Chapter 2. The Schrödinger Equation

<u>Classical waves</u>

$$\Psi_1(x,t) = A\sin[2\pi(\frac{x}{\lambda} - \frac{t}{T}) + \phi] = A\sin(kx - \omega t + \phi)$$

$$\Psi_2(x,t) = B\cos(kx - \omega t + \phi)$$

$$\Psi_3(x,t) = C[\cos(kx - \omega t + \phi) + i\sin(kx - \omega t + \phi)] = Ce^{-i(kx - \omega t + \phi)}$$

<u>Wave equation:</u>

$$\frac{d^2\Psi}{dx^2} + \frac{4\pi^2}{\lambda^2}\Psi = 0 \qquad \text{(standing wave)}$$

Recall $\lambda = h/p$ and $p^2 = 2m[E - V(x)]$, we have

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

where $V(x)$ is the potential. Rearrange, we have

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V(x)\Psi = E\Psi$$

This is the time-dependent <u>Schrödinger equation</u>, the fundamental equation in quantum mechanics.

Quantum operators

An operator represents a mathematic operation

$$\hat{O}f(x) = g(x)$$

Multiplication:

$$x \rightarrow x \times f(x)$$

Differentiation:

$$\frac{d}{dx} \rightarrow \frac{d}{dx} f(x)$$

In quantum mechanics, each <u>observable</u> corresponds to an <u>operator</u>.

<u>Coordinate operator:</u>

$$\hat{x} \rightarrow x \times$$

<u>Linear momentum operator:</u>

$$\hat{p}_x \rightarrow \frac{\hbar}{i}\frac{d}{dx} \qquad (\hbar = h/2\pi = 1.055 \times 10^{-34}\, Js)$$

<u>Kinetic energy operator</u>

$$\hat{T}_x = \frac{\hat{p}_x^2}{2m} \rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

Hamiltonian (energy) operator:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + V(x) \to -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

If a function $\psi_n(x)$ satisfies the eigenequation

$$\hat{O}\psi_n(x) = o_n\psi_n(x),$$

it is called an eigenfunction of the operator $\hat{O}$ with the constant o_n as its eigenvalue.

Schrödinger equation is an eigenequation:

$$\hat{H}\Psi = E\Psi$$

An operator may have more than one eigenfunction/eigenvalue.

Example:

$$\frac{d^2}{dx^2}\sin(kx) = -k^2\sin(kx)$$

So, $\sin(kx)$ is said to be an eigenfunction of the operator d^2/dx^2 with $-k^2$ as the eigenvalue.

If the eigenvalues of two eigenfunctions are the same, these two eigenstates are called degenerate (example: $\sin kx$ and $\cos kx$).

Application of a quantum operator to a system corresponds to a measurement. Each measurement yields an observable that is an eigenvalue of the corresponding operator.

The eigenvalues of a quantum operator are always real.

The eigenfunctions of a quantum operator are orthogonal:

$$\int_{-\infty}^{\infty} \psi_n^*(x)\psi_m(x)dx = 0 \qquad \text{for } n \neq m$$

where * is the complex conjugate.

They form a complete set, which means that any function can be expressed as a linear combination of the eigenfunctions:

$$\Psi(x) = \sum_{n=1}^{\infty} b_n \psi_n(x)$$

Fourier sine (and cosine) functions:

$$\int \sin(nx)\sin(mx)dx = 0 \quad \text{for } n \neq m$$

$$\Psi(x) = \sum_{n=1}^{\infty} b_n \sin(nx)$$

where the expansion coefficient is

$$b_n = \int \Psi(x)\sin(nx)dx$$