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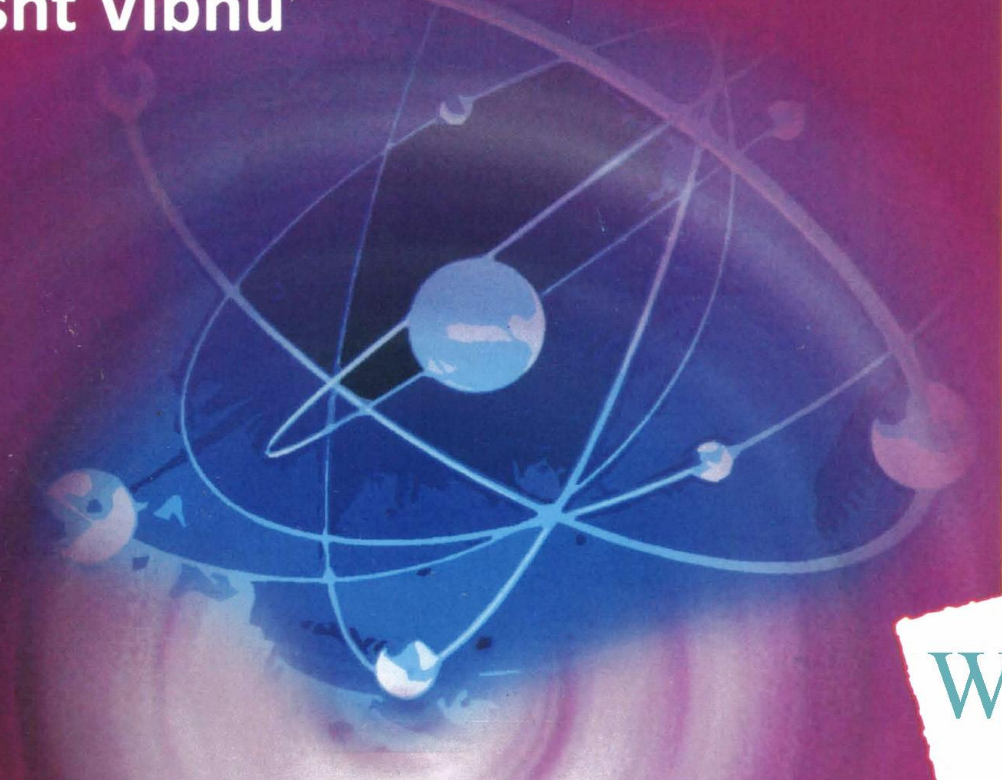
ENGINEERING PHYSICS

Volume II

Vishal Singh Chandel
Isht Vibhu



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Engineering Physics

Volume-II

Vishal Singh Chandel
Senior Lecturer
Department of Physics
Integral University
Kursi Road, Lucknow - 226 026 (UP), India

Isht Vibhu
Lecturer
Department of Physics
Yuvraj Dutt Mahavidyalaya
Lakhimpur Kheri - 262 701 (UP), India

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"This page is Intentionally Left Blank"

Unit - I

Wave Mechanics and X-ray Diffraction

If you are not confused by quantum mechanics, then you have not understood it.

Niels Bohr

❖❖❖

I do not like it, and I am sorry I ever had anything to do with it.

Erwin Schrödinger

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Chapter 1
Wave Mechanics

Wave particle duality, de-Broglie matter waves, Phase and Group velocities, Davission-Germer experiment, Heisenberg uncertainty principle and its applications, Wave function and its significance, Schrodinger's wave equation - particle in one dimensional box

1.1 de Broglie's Hypothesis

In order to explain the phenomenon of photoelectric effect, Einstein, in 1905 revolutionarized the quantum hypothesis of Planck and propounded that not only production but also propagation of electromagnetic waves is in the packets of energy i.e. quanta or photons. Thus, it was established that light has dual character — wave as well as particle.

In 1924, de Broglie suggested that matter, like light, has a dual character (particle and wave like) and that the relation between momentum p of the matter particle with the wavelength λ of associated matter wave is

$$\lambda = h/p, \; h = \text{Planck's constant.}$$

λ is called de Broglie wavelength

As in case of electromagnetic (e m) waves, the wave and particle aspects of moving bodies can never be observed at the same time. We therefore cannot ask which is the correct description. All that can be said is that in certain situation a moving body resembles a wave and in others it resembles a particle. Which set of properties is most conspicuous depends on how its de Broglie wavelength compares with its dimensions and dimensions of whatever it interacts with.

