Chapter two

Elementary properties of quantum mechanics

3.1 Introduction

In chapter one and two we introduced:

- the concept of the wave function $\Psi(\boldsymbol{r}, t)$, which is assumed to describe the dynamical state of a particle (or a physical system).
- Then we saw that a particle can be represented by a wave packet which is formed by superposing plane waves of different wave numbers.

Now, we need a wave equation, by solving it we obtain the wave function at any point (r, t) in space and time, given suitable initial and boundary conditions.

The equation must satisfy the following restrictions:

1. It must be *linear* and *homogeneous* so that the *superposition principle* holds. That is, if Ψ_1 and Ψ_2 are solutions of the equation, any linear combination $a_1\Psi_1 + a_2\Psi_2$ must also be a solution.
2. It must be a differential equation of the first order with respect to time, so that the evolution of the system is completely determined if the wave function is known at a given initial time.
3. It must be consistent with the Planck-Einstein relation $E = \hbar\omega$, the de Broglie relation $\mathbf{p} = \hbar\mathbf{k}$, and the correspondence principle.

Correspondence principle: The quantum theory must approach classical theory in the limit $n \rightarrow \infty$, where n is a quantum number.

The equation was discovered by Erwin Schrodinger in 1926 and is called the ***Schrodinger equation***.

To apply Schrodinger equation, we must understand some of the task properties of wave functions and the Operators.

3.2 Interpretation, Normalization and Quantization of the Wavefunction

In Quantum Mechanics, a "particle" (e.g. an electron) does not follow a definite trajectory $\boldsymbol{r}(t), \boldsymbol{p}(t)$ 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 $\Psi(x)$

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

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

Interpretation of the Wavefunction

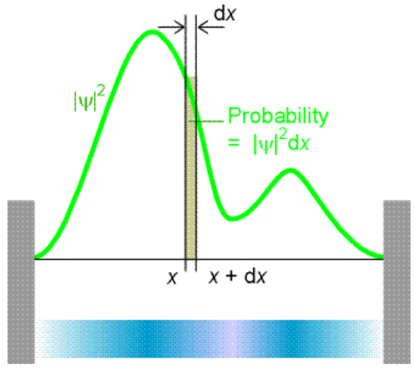
- In QM, a "particle" is distributed in space like a wave.
- We cannot define a position for the particle.
- Instead, we define a probability of finding the particle at any point in space.

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 $\Psi(\mathrm{x})$, the probability of finding the particle in the infinitesimally small region dx between x and $x + dx$ is:

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



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

$|\Psi(\mathrm{x})|$ 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

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

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

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

Quantization of the Wavefunction

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

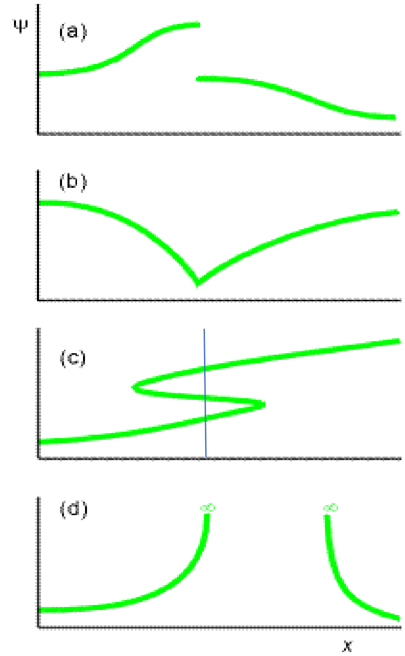
(a) Ψ must be continuous (no breaks).

(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.



3.3 Operators and Observables

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

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

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

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

This is an eigenvalue equation and can be rewritten as:

$\hat{\boldsymbol{A}}\Psi$: Operator $\hat{\boldsymbol{A}}$ 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.

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

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

- 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.

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

$$\frac{d}{dx}(x^3) = 3x$$

So

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

- 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 $\frac{d^2}{dx^2}$