

Quantum Mechanics

- **Heisenberg's Uncertainty Principle:**

Statement: It is not possible to determine both the position and momentum of a particle simultaneously and accurately.

(OR)

The product of uncertainties inherently present in measuring the position and momentum of a particle is always equal to or greater than $h/4\pi$.

$$\text{i.e. } \Delta x \cdot \Delta p \geq h/4\pi$$

Heisenberg's uncertainty principle is also applicable for other pairs of conjugate variables such as energy & time and angular position & angular momentum.

Heisenberg's uncertainty relationships:

$$(1) \quad \Delta x \cdot \Delta p \geq h/4\pi$$

$$(2) \quad \Delta \theta \cdot \Delta L \geq h/4\pi$$

$$(3) \quad \Delta t \cdot \Delta E \geq h/4\pi$$

- **Explanation:**

Heisenberg's uncertainty principle is a natural consequence of wave nature of matter. When we consider the particle as a wave group, there are fundamental limits to the accuracy with which we can determine the particle properties like position and momentum,

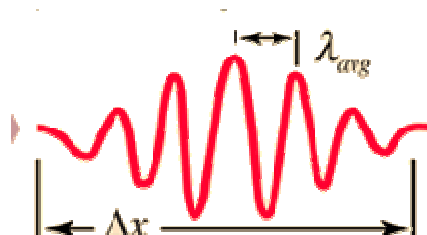
Let us consider an individual wave which can extend from $x = -\infty$ to $x = +\infty$.

This wave has a precisely defined wavelength (λ) and hence its momentum ($P = h / \lambda$) can be determined precisely.

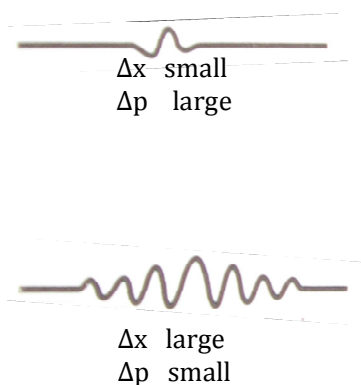
i.e. the uncertainty in the momentum, $\Delta p = 0$.

However, the amplitude of the wave is the same at all points from $x = -\infty$ to $x = +\infty$. (i.e. the wave packet extends from $x = -\infty$ to $x = +\infty$). Hence the location of the

particle becomes uncertain. In other words, the uncertainty in determining the position is, $\Delta x = \infty$.



In order to localize the particle and reduce the uncertainty in position (Δx), the wave packet must be very narrow. A narrow wave packet is formed only when large number of waves of different wavelengths overlaps. In such case, wavelength measurement becomes uncertain and hence this introduces uncertainty in the momentum. A large number of waves will result in lesser Δx and higher value of Δp and vice versa.



A more rigorous Fourier analysis of the waves will give us the relationship

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

This is the statement of Heisenberg's uncertainty principle.

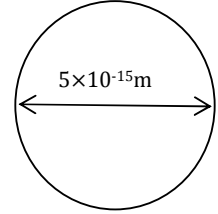
Uncertainties involved in the measurements are inherent in nature and not due to inaccuracy of the measuring instruments. This arises from wave properties of the material particles.

- **Applications of Heisenberg's uncertainty principle**

(i) To show that electrons cannot exist within the atomic nucleus:

The diameter of an atomic nucleus is $\approx 5 \times 10^{-15} \text{ m}$.

Suppose an electron exists inside the atomic nucleus, the uncertainty in determining its position must be less than $5 \times 10^{-15} \text{ m}$ (i.e. $\Delta x < 5 \times 10^{-15} \text{ m}$).



Then by Heisenberg's uncertainty principle, the uncertainty in determining its momentum must be, $\Delta p \geq h/4\pi \cdot \Delta x$

$$\therefore \Delta p > 6.6 \times 10^{-34} / 4 \times 3.14 \times 5 \times 10^{-15}$$

$$\Delta p > 1.05 \times 10^{-20} \text{ kg m s}^{-1}$$

The momentum of electron cannot be less than uncertainty in its momentum.

$$\text{i.e. } p \geq \Delta p$$

$$\therefore p \geq 1.05 \times 10^{-20} \text{ kg m s}^{-1}$$

The relativistic mass of electron is given by, $m = m_0 / \sqrt{1 - (v^2/c^2)}$

where m_0 is the rest mass of electron.

