

Schrödinger equation

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1 Introduction

The Schrödinger's equation is a cornerstone in quantum mechanics, providing a mathematical framework to describe the behavior of particles at the quantum level. It was developed by Austrian physicist Erwin Schrödinger in 1925 and stands as one of the fundamental equations in physics.

Quantum mechanics is a branch of physics that deals with the behavior of very small particles, such as atoms and subatomic particles. Unlike classical mechanics, which governs the motion of larger objects, quantum mechanics introduces the concept of wave-particle duality, where particles exhibit both wave-like and particle-like characteristics.

Central to Schrödinger's equation is the concept of the wave function (Ψ), a mathematical description of a particle's state. The square of the wave function ($|\Psi|^2$) provides the probability density of finding a particle in a particular region of space.

Time-dependent Schrödinger's equation

The time-dependent Schrödinger's equation is expressed as:

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \quad (1)$$

Here:

- i is the imaginary unit,
- \hbar is the reduced Planck constant,
- m is the particle mass,
- $\frac{\partial \Psi}{\partial t}$ is the partial derivative of the wave function with respect to time,
- \hat{H} is the Hamiltonian operator,
- Ψ is the wave function.

The reduced Planck constant, denoted as \hbar , is defined as:

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

Here:

- h is the Planck constant, a fundamental constant in quantum mechanics,
- π is the mathematical constant representing the ratio of a circle's circumference to its diameter,
- \hbar is the reduced Planck constant, which is simply h divided by 2π .

The time-independent Schrödinger's equation is expressed as:

Time-Independent Schrödinger Equation

The Schrödinger equation is a fundamental equation in quantum mechanics that describes the behavior of quantum systems. For stationary states, where the energy of the system does not change with time, the time-independent Schrödinger equation is employed.

The time-independent Schrödinger equation is given by:

$$\hat{H}\Psi = E\Psi \quad (2)$$

Here:

- \hat{H} is the Hamiltonian operator,
- Ψ is the wave function,
- E is the energy associated with a particular state.

This equation describes the behavior of a quantum system in terms of its wave function and energy. The time-independent Schrödinger equation can be expressed as:

$$\hat{H}\Psi = E\Psi \quad (3)$$

The Hamiltonian operator \hat{H} includes kinetic and potential energy terms. In one dimension, it takes the form:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \quad (4)$$

Here:

- x is the spatial coordinate,
- $V(x)$ is the potential energy.

Schrödinger's equation is applied in diverse fields, including quantum chemistry, solid-state physics, and quantum computing. It underpins the understanding of atomic and molecular structures, electronic behaviors, and the development of quantum technologies.

In summary, Schrödinger's equation is a foundational equation in quantum mechanics, providing a mathematical framework for understanding the behavior of particles on the quantum scale.

2 Derivation of Schrödinger's Equation

Time-Independent Schrödinger Equation

The total energy (E) of a classical system is the sum of kinetic energy (KE) and potential energy (PE):

$$E = KE + PE \quad (5)$$

Considering the classical expression for kinetic and potential energy:

$$E = \frac{1}{2}mv^2 + V \quad (6)$$

where V is the potential energy. This classical energy expression can be redefined in terms of momentum (p):

$$\frac{p}{2m} = \frac{1}{2}mv^2 \quad (7)$$

This leads to the expression:

$$E = \frac{p^2}{2m} + u \quad (8)$$

Now, let's define Ψ as a wave function:

$$\Psi = e^{i(kx - \omega t)} \quad (9)$$

Taking the second derivative with respect to x , we find:

$$\frac{d^2\Psi}{dx^2} = (ik)^2\Psi \quad (10)$$

Based on the definitions of k and p :

$$k = \frac{2\pi}{\lambda} \quad (11)$$

$$p = \frac{h}{\lambda} = \frac{hk}{2\pi} = \hbar k \quad (12)$$

We obtain:

$$\frac{d^2\Psi}{dx^2} = -\frac{p^2}{\hbar^2}\Psi \quad (13)$$

which can be rewritten as:

$$-\hbar^2 \frac{d^2\Psi}{dx^2} = p^2\Psi \quad (14)$$

Multiplying Ψ on both sides of (8) gives:

$$E\Psi = \frac{p^2}{2m}\Psi + V\Psi \quad (15)$$

Thus, we arrive at the time-independent Schrödinger equation:

$$E\Psi = -\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V\Psi \quad (16)$$

Energy in Terms of Frequency

Consider the energy (E) of a photon with frequency (f) given by Planck's equation:

$$E = \hbar\omega = \hbar f \quad (17)$$

Similar to the previous derivation, we use the wave function Ψ :

$$\Psi = e^{i(kx - \omega t)} \quad (18)$$

Taking the derivative with respect to t for Ψ gives:

$$\frac{d\Psi}{dt} = -i\omega\Psi \quad (19)$$

Multiplying Ψ on both sides of (17) gives:

$$E\Psi = \hbar\omega\Psi \quad (20)$$

Then we have:

$$-\frac{i}{\hbar}E\Psi = -i\omega\Psi = \frac{d\Psi}{dt} \quad (21)$$

Then we have:

$$E\Psi = \frac{\hbar}{-i} \frac{d\Psi}{dt} = i\hbar \frac{d\Psi}{dt} \quad (22)$$

From the previous derivation of the time-independent Schrödinger's equation, we have:

$$E\Psi = -\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V\Psi \quad (23)$$

Which finally gives the time-dependent Schrödinger's equation:

$$-i\hbar \frac{d\Psi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V\Psi \quad (24)$$

3 Solving the One-Dimensional Schrödinger Equation for an Infinite Potential Well

The Schrödinger Equation

The time-independent Schrödinger equation for a particle in an infinite potential well is given by:

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

where $V(x) = 0$ for $0 < x < L$ and $V(x) = \infty$ otherwise.

Inside the Well ($0 < x < L$)

Inside the well, the Schrödinger equation simplifies to:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$

Let $k = \frac{2m(E-V)}{\hbar^2}$

$$-\frac{d^2\psi}{dx^2} = k^2\psi$$

with the general solution:

$$\psi(x) = A \sin(kx) + B \cos(kx)$$

Boundary Conditions

Applying boundary conditions at $x = 0$ and $x = L$:

$$\begin{aligned} \text{At } x = 0 : \quad \psi(0) &= 0, & \frac{d\psi}{dx}(0) &= 0 \\ \text{At } x = L : \quad \psi(L) &= 0, & \frac{d\psi}{dx}(L) &= 0 \end{aligned}$$

Solving for k , we find $k = \frac{n\pi}{L}$.

Allowed Energies

The allowed energies are quantized:

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

Wave Functions

To find the normalization constant A for the wave function $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$, we need to ensure that the probability density $|\psi_n(x)|^2$ integrates to 1 over the entire well. The probability density is given by:

$$|\psi_n(x)|^2 = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right)$$

The normalization condition is expressed as:

$$\int_0^L |\psi_n(x)|^2 dx = 1$$

Performing the integration:

$$\begin{aligned} & \int_0^L \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) dx \\ &= \frac{2}{L} \int_0^L \frac{1 - \cos\left(\frac{2n\pi x}{L}\right)}{2} dx \\ &= \frac{1}{L} \left[x - \frac{L}{2n\pi} \sin\left(\frac{2n\pi x}{L}\right) \right]_0^L \\ &= \frac{1}{L} [L - 0] \\ &= 1 \end{aligned}$$

Therefore, the normalization constant A is $A = \sqrt{\frac{2}{L}}$, and the normalized wave function is:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

