$ ie $\frac{k_2}{k_1}$

Let us assume that the barrier is wide enough for ψ_{II} to be severely weakened between $x=0$ and $x=L$. This means that $k_2 L >> 1$ and

$$e^{k_2 L} >> e^{-k_2 L}$$

Hence eqn (5) can be approximated as

$$\frac{A}{F} = \left(\frac{1}{2} + \frac{ik_2}{4k_1}\right) e^{(+ik_1+k_2)L}$$

Now multiply (A/F) to $\left(\frac{A}{F}\right)^*$

$$\frac{AA^*}{FF^*} = \left(\frac{1}{4} + \frac{k_2^2}{16k_1^2}\right) e^{2k_2 L} \quad \text{——(6)}$$

Transmission Probabily $T = \dfrac{FF^* v_{III+}}{AA^* v_{I+}} = \left(\dfrac{AA^*}{FF^*}\right)^{-1}$ as $v_{III+} = v_{I+}$ kinetic energy is same on both sides of barrier.

$$\boxed{T = \left[\frac{16}{4+(k_2/k_1)^2}\right] e^{-2k_2 L}}$$

Here $\left(\dfrac{k_2}{k_1}\right)^2 = \dfrac{2m(U-E)/\hbar^2}{2mE/\hbar^2} = \dfrac{U}{E} - 1$

Approximate Transmission Probabilty, as term in bracket is always of the order 1.

$$T \approx e^{-2k_2 L}$$

HARMONIC OSCILLATOR: The condition for harmonic motion is the presence of a restoring force that acts to return the system to its equilibrium configuration when it is disturbed.

$$F = -kx \qquad \text{Hook's law}$$

From the second law of motion

$$-kx = m\frac{d^2x}{dt^2}$$

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0$$

Soln. $x = A\cos(2\pi\nu t + \phi)$

where ν, frequency of harmonic oscillator

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

The importance of the simple harmonic oscillator in both classical and modern physics lies not in the strict adherence of actual restoring forces to Hook's law, which is seldom true, but in the fact that these restoring forces reduce to Hook's law for small displacements x. As a result, any system in which something executes small vibrations about an equilibrium position behaves very much like a simple harmonic oscillator.

Use Maclaurin's series about the equilibrium

$$F(x) = F_{x=0} + \left(\frac{dF}{dx}\right)_{x=0} x + \frac{1}{2}\left(\frac{d^2F}{dx^2}\right)_{x=0} x^2 + \frac{1}{6}\left(\frac{d^3F}{dx^3}\right)_{x=0} x^3 + \cdots$$

$F_{x=0} = 0$ (equilibrium). For small x the term involving higher orders will be neglected.

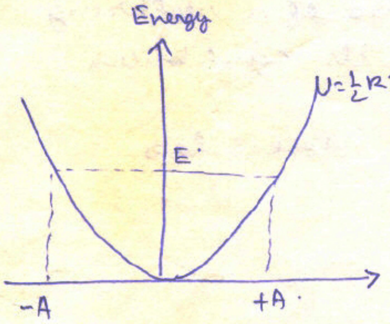
$$F(x) = \left(\frac{dF}{dx}\right)_{x=0} x$$

, $\left(\frac{dF}{dx}\right)_{x=0}$ is negative, as of course it is for any restoring force.

$\therefore$ $\boxed{F = -kx}$ which is Hook's law.

Potential energy

$$U(x) = -\int_0^x F(x)\,dx = k\int_0^x x\,dx = \frac{1}{2}kx^2$$



The Schrodinger wave eqn for oscillator

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\psi = 0$$

or $$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}\left(E - \frac{1}{2}kx^2\right)\psi = 0$$

Putting $\frac{8\pi^2 mE}{h^2} = \alpha$ and $\sqrt{\frac{8\pi^2 mk}{2h^2}} = \beta$

$$\frac{d^2\psi}{dx^2} + (\alpha - \beta^2 x^2)\psi = 0$$

Introducing a dimensionless independent variable such that

$\xi = \sqrt{\beta}\,x$ & solving. we will have

$$\frac{d^2\psi}{d\xi^2} + \left(\frac{\alpha}{\beta} - \xi^2\right)\psi = 0$$

To solve this equation, let us try solution

$\psi = c\,U\,e^{-\xi^2/2}$, where U is a fn of ξ.

