2.3 THE NEED FOR A WAVE FUNCTION

From the classical theory of waves. We know that waves are characterized by an amplitude function such that the intensity of the wave at any point is determined by the square of the amplitude.

Assuming that associated with each particle a wave function $\Psi(x, t)$ such that the absolute square of this function gives the intensity I:

$$I = |\Psi(x, t)|^2 = \Psi^*(x, t)\ \Psi(x, t)$$

where * denotes complex-conjugation.

For simplicity, we have taken

- One-dimensional wave function but the treatment can be easily generalized to 3D.
- $|\Psi(x, t)|$ is taken because the wave function is, in general, a complex quantity.
- The intensity I, is a real, positive quantity.

In the case of the double-slit experiment with particles,

At some point on the screen let,

Ψ_1 the wave function corresponding to the waves spreading from slit 1 with $I_1 = |\Psi_1|^2$

Ψ_2 the wave function corresponding to the waves spreading from slit 2 with $I_2 = |\Psi_2|^2$

I_1 , I_2 : The corresponding intensities on the screen when only one slit is open.

When both the slits are open, the resultant amplitude:

$$\Psi = \Psi_1 + \Psi_2$$

The resultant intensity is, therefore

$$I = |\Psi|^2 = |\Psi_1 + \Psi_2|^2$$

Let us write

$$\Psi_1 = |\Psi_1|e^{i\alpha_1},\ \Psi_2 = |\Psi_2|e^{i\alpha_2}$$

where $|\Psi_1|, |\Psi_2|$ are the absolute values and α_1, α_2 are the phases of the two wave functions, respectively. Then

$$|\Psi_1|^2 = \Psi_1^*\ \Psi_1 \quad \text{and} \quad |\Psi_2|^2 = \Psi_2^*\Psi_2$$

This gives

$$
\begin{aligned}
I &= (\Psi_1 + \Psi_2)^*\ (\Psi_1 + \Psi_2) \\
&= \Psi_1^*\Psi_1 + \Psi_2^*\Psi_1 + \Psi_1^*\Psi_2 + \Psi_2^*\Psi_2 \\
&= |\Psi_1|^2 + |\Psi_2|^2 + \Psi_1^*\Psi_2 + \Psi_2^*\Psi_1 \\
&= |\Psi_1|^2 + |\Psi_2|^2 + |\Psi_1|\ |\Psi_2|\ (e^{-i(\alpha_1 - \alpha_2)} + e^{i(\alpha_1 - \alpha_2)}) \\
&= I_1 + I_2 + 2\sqrt{I_1 I_2}\ \cos(\alpha_1 - \alpha_2)
\end{aligned}
$$

This shows that $I \neq I_1 + I_2$,

$2\sqrt{I_1 I_2} \cos(\alpha_1 - \alpha_2)$ is the *interference* term.

We shall see in later that the wave function satisfies a linear equation which is known as the Schrödinger equation.

The quantum mechanical wave function $\Psi(x,t)$ is an abstract quantity.

Max Born, in 1926, suggested that the wave function must be interpreted statistically.as follows:

If a particle is described by a wave function $\Psi(x,t)$, then the probability $P(x)\,dx$ of finding the particle within an element dx about the point x at time t is;

$$\boxed{P(x)\,dx = |\Psi(x,t)|^2\,dx}$$

The quantity

$$P(x) = |\Psi(x,\ t)|^2 = \Psi^*(x,\ t)\Psi(x,\ t)$$

is, naturally, called the **position probability density**.

Since the probability of finding the particle somewhere must be unity, the wave function should be normalized so that

$$\boxed{\int_{-\infty}^{\infty} \Psi^* \Psi\,dx = 1}$$

That is, the wave function should be *square integrable*.

2.4 Wave Packet and the Uncertainty Principle

From the de Broglie relation; $\quad p = \dfrac{h}{\lambda} = \hbar k$

where $k = 2\pi/\lambda = propagation\ constant$ or the *wave number*.

E is the energy of the particle

ν is the frequency of the associated wave

$E = h\nu = \hbar\omega$ is the Planck-Einstein relation

$\omega = 2\pi\nu$ is the angular frequency of the wave.

Let us consider a plane, monochromatic wave as a wave function to be associated with a particle,

$$\Psi(x,\ t) = A e^{i(kx - \omega t)}$$

Which represents a simple harmonic disturbance of wavelength λ and frequency ν, travelling towards the positive x-direction with velocity, $v_{ph} = \dfrac{\omega}{k} = $ *phase velocity*.