Squaring this equation and rearranging the terms, we obtain

$$m^2 [c^2 - v^2] = m_0^2 c^2$$

Multiplying on both sides with c^2 we get,

$$m^2 c^4 - m^2 c^2 v^2 = m_0^2 c^4 \quad \text{or} \quad E^2 = E_0^2 + p^2 c^2$$

Therefore, energy of electron, $E = \sqrt{E_0^2 + P^2 c^2}$

Substituting $p = 1.05 \times 10^{-20}$ in this, we get the total energy of electron inside the nucleus.

$$E = \sqrt{\{9.1 \times 10^{-31} \times (3 \times 10^8)^2\}^2 + \{(1.05 \times 10^{-20})^2 \times (3 \times 10^8)^2\}}$$

$$E = 20 \text{ MeV}$$

If an electron has 20 MeV of energy, it will escape from the nucleus because the maximum binding energy of a nucleon is about 8 MeV. Also experiments on beta decay show that even the electrons associated with unstable nucleus have energy of the order of 3-4 MeV. Hence an electron cannot be confined within the atomic nucleus.

- **Wave function (Ψ):**

Matter waves are represented by a complex function, $\Psi(x,t)$, which is called wave function. The wave function Ψ provides all possible information about the particle which is associated with wave-character. The state of the system is described or represented by Ψ which is a function of space and time coordinates.

The wave function Ψ has no direct physical meaning. According to Max Born interpretation, square of the wave function represents the probability of locating the particle (i.e. probability density) in a given region.

The well behaved wave function should satisfy the following conditions or Properties:

- (i) Ψ should be finite.
- (ii) Ψ should be single valued.
- (iii) Ψ and its first derivative should be continuous.
- (iv) Ψ should be normalizable.

$$\text{i.e. } \int_{-\infty}^{+\infty} \Psi_x^* \Psi_x dx = 1 \quad (\text{OR}) \quad \int_{-\infty}^{+\infty} \Psi_x^2 dx = 1$$

The above condition is called **normalization condition**. A wave function which satisfies above equation is said to be normalized.

- **Schrodinger's time independent wave equation in one dimension:**

The classical wave equation that describes any type of wave motion can be given as

$$\frac{\partial^2 y(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y(x, t)}{\partial t^2}$$

Where y is a variable quantity that propagates in 'x' direction with a velocity 'v'.

Matter waves should also satisfy a similar equation. Hence we can write the equation for matter waves as:

$$\frac{\partial^2 \Psi(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi(x, t)}{\partial t^2} \dots \dots (i)$$

We can eliminate the time dependence from the above equation by assuming a suitable form of the wave function and making appropriate substitutions.

Let $\Psi(x, t) = \Psi_x e^{-i\omega t} \dots \dots \dots (ii)$

where, Ψ_x depends only on 'x,' and $e^{-i\omega t}$ depends only on 't'.

Differentiate eqn. (ii) w.r.t. 'x' successively to obtain

$$\frac{\partial \Psi(x, t)}{\partial x} = \frac{\partial \Psi_x}{dx} e^{-i\omega t} \text{ and}$$

$$\frac{\partial^2 \Psi(x, t)}{\partial x^2} = \frac{\partial^2 \Psi_x}{\partial x^2} e^{-i\omega t} \dots \dots \dots (iii)$$

Differentiate eqn.(ii) w.r.t. 't' to obtain

$$\frac{\partial \Psi(x, t)}{\partial t} = (-i\omega) \Psi_x e^{-i\omega t}$$

$$\frac{\partial^2 \Psi(x, t)}{\partial t^2} = (-i\omega)^2 \Psi_x e^{-i\omega t} \dots \dots \dots (iv)$$

Substituting (iii) and (iv) in eqn. (i), we obtain

$$\frac{\partial^2 \Psi_x}{\partial x^2} e^{-i\omega t} = -\frac{\omega^2}{v^2} \Psi_x e^{-i\omega t} \dots \dots (v)$$

