SCHROGINGER EQUATION

B. TECH. - I

THE TIME-DEPENDENT SCHRODINGER EQUATION

For a particle in a potential $V(x,t)$ then $$E = \frac{p^2}{2m} + V(x,t)$$

and we have (KE + PE) × wavefunction = (Total energy) × wavefunction

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$ **TDSE**

Points of note:

1. The TDSE is one of the postulates of quantum mechanics. Though the SE cannot be derived, it has been shown to be consistent with all experiments.
2. SE is first order with respect to *time* (*cf*. classical wave equation).
3. SE involves the complex number *i* and so its *solutions are essentially complex*. This is different from classical waves where complex numbers are used imply for convenience – see later.

THE HAMILTONIAN OPERATOR

LHS of TDSE can be written as:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x,t)\Psi=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)\Psi=\hat{H}\Psi$$

where $\hat{H}$ is called the ***Hamiltonian operator*** which is the differential operator that represents the ***total energy*** of the particle.

Thus

$$\hat{H}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)=\frac{\hat{p}_x^2}{2m}+\hat{V}(x)$$

where the ***momentum operator*** is

$$\hat{p}_x=-i\hbar\frac{\partial}{\partial x}$$

Thus shorthand for TDSE is:

$$\hat{H}\Psi=i\hbar\frac{\partial\Psi}{\partial t}$$

Suppose the potential is independent of time i.e. $V(x, t) = V(x)$ then TDSE is:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2} + V(x) = i\hbar\frac{1}{T}\frac{\partial T}{\partial t}$$

LHS involves variation of ψ with t while RHS involves variation of ψ with x. Hence look for a separated solution:

$$\Psi(x,t) = \psi(x)T(t)$$

then

$$-\frac{\hbar^2}{2m}T\frac{\partial^2\psi}{\partial x^2} + V(x)\psi T = i\hbar\psi\frac{\partial T}{\partial t}$$

Now divide by ψT:

LHS depends only upon x, RHS only on t. True for all x and t so both sides must equal a constant, E (E = separation constant).

Thus we have:

$$i\hbar\frac{1}{T}\frac{\partial T}{\partial t} = E$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2} + V(x) = E$$

TIME-INDEPENDENT SCHRÖDINGER EQUATION

Solving the time equation: $i\hbar \frac{1}{T}\frac{dT}{dt} = E \quad \Rightarrow \frac{dT}{T} = -\frac{iE}{\hbar}dt \quad \Rightarrow T(t) = Ae^{-iEt/\hbar}$

This is exactly like a wave $e^{-i\omega t}$ with $E = \hbar\omega$. Therefore $T(t)$ depends upon the energy E.

To find out what the energy actually is we must solve the space part of the problem....

The space equation becomes $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = E\psi$ or $\hat{H}\psi = E\psi$

This is the **time independent Schrödinger equation (TISE)** .