The plane wave $\Psi(x, t)$ represents a particle having a momentum $p = \hbar k$.

The probability density (the amplitude A is constant)

$$P = |\Psi(x, t)|^2 = A^2$$

P is independent of position. Thus, the particle has equal probability of being found anywhere.

So, the question is: *how to construct a wave function that can look like a particle?*

A particle can be represented by a wave packet.

A wave packet can be formed by superposing plane waves of different wave numbers in such a way that they interfere with each other destructively outside of a given region of space.

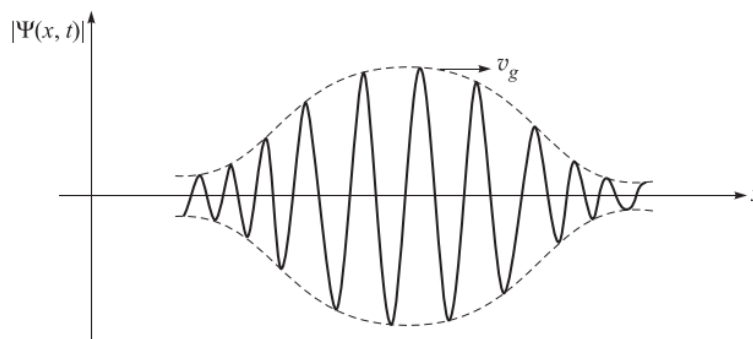Let $\Psi(x, t)$ be a one-dimensional wave packet formed by

of plane waves:

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)e^{i(kx - \omega t)} \, dk$$

where the amplitude A and the angular frequency ω depend on k.

a **wave packet** which moves with the *group velocity*

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

A wave packet propagating along the x-axis.

If Δx is the spatial extent of a wave packet and Δk is its wave number range, then it always happens that $\Delta x \, \Delta k \geq 1$ Heisenberg's uncertainty principle

2.5 HEISENBERG'S UNCERTAINTY PRINCIPLE

- In classical mechanics,

The position x and the momentum p of a particle are independent of each other and can be simultaneously measured precisely.

- In quantum mechanics,

a particle is represented by a wave packet. The particle may be found anywhere within the region where the amplitude of the wave function $\Psi(x)$ is nonzero.

How precisely we can determine the position and the momentum of a particle simultaneously?

By using the relation $\Delta x\, \Delta k \geq 1$ and $p = \hbar k$ we obtain $\Delta x\, \Delta p \geq \hbar$

This is Heisenberg's uncertainty relation for position and momentum.

It states that it is *not possible to specify both the position and the momentum of a particle simultaneously with arbitrary precision; the product of the uncertainties in the position and the momentum is always greater than a quantity of order $\hbar$.*

It is important to note that there is no uncertainty relation between one cartesian component of the position vector of a particle and a different cartesian component of the momentum.

$$\boxed{\begin{array}{l} \Delta x\, \Delta p_x \geq \hbar \\ \Delta y\, \Delta p_y \geq \hbar \\ \Delta z\, \Delta p_z \geq \hbar \end{array}}$$

Energy-Time Uncertainty Relation

The energy E of a free particle of mass m and momentum p is

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

If Δp is the uncertainty in momentum then the uncertainty in energy is

$$\Delta E = \frac{2p}{2m}\, \Delta p = \frac{p}{m}\, \Delta p = v\, \Delta p$$

where v is the velocity of the particle.

The uncertainty in time $\Delta t = \frac{\Delta x}{v}$

Multiplying the two,

$$\Delta E\, \Delta t = (v\Delta p)\left(\frac{\Delta x}{v}\right) = \Delta x\, \Delta p \geq \hbar$$

or
$$\Delta E \Delta t \geq \hbar$$

PROBLEM: Calculate the uncertainty in the momentum of a proton confined in a nucleus of radius $10^{-14} m$. From this result, estimate the kinetic energy of the proton.

Solution: If the proton is confined within a nucleus of radius r_0, then the uncertainty in its momentum is

$$\Delta p \approx \frac{\hbar}{r_0} = \frac{1.054 \times 10^{-34}}{10^{-14}} = \boxed{1.054 \times 10^{-20} \text{ kg m/s}}$$

Taking the momentum p to be of order Δp, the kinetic energy of the proton is given by

$$E = \frac{p^2}{2m} \approx \frac{\hbar^2}{2mr_0^2}$$

where m is the mass of the proton. Substituting the values,

$$E \approx \frac{(1.054 \times 10^{-34})^2}{2 \times 1.67 \times 10^{-27} \times (10^{-14})^2}$$

$$= 0.3326 \times 10^{-13} \text{ J}$$

$$= \frac{0.3326 \times 10^{-13}}{1.6 \times 10^{-13}} \text{ MeV}$$

$$= \boxed{0.21 \text{ MeV}}$$

PROBLEM: The lifetime of a nucleus in an excited state is $10^{-12}s$. Calculate the probable uncertainty in the energy and frequency of a γ-ray photon emitted by it.

