IDHAYA COLLEGE FOR WOMEN KUMBAKONAM – 612 001



DEPARTMENT OF PHYSICS

SEMESTER : II

CLASS : I MSc PHYSICS

SUBJECT- INCHARGE : Mr. N. MAHENDRAN

SUBJECT NAME : QUANTUM MECHANICS

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TOPIC : SCHRODINGER EQUATION

Schrodinger Equation

What is the Schrodinger Equation.

The Schrödinger equation (also known as Schrödinger's wave equation) is a partial differential equation that describes the dynamics of quantum mechanical systems via the wave function. The trajectory, the positioning, and the energy of these systems can be retrieved by solving the Schrödinger equation.

Schrödinger Wave Equation Derivation (Time-Dependent)

Considering a complex plane wave:

$$\Psi(x,t) = Ae^{i(kx-\omega t)}.$$

Now the Hamiltonian of a system is

$$H = T + V$$

Where 'V' is the potential energy and 'T' is the kinetic energy. As we already know that 'H' is the total energy, we can rewrite the equation as:

$$E = \frac{p^2}{2m} + V(x).$$

➤ Now taking the derivatives,

$$egin{aligned} rac{\partial \Psi}{\partial t} &= -i \omega A e^{i(kx-\omega t)} = -i \omega \Psi(x,t) \ rac{\partial^2 \Psi}{\partial x^2} &= -k^2 A e^{i(kx-\omega t)} = -k^2 \Psi(x,t) \end{aligned}$$

We know that,

$$p=rac{2\pi\hbar}{\lambda}$$
 and $k=rac{2\pi}{\lambda}$

where ' λ ' is the wavelength and 'k' is the wave number.

We have

$$k = \frac{p}{\hbar} .$$

Therefore,

$$rac{\partial^2 \Psi}{\partial x^2} = -rac{p^2}{\hbar^2} \, \Psi(x,t).$$

Now multiplying $\Psi(x, t)$ to the Hamiltonian we get,

$$E\Psi(x,t) = rac{p^2}{2m} \, \Psi(x,t) + V(x) \Psi(x,t).$$

The above expression can be written as:

$$E\Psi(x,t) = rac{-\hbar^2}{2m} \, rac{\partial^2 \Psi}{\partial x^2} + V(x) \Psi(x,t).$$

We already know that the energy wave of a matter wave is written as

$$E=\hbar\omega$$

So we can say that

$$E\Psi(x,t) = rac{\hbar\omega}{-i\omega} \, \Psi(x,t).$$

Now combining the right parts, we can get the Schrodinger Wave Equation.

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

This was the Derivation of Schrödinger Wave Equation (time-dependent).

In the discussion of the particle in an infinite potential well, it was observed that the wave function of a particle of fixed energy E could most naturally be written as a linear combination of wave functions of the form.

Schrödinger Wave Equation Derivation (Time-independents)

The Schr odinger wave equation of the form $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$

➤ Where the space and the time dependence of the complete wave function are contained in separate factors1.

The idea now is to see if this guess enables us to derive an equation for $\psi(x)$, the spatial part of the wave function.

If we substitute this trial solution into the Schr odinger wave equation, and make use of the meaning of partial derivatives, we get:

$$\hbar^2 2m d^2 \psi/(x) dx^2 e^{-iEt/h} + V(x)\psi(x)e^{-iEt/h} = i\hbar -iE/\hbar e^{-iEt/h} \psi(x) = E\psi(x)e^{-iEt/h}$$

The factor exp[-iEt/ ħ]cancels from both sides of the equation, giving

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

> If we rearrange the terms, we end up with

$$\hbar^2/2m d^2\psi(x)/dx^2 + (E \hbar - V(x)) \psi(x) = 0$$

which is the time independent Schrödinger equation The time dependent Schrödinger equation for one spatial dimension is of the form

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

For a free_particle where U(x) = 0 the wave function solution can be put in the form of a plane wave

$$\Psi(x,t) = Ae^{ikx - i\omega t}$$

For other problems, the potential U(x) serves to set boundary conditions on the spatial part of the wavefunction and it is helpful to separate the equation into the time_independent Schrodinger equation and the relationship for time evolution of the wave function.

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t} \qquad \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + U(x)\Psi(x) = E\Psi(x)$$
Time evolution