# EEE 2105 Electrical Engineering Materials

Elementary Quantum Physics

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# 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

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

$$\int_{-\infty}^{\infty} \Psi^*(x,t) \Psi(x,t) \mathrm{d}x = 1 \qquad \begin{array}{c} \text{Normalization} \\ \text{condition} \end{array}$$

# 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

$$\Psi'(x,t) = rac{1}{\sqrt{\mathcal{N}}} \Psi(x,t)$$
 Normalized wave function

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

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  $\Psi$  evolves?

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

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

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

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

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

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

$$\frac{d\mathcal{N}(t)}{dt} = \int_{-\infty}^{\infty} \frac{\partial \rho(x,t)}{\partial t} dx$$

$$= \int_{-\infty}^{\infty} \left( \frac{\partial \Psi^*(x,t)}{\partial t} \Psi(x,t) + \Psi^*(x,t) \frac{\partial \Psi(x,t)}{\partial t} \right) dx$$

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.

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#### 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

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

# Time evolution of probability density

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

# Conservation of probability

$$\frac{d\mathcal{N}(t)}{dt} = \int_{-\infty}^{\infty} \frac{\partial \rho(x,t)}{\partial t} dx$$

$$= -\int_{-\infty}^{\infty} \frac{\partial J(x,t)}{\partial x} dx$$

$$= -[J(\infty,t) - J(-\infty,t)]$$

#### Probability current

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

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

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

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

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

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

$$= 0$$

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

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

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