1.1.1 Concept of Wave Packet

The amplitude of the de Broglie wave that correspond to a moving a body reflects the probability that it will be found at a particular place at a particular time. It is clear that de Broglie wave cannot be represented simply by the usual formula for plane monochromatic wave $y = A \cos (kx - \omega t)$, which describes an infinite series of wave all with the same amplitude A. Moreover, the phase velocity of monochromatic de Broglies wave is greater than the velocity of light so special theory of relativity restricts that a particle in motion can not be described (represented) by a monochromatic wave.

It is noteworthy that at any given instant of time, the effect of the particle in motion is significant over a small region. In wave mechaincs, when waves of slightly differing frequencies interfere, a sort of bunching or packet formation occurs. These wavegroups or wavepacketes have limited spatial existence. This suggest that it might be possible to use concentrated buches of waves to describe localized particles of matter and quanta of radiation.

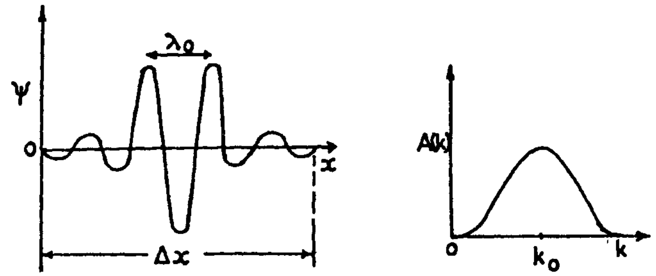

Fig. 1.1

1.1.2 Expression for group velocity:

Following figure shows how wavegroups are formed because of interference between two plane harmonic waves of **equal amplitudes** but **slightly different frequencies** travelling from left to right.

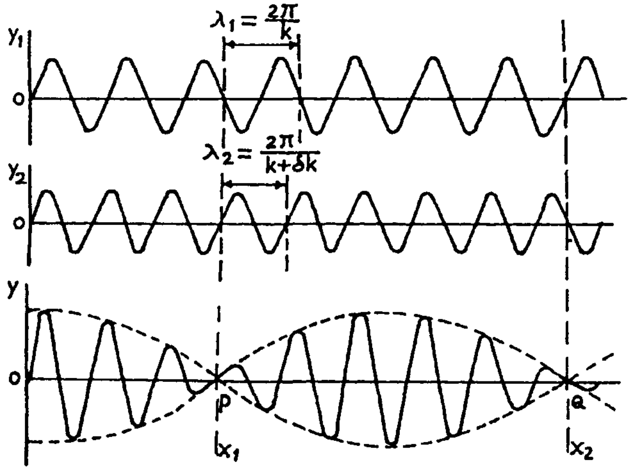

Fig. 1.2

When such a group travels in a dispersive medium, the phase velocities of different component are different. The observed velocity is however the velocity with which the maximum amplitude of the group advances in medium. This is called the 'group velocity'. The individual waves travel 'inside' the group with their phase velocities.

Let us consider a wave group consisting of two components of equal amplitude a but slightly different angular frequencies ω_1 and ω_2, and propagation constants k_1 and k_2. It ω_1 and ω_2 differ only slightly, we can write

$$\omega_2 = \omega_1 + \Delta\omega$$

$$k_2 = k_1 + \Delta k$$

where $\Delta\omega \to 0$ and $\Delta k \to 0$

Their separate displacements are given as

$$y_1 = A \sin(\omega_1 t - k_1 x)$$

and $$y_2 = A \sin\{(\omega + \Delta\omega t)t - (k_1 + \Delta k)x\}$$

Their superposition gives

$$y = y_1 + y_2$$

$$= 2A\sin\left\{\omega_1 t - k_1 x + \frac{\Delta\omega t - \Delta kx}{2}\right\} \times \cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)$$

(using the trigonometric relation $\sin A + \sin B = 2\sin\frac{A+B}{2}\cos\frac{A-B}{2}$)

for small values of $\Delta\omega$ and ΔK, we can write $y \cong R\sin(\omega_1 t - k_1 x)$

where

$$R = 2A\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right) \text{ is the amplitude.}$$

This represents a wavesystem similar to the component ones, but with an oscillating amplitude k, which is modulated both is space and time by a slowly varying envelope of frequency $\frac{\Delta\omega}{2}$ and propagation constant $\frac{\Delta k}{2}$ and has a maximum value 2A.

