Quantum Mechanics I

PHY 3103

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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

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

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

Normalization condition

Properties of wave function

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

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

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

Normalizing the wave function

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

Normalizable wave function

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

Normalized wave function

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

Time evolution of wave function

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

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

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,

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

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

Time evolution of wave function

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

Probability density

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

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

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

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

Conservation of probability

Conservation of probability

$$\frac{\mathrm{d}\mathcal{N}(t)}{\mathrm{d}t} = \int_{-\infty}^{\infty} \frac{\partial \rho(x,t)}{\partial t}\mathrm{d}x$$
$$= \int_{-\infty}^{\infty} \left(\frac{\partial \Psi^*(x,t)}{\partial t}\Psi(x,t) + \Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial t} \right) \mathrm{d}x$$

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

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

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

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

Probability current

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

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

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

$$\boxed{J(\infty,t) = J(-\infty,t) = 0}$$

Time evolution of wave function

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

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.

Time evolution of wave function

$$\boxed{\frac{\mathrm{d}\mathcal{N}}{\mathrm{d}t} = 0}$$

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.