

PHY 3101

Electrical Engineering Materials

Elementary Quantum Physics

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Time evolution of wave function



Wave function and Schrödinger equation

The wave function $\Psi(x, t)$ that describes the quantum mechanics of a particle of mass m moving in a potential $V(x, t)$ satisfies the Schrödinger equation

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



Interpretation of wave function

The interpretation of the wave function arises by defining probability density

$$\rho(x, t) \equiv \Psi^*(x, t)\Psi(x, t) = |\Psi(x, t)|^2$$

$$\int_{-\infty}^{\infty} \Psi^*(x, t)\Psi(x, t)dx = 1$$

Normalization
condition



Properties of wave function

If a wave function has well-defined non-zero limits as $x \rightarrow \pm\infty$, the integral around infinity would produce an infinite result.

$$\lim_{x \rightarrow \pm\infty} \Psi(x, t) = 0$$

$$\left| \lim_{x \rightarrow \pm\infty} \frac{\partial \Psi(x, t)}{\partial x} \right| < \infty$$

Normalizing the wave function

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = \mathcal{N} \neq 1$$

Normalizable wave function

$$\Psi'(x, t) = \frac{1}{\sqrt{\mathcal{N}}} \Psi(x, t)$$

Normalized wave function

$$\int_{-\infty}^{\infty} |\Psi'(x, t)|^2 dx = \frac{1}{\mathcal{N}} \int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = \frac{1}{\mathcal{N}} \times \mathcal{N} = 1$$

Time evolution of wave function

Suppose we have a normalized wave function at an initial time $t = t_0$

$$\int_{-\infty}^{\infty} \Psi^*(x, t_0) \Psi(x, t_0) dx = 1.$$

Will it remain normalized as time goes on and Ψ evolves?

Time evolution of wave function

Since $\Psi(x, t_0)$ and the Schrödinger equation determine Ψ for all times. Do we have for a later time t ,

$$\int_{-\infty}^{\infty} \Psi^*(x, t) \Psi(x, t) dx = 1?$$

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

Time evolution of wave function

$$\rho(x, t) \equiv \Psi^*(x, t)\Psi(x, t) = |\Psi(x, t)|^2 \quad \text{Probability density}$$

$$\mathcal{N}(t) \equiv \int_{-\infty}^{\infty} \rho(x, t) dx$$

We have: $\mathcal{N}(t_0) = 1$

Need to show: $\mathcal{N}(t) = 1$

$$\frac{d\mathcal{N}(t)}{dt} = 0$$

Conservation of probability

Conservation of probability

$$\begin{aligned}\frac{d\mathcal{N}(t)}{dt} &= \int_{-\infty}^{\infty} \frac{\partial \rho(x, t)}{\partial t} dx \\ &= \int_{-\infty}^{\infty} \left(\frac{\partial \Psi^*(x, t)}{\partial t} \Psi(x, t) + \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial t} \right) dx\end{aligned}$$

Note that $\mathcal{N}(t)$ is a function only of t , so we used a total derivative but $\rho(x, t)$ is a function of x as well as t , so a partial derivative is used.

The Schrödinger equation

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

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

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

Time evolution of probability density

$$\begin{aligned}\frac{\partial \rho(x, t)}{\partial t} &= \frac{\partial}{\partial t} [\Psi^*(x, t) \Psi(x, t)] \\&= \frac{\partial \Psi^*(x, t)}{\partial t} \Psi(x, t) + \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial t} \\&= -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} \Psi + \frac{i}{\hbar} V(x, t) \Psi^* \Psi + \frac{i\hbar}{2m} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} \Psi^* V(x, t) \Psi \\&= -\frac{i\hbar}{2m} \left(\frac{\partial^2 \Psi^*}{\partial x^2} \Psi - \Psi^* \frac{\partial^2 \Psi}{\partial x^2} \right)\end{aligned}$$

Time evolution of probability density

$$\begin{aligned}\frac{\partial \rho(x, t)}{\partial t} &= -\frac{i\hbar}{2m} \left(\frac{\partial^2 \Psi^*}{\partial x^2} \Psi + \frac{\partial \Psi^*}{\partial x} \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial \Psi}{\partial x} \frac{\partial \Psi^*}{\partial x} \right) \\&= \frac{\partial}{\partial x} \left[-\frac{i\hbar}{2m} \left(\frac{\partial \Psi^*}{\partial x} \Psi - \Psi^* \frac{\partial \Psi}{\partial x} \right) \right] \\&= -\frac{\partial}{\partial x} \left[-\frac{i\hbar}{2m} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) \right] \\&= -\frac{\partial J(x, t)}{\partial x}\end{aligned}$$

Conservation of probability

$$\begin{aligned}\frac{d\mathcal{N}(t)}{dt} &= \int_{-\infty}^{\infty} \frac{\partial \rho(x, t)}{\partial t} dx \\ &= - \int_{-\infty}^{\infty} \frac{\partial J(x, t)}{\partial x} dx \\ &= -[J(\infty, t) - J(-\infty, t)]\end{aligned}$$

Probability current

$$J(x, t) = \frac{\hbar}{2im} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right)$$

$$\lim_{x \rightarrow \pm \infty} \Psi(x, t) = 0$$

$$\left| \lim_{x \rightarrow \pm \infty} \frac{\partial \Psi(x, t)}{\partial x} \right| < \infty$$

$$J(\infty, t) = J(-\infty, t) = 0$$

Time evolution of wave function

$$\begin{aligned}\frac{d\mathcal{N}(t)}{dt} &= -[J(\infty, t) - J(-\infty, t)] \\ &= 0\end{aligned}$$

Hence \mathcal{N} is constant (independent of time) and if Ψ is normalized at time $t = t_0$, it remains normalized for all future time.

Time evolution of wave function

$$\frac{d\mathcal{N}}{dt} = 0$$

Hence \mathcal{N} is constant (independent of time) and if Ψ is normalized at time $t = t_0$, it remains normalized for all future time.