The velocity with which this envelope moves, is the same as the velocity of the maximum amplitude of the group and is given by

$$v_g = \frac{\Delta\omega/2}{\Delta k/2} = \frac{\Delta\omega}{\Delta k}$$

If a group contains a number of frequency components in an infinitesimally small frequency interval, then the expression for the group velocity becomes

$$v_g = \text{limit}_{\Delta k \to 0} \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk} \tag{1.1}$$

This is the general expression for group velocity.

Also, phase velocity is given as

$$\because v_p = \frac{\omega}{k} = v_\lambda \text{ which gives } \omega = kv_p$$

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

$$= v_p + \frac{2\pi}{\lambda}\frac{dv_p}{d\lambda}.\frac{d\lambda}{dk}$$

$$= v_p + \frac{2\pi}{\lambda}\frac{dv_p}{d\lambda}\left(-\frac{2\pi}{k^2}\right) \qquad \left(\because k = \frac{2\pi}{\lambda}\right)$$

$$= v_p - \frac{4\pi^2}{\lambda k^2}\frac{dv_p}{d\lambda}$$

$$= v_p - \frac{4\pi^2}{\lambda \frac{4\pi^2}{\lambda^2}}\frac{dv_p}{d\lambda}$$

$$v_g = v_p - \lambda\frac{dv_p}{d\lambda} \tag{1.2}$$

This is the relation between group velocity v_g and wave velocity v_p in a dispersive medium.

1.1.3 Derivation of de Broglie relationship

de Broglie assumed that –

(1) The frequency ν of the wave associated with a particle in motion and the total relativistic energy E of the particle are related by the relation.

$$h\nu = E = \hbar\omega \tag{1.3}$$

(2) The particle in motion is considered as a wave packet of small extension formed by the superposition of a large number of wave lengths slightly different from the associated wavelength λ and centred about it such that

particle velocity = group velocity, i.e.

$$v = v_g = \frac{d\omega}{dk} \tag{1.4}$$

here ω = angular frequency

$= 2\pi\nu$

$$= \frac{E}{h/2\pi} \qquad \text{(from equation 1.3)}$$

$$= \frac{E}{\hbar}$$

$$= \frac{\sqrt{p^2c^2 + m_o{}^2c^4}}{\hbar} \qquad \left[\begin{array}{l} \because E = \sqrt{p^2c^2 + m_o{}^2c^4} \\ \text{here} \\ p = \text{relativistic momentum} \\ \quad = \dfrac{m_o v}{\sqrt{1 - v^2/c^2}} \end{array}\right]$$

we need a relationship between p and λ (or k) so we try to replace ω by p, as follows, in the relation given in equaiton (1.4).

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

$$v = \frac{d}{dk}\left(\frac{E}{h}\right)$$

$$= \frac{1}{h}\frac{d}{dk}\left(\sqrt{p^2c^2 + m^2{}_oc^4}\right)$$

$$= \frac{1}{h}.\left(\frac{1}{\not{2}\sqrt{p^2c^2 + m^2{}_oc^4}}.\not{2}pc^2\frac{dp}{dk}\right)$$

$$= \frac{p\not{c}^2}{h(m\not{c}^2)}\frac{dp}{dk} \qquad \left(E = \sqrt{p^2c^2 + m_o{}^2c^4} = mc^2\right)$$

$$\not{v} = \frac{(\not{m}\not{v})}{h\not{m}}\frac{dp}{dk} \qquad (p = mv)$$

$$hdk = dp$$

on integrating

$$hk = p + c, \text{here} \quad c = \text{constant of integration}$$

If we choose $k = 0$ when $p = 0, c = 0$

hence $hk = p$

$$p = \frac{h}{2\pi}.\frac{2\pi}{\lambda}$$

$$p = \frac{h}{\lambda} \qquad (1.5)$$

This is de Broglie's relation. It gives the relation between wave length of the matter wave associated with a particle moving with momentum p. Thus it couples the wave with the particle properties.

1.1.4 Group velocity of de Broglie wave and particle velocity

It can be shown that group velocity of the de Broglie wave packet associated with a moving body is equal to the velocity of the body.