We can cancel $e^{-i\omega t}$ on both sides to eliminate time dependence and get

$$\frac{\partial^2 \Psi_x}{\partial x^2} = -\frac{\omega^2}{v^2} \Psi_x = -k^2 \Psi_x \dots \dots (vi)$$

$$(or) \quad \frac{\partial^2 \psi_x}{\partial x^2} + k^2 \psi_x = 0 \quad \dots\dots (vii)$$

$$k = \frac{2\pi}{\lambda} \quad \text{and} \quad \lambda = \frac{h}{p}, \quad \therefore k^2 = \frac{4\pi^2 p^2}{h^2}$$

The total energy of the particle is the sum of kinetic and potential energy.

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

$$(or) \quad p^2 = 2m(E - V)$$

$$\therefore k^2 = 8\pi^2 m(E - V) / h^2$$

Substituting the value of k^2 in eqn.(vii) , we obtain the Schrodinger's time independent wave equation in one dimension as:

$$\frac{d^2 \psi_x}{dx^2} + \frac{8\pi^2 m(E - V)}{h^2} \psi_x = 0$$

Note: Eigen functions and Eigen values:

A system is defined by its energy, momentum, position etc. Once, the wave function Ψ corresponding to a system is known, the state of system can be determined. In order to find Ψ , the Schrödinger equation has to be solved. But, it is second order differential equation; there are not one but several solutions. All of them may not be correct wave functions which we are looking for. We have to select those wave functions which would correspond meaningfully to a physical system. Such acceptable well behaved wave functions which are finite, continuous, single valued and normalized are called **eigen functions** while the energies corresponding to these eigen functions are called **eigen values**. (*Eigen is the German word meaning proper or characteristic*).

- **Applications of Schrodinger's time independent wave equation**

1) **Particle in an infinite one dimensional potential well** (OR) **Particle in a box**

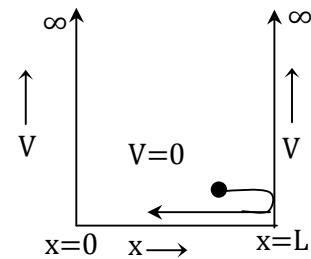
Consider a particle of mass 'm' confined to a one dimensional potential well of width 'L' and infinite wall height.

Let the potential energy of particle be, $V = \infty$ at $x=0$ and $x=L$. Let $V = 0$ for $0 < x < L$.

The walls are perfectly rigid and the probability of finding the particle is zero at the walls.

Hence, the boundary conditions are, $\Psi_x = 0$ at $x = 0$ and also $\Psi_x = 0$ at $x = L$.

The one dimensional time independent Schrodinger's wave equation is



$$\frac{d^2\Psi_x}{dx^2} + \frac{8\pi^2m(E-V)}{h^2} \Psi_x = 0$$

We can substitute $V=0$, since the particle is free to move inside the potential well.

$$\frac{d^2\Psi_x}{dx^2} + \frac{8\pi^2mE}{h^2} \Psi_x = 0$$

$$\text{Let } \left(\frac{8\pi^2mE}{h^2} \right) = k^2$$

Then, the Schrodinger's wave equation is, $\frac{d^2\Psi(x)}{dx^2} + k^2\Psi(x) = 0$

The above equation represents simple harmonic motion and the general solution of it is

$$\Psi_x = A \sin kx + B \cos kx \quad \dots\dots\dots(1)$$

Applying the boundary condition, $\Psi_x = 0$ at $x = 0$, we get

$$0 = A.0 + B$$

$$\therefore B = 0$$

Substituting the condition $\Psi_x = 0$ at $x = L$, we get

$$A \sin kL = 0.$$

Here $A \neq 0$ because it leads to trivial solution, $\Psi_x = 0$ in the entire box which is not correct.

$$\therefore \sin kL = 0$$

This implies that, $kL = 0, \pi, 2\pi, 3\pi, \dots \dots n\pi$

$$(OR) \quad k = \frac{n\pi}{L} \quad \text{where } n = 1, 2, 3, \dots \dots \text{ is a positive integer.}$$

This is called quantization condition.