Solution: The energy-time uncertainty relation is

$$\Delta E \, \Delta t \approx \hbar$$

Therefore, the uncertainty in energy is

$$\Delta E \approx \frac{\hbar}{\Delta t} = \frac{1.054 \times 10^{-34}}{10^{-12}} = \boxed{1.054 \times 10^{-22} \text{ J}}$$

The uncertainty in frequency is

$$\Delta \nu = \frac{\Delta E}{h} = \frac{1.054 \times 10^{-22}}{6.625 \times 10^{-34}} = \boxed{1.59 \times 10^{11} \text{ Hz}}$$

PROBLEM: Using the uncertainty principle, show that an alpha particle can exist inside a nucleus.

Solution: The radius of a typical nucleus is of the order of 10^{-14} m. If a particle is to exist within the nucleus, then the uncertainty in its position must be of this order:

$$\Delta x \approx 10^{-14} \text{ m}$$

Therefore, the uncertainty in the momentum of the particle must be

$$\Delta p \approx \frac{\hbar}{\Delta x} = \frac{1.054 \times 10^{-34}}{10^{-14}}$$

$$= 1.054 \times 10^{-20} \text{ kg m/s}$$

The momentum of the particle is at least of this order.

The rest mass of an α-particle is approximately four times the mass of a proton:

$$m = 4 \times 1.67 \times 10^{-27} \text{ kg}$$

The speed of the α-particle would be

$$v = \frac{1.054 \times 10^{-20}}{4 \times 1.67 \times 10^{-27}} = 1.58 \times 10^6 \text{ m/s}$$

With this speed the motion can be considered nonrelativistic. Therefore, the kinetic energy of the particle is at least

$$K = \frac{p^2}{2m} = \frac{(1.054 \times 10^{-20})^2}{2 \times 4 \times 1.67 \times 10^{-27}}$$

$$= 8.3 \times 10^{-15} \text{ J}$$

$$= \boxed{52 \text{ keV}}$$

2.6 summery about wavefunction

In Quantum Mechanics, a "particle" (e.g. an electron) does not follow a definite trajectory $r(t), p(t)$ but rather it is best described as being distributed through space like a wave.

Wavefunction $\Psi(x)$: is a wave representing the spatial distribution of a "particle".

- e.g. electrons in an atom are described by a wavefunction centred on the nucleus.

$\Psi(x)$: is a function of the coordinates defining the position of the classical particle

One-dimension (1D) time independent $\qquad \Psi(x)$

Three-dimension (3D) time independent $\qquad \Psi(r) = \Psi(x, y, z) = \Psi(r, \theta, \phi)$ (e.g. atoms)

Ψ may be time dependent e.g. $\Psi(x, t)$ and $\Psi(r, t) = \Psi(x, y, z, t) = \Psi(r, \theta, \phi, t)$

Interpretation of the Wavefunction

- In QM, a "particle" is distributed in space like a wave.

- We cannot define a position for the particle.

- Instead, we define a probability of finding the particle at any point in space.

The Born Interpretation (1926): *"The square of the wavefunction at any point in space is proportional to the probability of finding the particle at that point."*

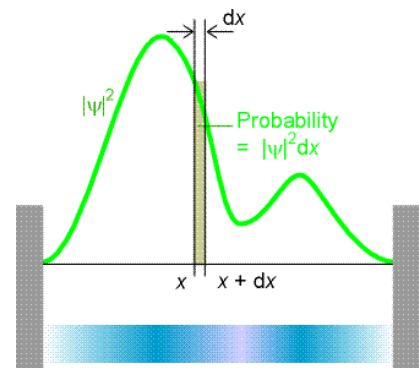**Note**: the wavefunction (Ψ) itself has no physical meaning.

