## 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

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



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  $x \to \pm \infty$ , 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

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



#### 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,

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

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



$$
\rho(x,t) \equiv \Psi^*(x,t)\Psi(x,t) = |\Psi(x,t)|^2
$$
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:  $\mathcal{N}(t) = 1$ 



Conservation of probability



### Conservation of probability

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

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.



#### 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

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



### Time evolution of probability density

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

$$
= \frac{\partial}{\partial x} \left[ -\frac{i\hbar}{2m} \left( \frac{\partial \Psi^*}{\partial x} \Psi - \Psi^* \frac{\partial \Psi}{\partial x} \right) \right]
$$

$$
= -\frac{\partial}{\partial x} \left[ -\frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) \right]
$$

$$
= -\frac{\partial J(x,t)}{\partial x}
$$



#### Conservation of probability





#### Probability current

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

$$
\lim_{x \to \pm \infty} \Psi(x, t) = 0 \qquad \qquad \left| \lim_{x \to \pm \infty} \frac{\partial \Psi(x, t)}{\partial x} \right| < \infty
$$

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



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

$$
= 0
$$

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.



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

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.