We get $\frac{d^2U}{d\xi^2} - 2\xi\frac{dU}{d\xi} + \left(\frac{\alpha}{\beta} - 1\right)U = 0$

If we replace $\frac{\alpha}{\beta} - 1$ by $2n$, this equation becomes Hermite polynomial. Then function $U(\xi)$ may be replaced by Hermite polynomial $H(\xi)$. Then we get

$$\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + 2nH = 0$$

Then solution

$$\psi = C H e^{-\xi^2/2}$$

Hence in general form

$$\psi_n(\xi) = C H_n(\xi)\, e^{-\xi^2/2} \quad \text{where } n = 0, 1, 2, 3 \ldots$$

Eigen values of energy

$$\frac{\alpha}{\beta} - 1 = 2n$$

$$\frac{\alpha}{\beta} = 2n+1 \qquad \text{Since } \alpha = \frac{8\pi^2 mE}{h^2} \text{ \& } \beta = \frac{2\pi}{h}\sqrt{mk}$$

we have

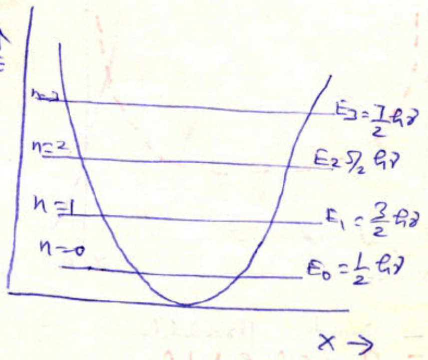
$$\frac{8\pi^2 mE}{h^2} \Big/ \frac{2\pi\sqrt{mk}}{h} = 2n+1 = 2\left(n+\tfrac{1}{2}\right)$$

or $\quad E = \left(n+\frac{1}{2}\right)\frac{h}{2\pi}\sqrt{k/m}$

or $\quad \boxed{E = \left(n+\frac{1}{2}\right)h\nu} \qquad n = 0, 1, 2, \ldots$

Wave mechanical harmonic oscillator can take only certain discreate energies separated by intervals $h\nu$. Thus discreate energy levels are equidistant.

Since eigen values of energies depend only upon quantum number n, the energy levels are non-degenerate.



For $n = 0$, $E_0 = \frac{1}{2}h\nu$

It is the lowest energy which the oscillator can have. This is called zero point energy.

Significance of Zero point energy:

For lowest (ground) state $n=0$, $E_0 = \frac{1}{2}h\nu$

Even if the temperature reduces to absolute zero, the oscillator would still have an amount of energy $\frac{1}{2}h\nu$.

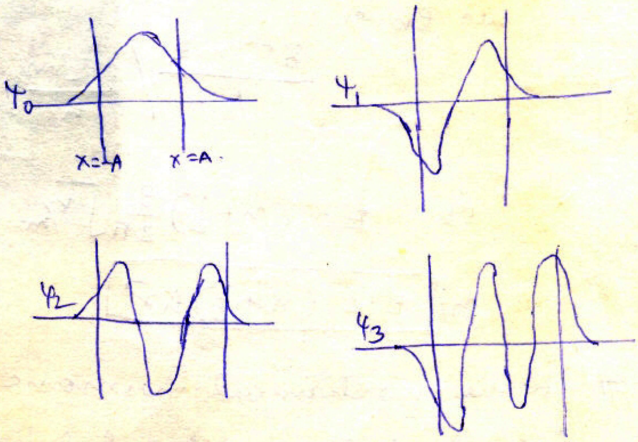
The existance of zero point energy is an important feature of wave mechanics and has been found to be experimentally true. Experiments in scattering of light by crystals at low temperatures show that when temperature is decreased, the intensity of scattered light due to thermal oscillations of the atom in crystal lattice, tends to a finite limit and remains unchanged with further decrease in temperature. It indicates that the oscillations of the atom in the crystal do not stop even at absolute zero.

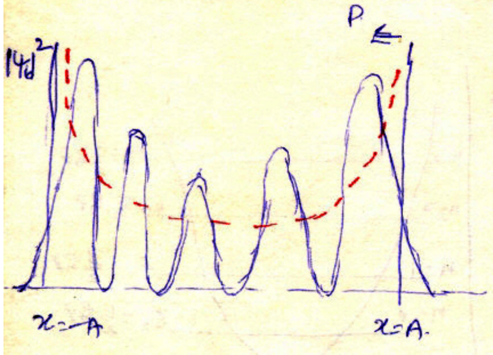
Wave functions:

$$\psi_n = \left(\frac{2m\nu}{\hbar}\right)^{1/4}\left(2^n n!\right)^{-1/2} H_n(\xi)\, e^{-\frac{\xi^2}{2}}$$

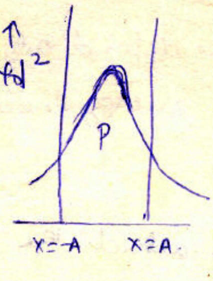
Six Hermite Polynomials

n	$H_n(y)$	α_n	E_n
0	1	1	$\frac{1}{2}h\nu$
1	$2y$	3	$\frac{3}{2}h\nu$
2	$4y^2-2$	5	$\frac{5}{2}h\nu$
3	$8y^3-12y$	7	$\frac{7}{2}h\nu$
4	$16y^4-48y^2+12$	9	$\frac{9}{2}h\nu$
5	$32y^5-160y^3+120y$	11	$\frac{11}{2}h\nu$





– Quantum Probability
– Classical Probability



In the limit of large quantum numbers, quantum Physics yields the same results as Classical Physics. (Correspondence Principle)

Exponential tails of $|\psi|^2$ beyond $x=\pm A$ also decrease in magnitude with increasing n.