If the wavefunction at point x is $\Psi(x)$, the probability of finding the particle in the infinitesimally small region dx between x and $x + dx$ is:

$$P(x) = |\Psi(x)|^2 = \Psi^*\Psi$$

$|\Psi(x)|^2$ is the **probability density**

$|\Psi(x)|$ is the magnitude of Ψ at point x

probability must be real and positive ($0 \leq P \leq 1$)

Normalization of the Wavefunction

We return now to the statistical interpretation of the wave function, which says that $p(x) = |\Psi(x,t)|^2$ is the probability density for finding the particle at point x, at time t. It follows that the integral of $|\Psi\Psi^*|^2$ must be *1* (one) (the particle's got to be somewhere):

$$P_{tot} = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

Since the probability must be (one) for finding the particle somewhere, the wave function must be normalized.

For three dimensions

$$P_{tot} = \int_{-\infty}^{\infty} |\Psi(x,y,z,t)|^2 dxdydz = \int_{-\infty}^{\infty} |\Psi(r,t)|^2 dr = 1$$

In this case, Ψ is said to be a normalized wavefunction

How to Normalize the Wavefunction

If Ψ is not normalized, then:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = N \qquad\qquad N \neq 1$$

A corresponding normalized wavefunction (Ψ_{norm}) can be defined:

$$\Psi_{norm} = \frac{1}{\sqrt{N}} \Psi$$

such that $\qquad\qquad \int_{-\infty}^{\infty} |\Psi_{norm}(x,t)|^2 dx = 1$

The factor ($\frac{1}{\sqrt{N}}$) is known as the **normalization constant**.

Quantization of the Wavefunction

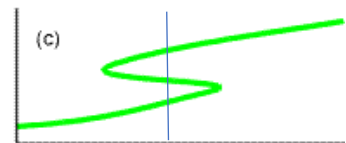The Born interpretation of y places restrictions on the form of the wavefunction:

   (a) Ψ must be continuous (no breaks).

   (b) The gradient of Ψ is $\left(\frac{d\Psi}{dx}\right)$ must be continuous.
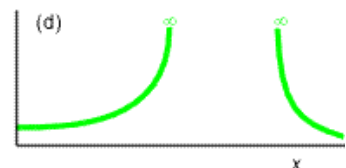
   (c) Ψ must have a single value at any point in space.

   (d) Ψ must be finite everywhere.
   (e) Ψ cannot be zero everywhere.

Operators and Observables

If Ψ is the wavefunction representing a system, we can write:

$$\hat{A}\Psi = a\Psi$$

Where a: **Observable property** of system (e.g. energy, momentum, dipole moment …)

  $\hat{A}$: **Operator** corresponding to observable a.

This is an eigenvalue equation and can be rewritten as:

$\widehat{A}\Psi$: Operator $\widehat{A}$ acting on function Ψ (**eigenfunction**)

$a\Psi$: function Ψ multiplied by a number a (**eigenvalue**)

(**Note:** Ψ can't be cancelled).

Examples:

1- If $\hat{A} = \frac{d}{dx}$ and $\Psi = e^{mx}$. Is the function Ψ an eigenfunction for the Operator $\hat{A}$. Show that.

$$\hat{A}\Psi = a\Psi$$
$$\frac{d}{dx}(e^{mx}) = me^{mx} = m\Psi$$

- The function e^{mx} is an eigenfunction for the Operator $\frac{d}{dx}$
- The magnitude m is the eigenvalue for the Operator $\frac{d}{dx}$

2- If $\hat{A} = \frac{d}{dx}$ and $\Psi = x^3$. Is the function Ψ an eigenfunction for the Operator $\hat{A}$. Show that.

$$\hat{A}\Psi = a\Psi$$
$$\frac{d}{dx}(x^3) = 3x$$

So
$$\hat{A}\Psi \neq a\Psi$$

- The function x^3 is not an eigenfunction for the Operator $\frac{d}{dx}$

3- If $\hat{A} = \frac{d^2}{dx^2}$ and $\Psi = \sin ax$. Is the function Ψ an eigenfunction for the Operator $\hat{A}$. Show that.

$$\frac{d^2}{dx^2}(\sin ax) = \frac{d}{dx}\left(\frac{d}{dx}(\sin ax)\right) = \frac{d}{dx}(a \cos ax) = -a^2 \sin ax$$

$$\frac{d^2}{dx^2}(\sin ax) = -a^2 \sin ax$$

- The function $(\sin ax)$ is an eigenfunction for the Operator $\frac{d^2}{dx^2}$
- The magnitude $(-a^2)$ is the eigenvalue for the Operator $\frac{d^2}{dx^2}$