



Quantum Mechanics in Medicine

Presented by

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Third-year students

3.4 The Time Dependent Schrödinger Equation

To begin with, we consider the one-dimensional motion of a free particle of mass m , moving in the positive x direction with momentum p and energy E . Such a particle can be described by the monochromatic plane wave

$$\Psi(x, t) = A e^{i(px-Et)/\hbar} \quad \dots(3.1)$$

where A is a constant. Differentiating with respect to t , we have

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar} \Psi \quad \dots(3.2)$$

or
$$i\hbar \frac{\partial \Psi}{\partial t} = E\Psi \quad \dots(3.3)$$

Differentiating twice with respect to x , we have

$$-i\hbar \frac{\partial \Psi}{\partial x} = p\Psi \quad \dots(3.4)$$

and
$$-\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} = p^2\Psi \quad \dots(3.5)$$

or
$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = \frac{p^2}{2m} \Psi \quad \dots(3.6)$$

Now, for a nonrelativistic free particle

$$E = \frac{p^2}{2m} \quad \dots(3.7)$$

Therefore;

$$\boxed{i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2}} \quad \dots(3.8)$$

This is the one-dimensional time-dependent Schrödinger equation for a free particle.

Since the Schrodinger equation is linear and homogeneous, it will also be satisfied by the wave packet

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int \phi(p) e^{i(px-Et)/\hbar} dp \quad \dots(3.9)$$

which is a linear superposition of plane waves and is associated with a ‘localised’ free particle. We have

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \frac{1}{\sqrt{2\pi\hbar}} \int E \phi(p) e^{i(px-Et)/\hbar} dp$$

and

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} = \frac{1}{\sqrt{2\pi\hbar}} \int \frac{p^2}{2m} \phi(p) e^{i(px-Et)/\hbar} dp$$

The righthand sides of the above two equations are equal, (where $E = \frac{p^2}{2m}$) and hence we obtain equation (3.8).

To see how it satisfies the **correspondence principle**, we note that this equation is the quantum mechanical ‘translation’ of the classical equation ($E = \frac{p^2}{2m}$), where the energy E, and the momentum p are represented by differential operators

and

$$\boxed{\begin{aligned} \hat{E} &= i\hbar \frac{\partial}{\partial t} \\ \hat{p} &= -i\hbar \frac{\partial}{\partial x} \end{aligned}} \quad \dots(3.10)$$

respectively, acting on the wave function:

$$\hat{E} \Psi(x, t) = \frac{\hat{p}^2}{2m} \Psi(x, t) \quad \dots(3.11)$$

The expression for the plane wave in three dimensions

$$\Psi(\mathbf{r}, t) = A e^{i(\mathbf{p}\cdot\mathbf{r}-Et)/\hbar} \quad \dots(3.12)$$

The **operator representation** of **p** would be

$$\boxed{\hat{\mathbf{p}} = -i\hbar \nabla} \quad \dots(3.13)$$

which is equivalent to

$$\begin{cases} \hat{p}_x = -i\hbar \frac{\partial}{\partial x} \\ \hat{p}_y = -i\hbar \frac{\partial}{\partial y} \\ \hat{p}_z = -i\hbar \frac{\partial}{\partial z} \end{cases} \quad \dots(3.14)$$

Therefore, the Schrödinger equation becomes

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t) \quad \dots(3.15)$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

3.5 Particle in a Force-field

The case of a particle acted by a force which is derivable from a potential $V(\mathbf{r}, t)$. According to classical mechanics, the total energy of the particle would be given by;

$$E = \frac{p^2}{2m} + V(\mathbf{r}, t) \quad \dots(3.16)$$

Since V does not depend on E or p , the above discussion for the free particle suggests that the wave function should satisfy

$$\hat{E}\Psi = \left(\frac{\hat{p}^2}{2m} + V \right) \Psi \quad \dots(3.17)$$

so that, the Schrödinger equation generalizes to

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left(-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}, t) \right) \Psi(\mathbf{r}, t) \quad \dots(3.18)$$

(Time-dependent Schrödinger equation)

The operator on the right-hand side is called the **Hamiltonian operator** and is denoted by the symbol **H**:

$$H = -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}, t) \quad \dots(3.19)$$

(Hamiltonian operator)

The name follows from the fact that **in classical mechanics the sum of the kinetic and the potential energies of a particle is called its Hamiltonian.**

3.6 Statistical Interpretation of The Wave Function and Conservation of Probability

If a particle is described by a wave function $\Psi(\mathbf{r}, t)$, then the probability of finding the particle, at time t , within the volume element $d\mathbf{r} = dx dy dz$ about the point $\mathbf{r} \equiv (x, y, z)$ is

$$P(\mathbf{r}, t) d\mathbf{r} = |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = \Psi^*(\mathbf{r}, t) \Psi(\mathbf{r}, t) d\mathbf{r} \quad \dots(3.20)$$

The quantity

$$P(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2 = \Psi^*(\mathbf{r}, t) \Psi(\mathbf{r}, t) \quad \dots(3.21)$$

is obviously called the **position probability density**. Since the probability of finding the particle somewhere at time t is unity, the **normalization condition**,

$$\boxed{\int |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1} \quad \dots(3.22)$$

where the integral extends over all space.

What happens as time changes.?

It is clear that the probability of finding the particle somewhere must remain **conserved**. That is, the normalization integral in (3.22) must be independent of time.

$$\frac{\partial}{\partial t} \int P(\mathbf{r}, t) d\mathbf{r} = \frac{\partial}{\partial t} \int \Psi^*(\mathbf{r}, t) \Psi(\mathbf{r}, t) d\mathbf{r} = 0 \quad \dots(3.23)$$

In order to prove this,

By use the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \quad \dots(3.24)$$

and its complex conjugate

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V\Psi^* \quad \dots(3.25)$$

where $V(\mathbf{r}, t)$ is assumed to be real.

Multiplying (3.24) by Ψ^* and (3.25) by Ψ on the left and then subtracting, we get

$$i\hbar \left[\Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t} \right] = -\frac{\hbar^2}{2m} [\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*] \quad \dots(3.26)$$

Now, consider the time derivative of the integral of $\Psi^* \Psi$ over a finite volume V . We have,

$$\begin{aligned} \frac{\partial}{\partial t} \int_V \Psi^* \Psi d\mathbf{r} &= \int_V \left[\left(\Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t} \right) \right] d\mathbf{r} \\ &= \frac{i\hbar}{2m} \int_V [(\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*)] d\mathbf{r} \end{aligned}$$

$$\text{By using (3.26)} \quad = \frac{i\hbar}{2m} \int_V \nabla \cdot (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) d\mathbf{r} \quad \dots(3.27)$$

Let us define a vector

$$\mathbf{j}(\mathbf{r}, t) = \frac{-i\hbar}{2m} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) \quad \dots(3.28)$$

Substituting in (3.27),

$$\frac{\partial}{\partial t} \int_V P(\mathbf{r}, t) d\mathbf{r} = - \int_V \nabla \cdot \mathbf{j} d\mathbf{r} \quad \dots(3.29)$$

Using Green's theorem (also called Gauss' divergence theorem) we can convert the volume integral on the right into an integral over the surface S bounding the volume V :

$$\frac{\partial}{\partial t} \int_V P(\mathbf{r}, t) d\mathbf{r} = - \int_S \mathbf{j} \cdot d\mathbf{S} \quad \dots(*)$$

Since a square integrable wave function vanishes at large distances, the surface integral becomes zero and hence (3.23) is proved.