Quantum mechanics is the description of the behaviour of matter and light in all its details and in particular of the happening on ~~its~~ an atomic scale. Things on a very small scale behave like nothing that you have direct experience about.

— Feynman

Old quantum theory:

→ Plancks constant -- for explaining blackbody radiation.

→ Bohr-sommerfeld quantization rules. (an atomic system can exist in particular stationary or quantized states. Each of which corresponds to a definite energy of the system. second postulates was $E = h\nu$; $L = \hbar$)

→ De broglie wave: $\lambda = \frac{h}{p}$

Limitations:

□ It can not be applied to a periodic system.

□ It provides only a qualitative and incomplete treatment of the intensities of the spectral lines

□ Can not give the satisfactory account of the dispersion of light

□ Rotational spectra of diatomic molecule.

□ It was difficult to understand conceptually why the electrostatic interaction between a hydrogen nucleus an electron should be effective when the ability of the accelerated electron to emit electromagnetic radiation disappeared in stationary state

The schrödinger equation

In classical mechanics Newton's second law of motion is used to decribe the physical system at each time instant

In quantum mechanics the anologue of Newton's law is Schrodinger's equation.

If a particle like an electron behaves as a wave then the equation of wave motion could be successfully applied to it

The form of schrodinger equation depends on the physical situation.

The most general form is the time dependent schrodinger equation which gives a description of a system evolving with time.

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

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

The potential energy has to be specified to solve this equation different potential energy functions result in different wave function just as different forces lead to different trajectories in classical mechanics

Since this function represents the wave nature of particle it mainly should be the function of wave, thats why it is called wave function $\psi(x,t)$

□ Formulate the following eq^n $i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi$

Let us consider a particle of mass m moves along the x direction then the wave function is given by

$$\psi = Ae^{-i(\omega t - kx)}$$

we know
$\omega = 2\pi\nu$
$k = \frac{2\pi}{\lambda}$

$$\therefore \quad \psi = Ae^{-i(2\pi\nu t - \frac{2\pi}{\lambda}x)} \text{ —— (2)}$$

again $E = h\nu$

or, $\nu = \frac{E}{2\pi\hbar}$

$\lambda = \frac{h}{p}$

$= \frac{2\pi\hbar}{p}$

Putting the values in (2)

$$\psi = Ae^{-i\left(\frac{Et}{\hbar} - \frac{px}{\hbar}\right)} \text{ —— (3)}$$

differentiating (3) w.r.t x

$$\frac{\partial \psi}{\partial x} = \frac{ip}{\hbar} Ae^{-i\left(\frac{Et}{\hbar} - \frac{px}{\hbar}\right)}$$

again differentiating w.r.t. x

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2} Ae^{-i\left(\frac{Et}{\hbar} - \frac{px}{\hbar}\right)}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi \qquad \text{or, } p^2\psi = \hbar^2 \frac{\partial^2 \psi}{\partial x^2} \text{ —— (4)}$$

differentiating (3) w.r.t t

$$\frac{\partial \psi}{\partial t} = \frac{E}{\hbar} Ae^{-i\left(\frac{Et}{\hbar} - \frac{px}{\hbar}\right)}$$

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar}\psi$$

$$\text{or, } E\psi = i\hbar \frac{\partial \psi}{\partial t} \text{ —— (5)}$$

But the energy of a particle is

$$E = T + V$$

$$\text{or, } E\psi = \frac{p^2}{2m}\psi + V(\psi) \quad \text{——(6)}$$

Putting the values from eq^n (4) and (5)

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

This is the schrodinger time dependent 1D equation

Thus for 3D

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + \vec{V}\psi$$

$$\text{or } i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + \vec{V}(\psi)$$

But $\hat{H} = \frac{\hbar^2}{2m}\nabla^2\psi + \vec{V}$ and $\hat{E} = i\hbar\frac{\partial\psi}{\partial t}$

Hence

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