➤ **Eigen values:**

$$\text{We have, } \left(\frac{8\pi^2 m E}{h^2} \right) = k^2 \Rightarrow E = \frac{h^2 k^2}{8\pi^2 m}$$

Substituting $k = \frac{n\pi}{L}$, we get energy Eigen values,

$$E_n = \frac{k^2 h^2}{8\pi^2 m} = \frac{n^2 \pi^2 h^2}{8\pi^2 m L^2}$$

$$(OR) \quad E_n = \frac{n^2 h^2}{8mL^2}$$

Here n is the quantum number corresponding to a given energy level.

$n=1$ corresponds to the ground state, $n=2$ corresponds to the first excited state and so on.

From above equation it is clear that the energy of the particle confined in a box can have only certain discrete values i.e., energy of the particle is quantized.

➤ **Eigen functions:**

From equation (1), the allowed wave functions are

$$\Psi_x = A \sin \left(\frac{n\pi}{L} x \right)$$

The constant A can be evaluated from normalization condition, $\int_0^L \Psi_x^2 dx = 1$

$$\text{i.e.} \quad \int_{x=0}^{x=L} A^2 \sin^2(n\pi x/L) dx = 1$$

using the trigonometric identity $\sin^2 \theta = (1 - \cos 2\theta)/2$, we get

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

$$\text{after integration we obtain,} \quad \frac{A^2}{2} \left[x - \frac{L}{2n\pi} \sin(2n\pi x/L) \right]_0^L = 1$$

$$\frac{A^2 L}{2} = 1 \quad (\text{OR}) \quad A = \sqrt{2/L}$$

$$\text{Hence, the eigen functions are} \quad \Psi_n(x) = \sqrt{2/L} \sin\left(\frac{n\pi}{L} x\right)$$

➤ **Graphical representation** of E_n , $\Psi_n(x)$ and $P_n(x)$ for $n = 1, 2$ and 3 quantum states.

Eigen values

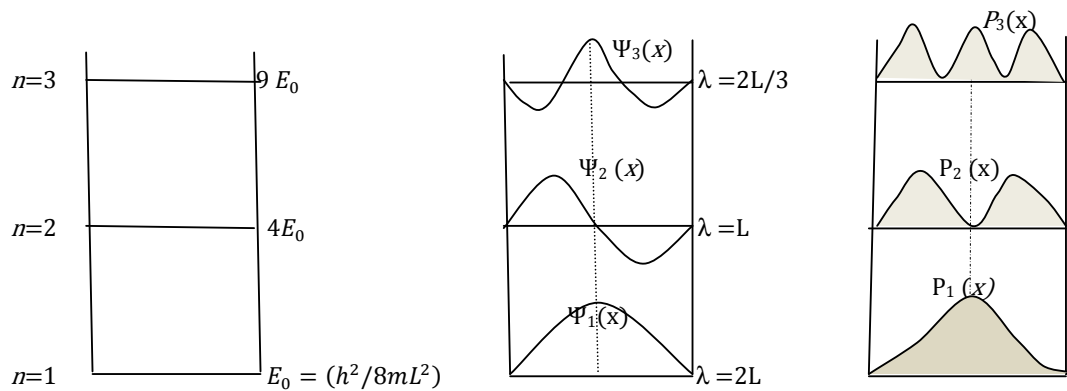
Eigen functions

Probability densities

$$E_n = n^2 h^2 / 8mL^2$$

$$\Psi_n(x) = \sqrt{2/L} \sin(n\pi x/L)$$

$$P_n(x) = \frac{2}{L} \sin^2(n\pi x/L) dx$$



Note:

- The wave length ' λ ' of the matter waves satisfies the condition for stationary waves.

$$k = n\pi/L = \frac{2\pi}{\lambda} \quad \text{or} \quad \frac{n\lambda}{2} = L$$

- Probability densities:

The probability of finding the particle in a small region ' dx ' in a given quantum state ' n ' is

$$P_n(x) = \frac{2}{L} \sin^2(n\pi x/L) dx$$

$$\text{(OR)} \quad \int_{x_1}^{x_2} P_n(x) dx = \int_{x_1}^{x_2} \frac{2}{L} \sin^2(n\pi x/L) dx$$