We know that,

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

$$\text{where } p = \hbar k = \frac{h}{\lambda}$$

$$\text{and } E = \hbar\omega = \hbar\nu$$

For relativistic case,

$$p = \frac{m_0 v}{\sqrt{1 - v^2/c^2}} = mv$$

$$E = \frac{m_o c^2}{\sqrt{1 - v^2/c^2}} = mc^2$$

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

Here v is the velocity of the particle. We can write

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

$$= \hbar \frac{d\omega}{dp} \qquad (\because p = \hbar k)$$

$$= \hbar \frac{d}{dp}\left(\frac{E}{\hbar}\right) \qquad \left(\because \omega = \frac{E}{\hbar}\right)$$

$$v_g = \frac{dE}{dp}$$

$$= \frac{d}{dp}\sqrt{p^2c^2 + m_0^2c^4}$$

$$= \frac{1}{\cancel{2}\sqrt{p^2c^2 + m_0^2c^4}} \cdot \cancel{2}pc^2$$

$$= \frac{pc^2}{E} = \frac{(\cancel{m}v)\cancel{c^2}}{\cancel{m}\cancel{c^2}}$$

$$v_g = v \qquad (1.8)$$

1.1.5 Insignificance of phase Velocity for Matter Waves

de Broglie wavelength associated with a particle of mass m and moving with velocity v is given by de Broglie relation

$$\lambda = \frac{h}{mv} \tag{1.9}$$

here h = planck's constant = 6.63×10^{-34} J sec. Total relativistic energy of the particle is

$$mc^2 = E = h\nu \tag{1.10}$$

here ν = de Broglie frequency.

so phase velocity of the de Broglie wave

$$v_p = \nu = \frac{\cancel{m}c^2}{\cancel{h}} \cdot \frac{\cancel{h}}{\cancel{m}v}$$

$$v_p = \frac{c^2}{v} \tag{1.11}$$

But we must have

v < c (From special theory of relativity)

$$\Rightarrow \frac{c}{v} > 1 \text{ for every value of v}$$

$$\Rightarrow c\,\frac{c}{v} > c$$

$$\Rightarrow \frac{c^2}{v} > c$$

$$\Rightarrow v_p > c$$

⇒ value of v_p violates the axioms of special theory of relativity.

⇒ phase velocity has no physical significance.

1.1.6 Davisson and Germer's experiment

This is an experiment to establish the wave nature of electrons.

Theoretical Foundation

de Broglie wavelength of an electron accelerated by a potential difference V (non -relativistically) is given as

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

$$\text{or } \lambda = \frac{h}{\sqrt{2m_e K}}$$

here h = Planck's constant

p = particale momentum

$= \sqrt{2mK}$

where

K = kinetic energy of particle = eV

and m = mass

$$\Rightarrow \lambda = \frac{h}{\sqrt{2m_e eV}}$$

K = eV

e = electronic charge

V = accelerating potential

If V is in volts then putting the values of h, m_e, e, we get

$$\lambda = \frac{12.28}{\sqrt{V}} \text{Å} \qquad (1.12)$$

$$h = 6.63 \times 10^{-34} \text{ J.sec.}, m_e = 9.1 \times 10^{-31} \text{ kg}, e = 1.6 \times 10^{-19} \text{ c}$$

for v~ 100 volts $\lambda \sim 1.228$Å

⇒ The wavelength of the waves associated with the beam of electron is of the same order as that of x - rays.

⇒ If such a beam of electrons is reflected from a crystal the reflected beam should show the same diffraction pattern as for x - rays of the same wavelenth.

Experimental Set up :

F = heated tungustun filament (as electron emitter)

p = accelerating plate (at a potential V w.r. to F)

C = nickel target with (1,1,1) plane face normal to the beam of electron.

D = electron detector, capable of rotating in a circle with axis at the point of incidence of electron beam on Ni crystal.

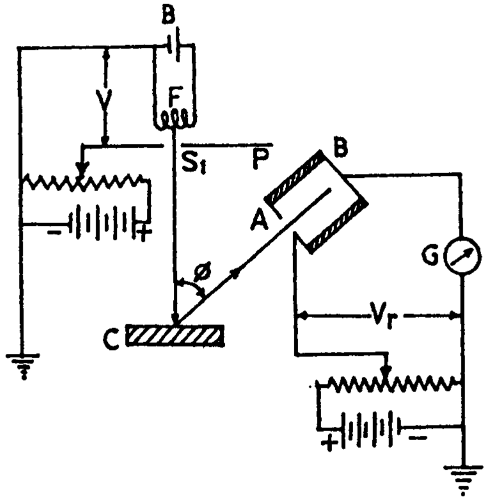

Fig. 1.3 (a) schematic setup for Davisson Germer experiment.

