



Quantum Mechanics in Medicine

Presented by

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Third-year students

Chapter two

Elementary properties of quantum mechanics

3.1 Introduction

In chapter one and two we introduced:

- the concept of the **wave function $\Psi(\mathbf{r}, t)$** , 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 $(\mathbf{r}, t)$ 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 $\mathbf{r}(t), \mathbf{p}(t)$ 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 $\Psi(\mathbf{r}) = \Psi(x, y, z) = \Psi(r, \theta, \phi)$ (e.g. atoms)

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

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:

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

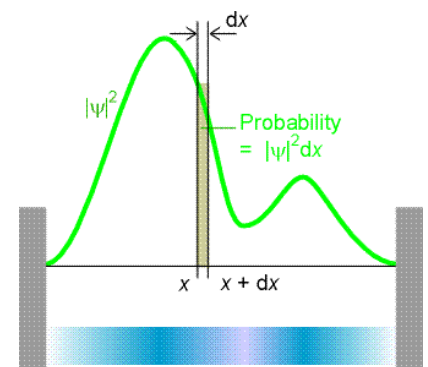
$|\Psi(x)|^2$ is the **probability density**

$|\Psi(x)|$ 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

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

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

How to Normalize the Wavefunction ?

If Ψ is not normalized, then:

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

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

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

such that

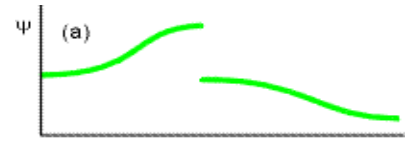
$$\int_{-\infty}^{\infty} |\Psi_{norm}(x, t)|^2 dx = 1$$

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

Quantization of the Wavefunction

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

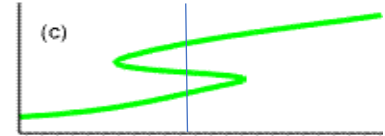
(a) Ψ must be continuous (no breaks).



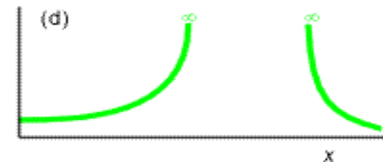
(b) The gradient of Ψ is $\left(\frac{d\Psi}{dx}\right)$ must be continuous.



(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:

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

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:

$\hat{A}\Psi$: Operator $\hat{A}$ 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 $\frac{d^2}{dx^2}$