Schrodinger Wave Equation

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Schrodinger Wave Equation

- Schrodinger wave equation describes the behaviour of a particle in a field of force or the change of a physical quantity over time. Erwin Schrödinger who developed the equation was even awarded the Nobel Prize in 1933.

- Schrodinger wave equation is a mathematical expression describing the energy and position of the electron in space and time, taking into account the matter wave nature of the electron inside an atom.

The wave Equation (Schrodinger's equation)- time dependent

Fundamental equation of Quantum Mechanics
(like second law motion of Newtonian mechanics F=ma)
Is a wave equation in the variable ψ

For standing wave equation in classical

$$y = A\cos(\omega t - kx) \quad 1$$

Let us consider the wave equivalent of a Free Particle in a straight path at constant speed

This wave is described by general solution

$$y = A\cos(\omega t - kx) - iA\sin(\omega t - kx) \quad 2$$

(If undamped, monochromatic harmonic wave in + x direction)
2 can be written in the form

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

Only real part of (2) has significance in the case of waves in a stretched string. 'y' means displacement , imaginary is discarded as irrelevant.

In quantum mechanics the wave function 'ψ' corresponds to the wave variable 'y' of wave motion in general.

However, ψ - is not measureable quantity and may therefore be complex

Wave equation

$$\Psi\left(x,t\right)=e^{i(kx-\omega t)}$$

Schrodinger time dependent wave equation

Wave equation

$$\Psi\left(x,t\right)=e^{i(kx-\omega t)}$$

From de Broglie

$$\lambda=\frac{h}{p}\Rightarrow k=\frac{2\pi}{\lambda}=\frac{2\pi\, p}{h}=\frac{p}{\hbar}$$

From Planck's

$$E=h\nu$$

$$E=h\frac{\omega}{2\pi}=\hbar\,\omega \qquad E/\hbar=\omega$$

$$\Psi\left(x,t\right)=e^{i\left(\frac{p}{\hbar}x-\frac{E}{\hbar}t\right)}$$

$$\psi=A\,Sin\frac{2\pi}{\lambda}(vt-x)$$

$$=A\,Sin\left(\underbrace{\frac{2\pi}{\lambda}v}_{f}t-\underbrace{\frac{2\pi}{\lambda}}_{k}x\right)$$

$$=A\,Sin\left(\omega t-kx\right)$$

$$\psi\left(x,t\right)=e^{i\left(\frac{p}{\hbar}x-\frac{E}{\hbar}t\right)} \qquad \frac{\partial\psi}{\partial x}=i\frac{p\psi}{\hbar}$$

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

$$p^2\psi=-\hbar^2\frac{\partial^2\psi}{\partial x^2}$$

$$\frac{\partial\psi}{\partial t}=-i\frac{E}{\hbar}\psi\Rightarrow E\psi=-\frac{\hbar}{i}\frac{\partial\psi}{\partial t}\Rightarrow E\psi=i\hbar\frac{\partial\psi}{\partial t}$$

Total Energy,

$$E=\frac{p^2}{2m}+V\left(x\right) \qquad E\psi=\frac{p^2}{2m}\psi+V\left(x\right)\psi$$

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

Time dependent Schrödinger

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

In three dimension

Time independent Schrödinger wave equation

ψ(x, y, z, t) be the wave function for de Broglie waves .
The differential equation of wave given as

$$\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)-\frac{1}{u^2}\frac{\partial^2\psi}{\partial t^2}=0$$

The solution of differential equation in terms of time as below:

$$\psi(x, y, z, t)=\psi_0(x, y, z,)\,e^{-i\omega t}$$

Differentiating twice w.r.t. time t $\quad \frac{\partial^2\psi}{\partial t^2}=-\omega^2\psi_0 e^{-i\omega t}$ Or $\frac{\partial^2\psi}{\partial t^2}=-\omega^2\psi$

$$\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+\frac{\omega^2}{u^2}\psi=0 \qquad \omega=2\pi\nu=2\pi\frac{u}{\lambda}$$

$$\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+\frac{4\pi^2}{\lambda^2}\psi=0$$

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From de Broglie relation $\lambda=\frac{h}{p}$

$$\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+\frac{4\pi^2p^2}{h^2}\psi=0$$

Total energy = Kinetic energy + Potential energy $\quad E=\frac{p^2}{2m}+V(x,y,z)$

p^2 = 2m (E-V)

$$\boxed{\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+\frac{8\pi^2m(E-V)}{h^2}\psi=0}$$

This is time independent Schrödinger wave equation

$$\boxed{\nabla^2\psi+\frac{2m}{\hbar^2}(E-V)\psi=0} \quad \textit{where } \nabla^2\equiv\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2} \textit{ and } \hbar=\frac{h}{2\pi}$$