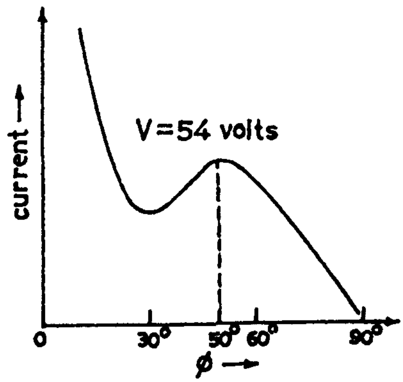

Fig 1.3. (b) results of Davisson and Germer experiment. (These are polar graphs such that the intensity at any angle is propotional to the distance of curve at the angle from the point of scattering.)

Classical Expectation

Continous variation of scattered electron intensity with angle, resulting in circles centred at the point of scattering.

Actual Results

Distinct maxima and minima were observed whose position depended upon the electron energy, and therefore on accelerating potential. In a particular case

V = 54V, a sharp maximum at θ = 50⁰ was obtained. The angle of incidence and angle fo scattering relative to family of Bragg's plane are both 65°.

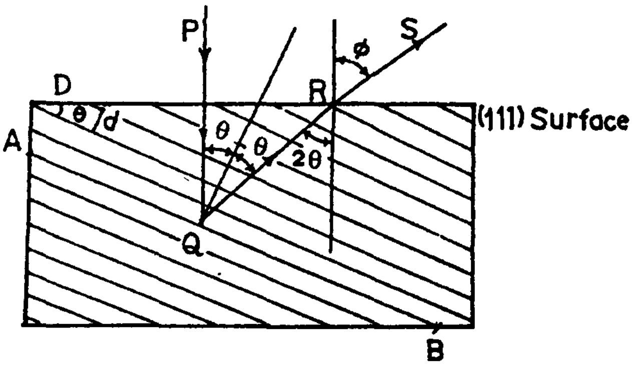

Fig. 1.4

spacing d = 0.091nm

n =1 (first order)

Bragg's condition gives

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

or λ =0.165 nm

also de Broglie wavelength λ_d

$$\Rightarrow \lambda_d = \frac{12.28}{\sqrt{54}} \text{ Å} = 1.66 \text{ Å} = 0.166 \text{ nm}$$

$$\Rightarrow \lambda_d \cong \lambda$$

Thus experiment of Davisson and Germer directly verifies de Broglie's hypothesis of the wave nature of moving bodies.

1.1.7. Application of de Broglie's Relation

(1) Particle in a box

consider the relativistic velocities. From a wave point of view, a particle trapped in box is like a standing wave. The wave variable (ψ) must be zero at the walls, since the wave stops here. Thus, only those values of the de Broglie wave length are permitted for which

$$n\left(\frac{\lambda}{2}\right) = L \text{ where L= width of the box}$$

and n = 1, 2, 3............

so K.E. of the particle in a box is

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

$$= \frac{h^2}{2m\lambda^2} \qquad \left(\because p = \frac{h}{\lambda}\right)$$

$$K.E. = \frac{n^2h^2}{8mL^2} \qquad \left(\because \lambda = \frac{2L}{h}\right) \qquad (1.13)$$

Following conclusions can be drawn from this equaiton

(1) A trapped particle can't have an arbitrary energy, as a free particle can. Its confinement leads to restriction on its wave function that allow the particle to have only certain specific energies and not the others. Exactly these energies depends on the mass of the particle and on the details of how it is trapped.

(2) A trapped particle can't have zero energy. Since the de Broglie wavelength of the particle is $\lambda = \frac{h}{mv}$, v = 0 means infinite wavelenth. But there is no way to reconcile an infinite wavelenth with a trapped particle, so such a particle must have at least some kinetic energy. This result of non-zero kinetic energy has no classical counterpart.

(3) Because h is small, quantisation of energy is conspicuous only when m and L are small. This is why we are not aware of energy quantisation in our own experience of day to day life.

(II) Quantization of energy levels in atoms

Bohr's quantization Condition

Bohr's ad- hoc assumption that the angular momentum of electron in orbit is integral multiple of $\hbar = \frac{h}{2\pi}$ i.e.

$mvr = n\hbar \ (n = 1, 2, 3)$

can be derived using de Broglie relation. For this purpose, we argue that

1. The motion of the electron in stationary orbit is represented by a matter wave of wavelength λ given by the de Broglie's relationship $\lambda = \frac{h}{p}$ where p is the linear momentum of the electron in the orbit.

2. An electron orbit contains an integral number of de Broglie's wavelength. This is clear from the accompanying figures as a fractional number of

wavelengths can not persist because destructive interference will occur. This means circumference of the orbit must be equal to integral multiple of de Broglie wavelength of the electron.

This means circumference of the orbit

$$= n\lambda \quad (n = 1, 2, 3......)$$

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

$$\Rightarrow pr = n\frac{h}{2\pi} = n\hbar$$

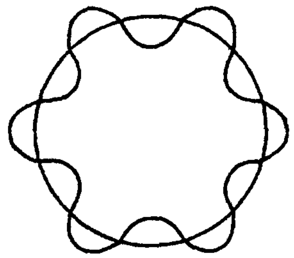

Fig. 1.5

$\Rightarrow$angular momentum = pr = n $\hbar$

Which is Bohr's condition.

1.2 Heisenberg's Uncertainty Particle

1.2.1 Statement

It is impossible to specify precisely and simultaneously the values of both members of particular pairs (canonically conjugate) of physical variables that describes the behavior of system.

Quantitavily, the order of magnitude of the product of the uncertainties in the knowledge of two variables (Δa and Δb say) must be at least $\frac{h}{2\pi}$ where 'h' is the Planck's constant. i.e.

$$\Delta a.\Delta b \geq \left(\frac{h}{2\pi}\right)$$

From classical mechanics it is found that a rectangular co-ordinate x (or y or z) of a particle and the corresponding component of momentum p_x (or p_y or p_z), a component L_z of angular momentum of a particle and it angular position ϕ in the perpendicular x-y plane, the energy E of the particular energy level and the time t at which it is mesured are some of such pair of variables called canonical conjugates. So Heisenberg's principle says that.

$$\begin{aligned} &\Delta x.\ \Delta p_x \geq \hbar \\ &\Delta y.\ \Delta p_y \geq \hbar \\ &\Delta z\ \Delta p_z \geq \hbar \\ &\Delta \tau_z\ \Delta \phi \geq \hbar \\ &\Delta E.\ \Delta t \geq \hbar \end{aligned} \qquad (1.15)$$

1.22 Derivation of Uncertainty Principle

If we define uncertainity as

$$\Delta x = <[<x^2> - <x>^2]>^{1/2} \tag{1.16}$$

And
$$\Delta p = <[<p^2> - <p>^2]>^{1/2} \tag{1.17}$$

And choose the normalized wave function ψ (x) centred around x = 0 initially, and has zero average momentum, we simplify above expression as

$$\Delta x = [<x^2>]^{1/2}$$

And
$$\Delta p = [<p^2>]^{1/2}$$

Here < > denotes expectation value

i.e.

$$<x^2> = \int_{-\infty}^{+\infty} \psi^* x^2 \psi dx$$
$$= \int_{-\infty}^{+\infty} (x\psi^*)(x\psi) dx$$
$$= \int_{-\infty}^{+\infty} (x\psi^*)(x\psi) dx$$

$$\Rightarrow (\Delta x)^2 = <x^2> = \int_{-\infty}^{+\infty} f^* f dx \tag{1.17}$$

$$\text{where } f^* = x\psi^* \text{ and } f = x\psi \tag{1.18}$$

also

$$<p>^2 = <p^2> = \int_{-\infty}^{+\infty} \psi^* \left(-i\hbar\frac{\partial}{\partial x}\right)^2 \psi \, dx$$
$$= -h^2 \int_{-\infty}^{+\infty} \psi^* \frac{d^2\psi}{dx^2} dx$$

If we difine a function $g(x) = -i\hbar \dfrac{\partial\psi}{\partial x}$ (1.19)

then $\int_{-\infty}^{+\infty} g^*(x)\, g(x)\, dx = \int_{-\infty}^{+\infty} \left(i\hbar \dfrac{\partial\psi^*}{\partial x}\right)\left(-i\hbar \dfrac{\partial\psi}{\partial x}\right) dx$

$$= \hbar^2 \int_{-\infty}^{\infty} \left(\frac{\partial\psi^*}{\partial x}\right)\left(\frac{\partial\psi}{\partial x}\right) dx$$