Modern Physics

Unit 2: Schrödinger Equation in 1 Dimension
Lecture 2.4: A Free Particle

Ron Reifenberger
Professor of Physics
Purdue University
Important Results...so far

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

Time-dependent Schrödinger Wave Equation in one dimension

When \( U(x) \) is independent of time, we have

\[ \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right] \Psi = E\Psi \]

Time-independent Schrödinger Wave Equation in one dimension - stationary states
Any physical constraints on $\Psi$?

- $\Psi(x) \to 0$ as $x \to \infty$
- $\Psi$ must be continuous function of $x$
- $\frac{\partial \Psi}{\partial x}$ must be continuous function of $x$

Energy cannot be infinite.

Since

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

this implies that

$$\frac{\partial^2 \Psi}{\partial x^2}$$

must be finite.
What is physical interpretation of $\Psi$?

Max Born (1926; Noble Prize 1954):

$\Psi(x)$ doesn't represent anything real, only its square has a physical meaning

$$P(x) = \text{Probability that particle is between } x-\Delta x/2 \text{ and } x+\Delta x/2$$

$$\equiv \left|\Psi(x)\right|^2 \Delta x$$

Since $\Psi(x)$ is complex number

$$\left|\Psi(x)\right|^2 = \Psi^*(x)\Psi(x)$$

Probability "density" =

$$\lim_{\Delta x \to 0} \frac{P(x)}{\Delta x} = \Psi^*(x)\Psi(x)$$

$\Psi$ is the wavefunction (or probability amplitude)

and

$\Psi \Psi^*$ (or $|\Psi|^2$) is the probability density
The arithmetic needs to be crystal clear


Remember $\Psi(x)$ is a complex number!

When confused, always split $\Psi$ into its real and imaginary parts:

$$|\Psi(x)|^2 = \Psi^*(x)\Psi(x) = \Psi(x)\Psi^*(x)$$

$$= [\text{Re}(\Psi(x)) + i\text{Im}(\Psi(x))][\text{Re}(\Psi(x)) - i\text{Im}(\Psi(x))]$$

$$= [\text{Re}(\Psi(x))]^2 + [\text{Im}(\Psi(x))]^2$$
FOUR IMPORTANT EXAMPLES

I. The Free Particle
II. Infinite Square Well
III. Finite Square Well
IV. Simple Harmonic Oscillator

These are four standard problems. The solutions must be known inside and out.
I. The free particle

Need to solve for particle of mass m:

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

Separation of Variables: \( \Psi(x,t) = \psi(x) e^{-iEt/\hbar} = \psi(x) e^{-i\omega t} \)

Time independent equation:

\[ \left[ U(x) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right] \psi = E\psi \]

If \( U(x) = U_0 = \text{constant} \):

\[ \frac{\partial^2 \psi}{\partial x^2} = -2m \frac{1}{\hbar^2} (E - U_0) \psi; \quad \text{assume} \quad 2m \frac{1}{\hbar^2} (E - U_0) > 0 \]

this is the free particle assumption
Possible Solutions?

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

\[ \Psi(x, t) = \left[ A \sin(kx) + B \cos(kx) \right] e^{-iEt/\hbar} \]

In quantum mechanics, \( A \) and \( B \) can be complex numbers. This increased flexibility means you can also write \( \psi(x) \) as:

\[ \psi(x) = Ce^{ikx} + De^{-ikx} \]

\[ \Psi(x, t) = \left[ Ce^{ikx} + De^{-ikx} \right] e^{-iEt/\hbar} = \psi(x) e^{-i\omega t} \]

Working it out:

\[ \psi(x) = A \sin(kx) + B \cos(kx) = A \left[ \frac{e^{ikx} - e^{-ikx}}{2i} \right] + B \left[ \frac{e^{ikx} + e^{-ikx}}{2} \right] \]

\[ = \left[ \frac{A}{2i} + \frac{B}{2} \right] e^{ikx} + \left[ \frac{B}{2} - \frac{A}{2i} \right] e^{-ikx} \]

\[ = Ce^{ikx} + De^{-ikx} \quad \text{where } C \text{ and } D \text{ can be complex numbers.} \]

The different forms of \( \psi(x) \) are useful in different situations, just like \( 3/8, 0.375, 37.5% \). Use the most convenient form for the problem at hand.
Picturing the time-dependent free particle wave function

Free particle wave function moving in +x; D=0, let k=k_x:

\[ \Psi(x,t) = Ce^{i(k_xx_0 - \omega t)} \]

\[ k_x \equiv \frac{2\pi}{\lambda}; \quad \omega \equiv 2\pi f \]

Need a physical condition to somehow fix the value of C

At some particular value of x=x_0 when t=0:

\[ C \cos k_xx_0 \]
\[ iC \sin k_xx_0 \]

At a fixed x=x_0, as t increases, the helical "wavefunction" rotates at -\omega t

Also, see Appendix in L1.02
What’s with the \(-\omega t\)?

If \(\omega t\) increases by \(+2\pi\), then \(x_0 \rightarrow x_0 - \Delta\) to keep the phase the same.

If \(\omega t\) decreases by \(-2\pi\), then \(x_0 \rightarrow x_0 + \Delta\) to keep the phase the same.

Motion in \(-x\) as \(t\) increases

Motion in \(+x\) as \(t\) increases

Defining positive rotation
Free-particle Energy Eigenvalues?

\[ \frac{\partial^2 \psi}{\partial x^2} = -\frac{2m}{\hbar^2} (E - U_o) \psi \]

\[ \frac{\partial^2}{\partial x^2} \left( C e^{ik_xx} \right) = -C k_x^2 e^{ik_xx} = -k_x^2 \psi \]

\[ \frac{\hbar^2 k_x^2}{2m} = (E - U_o); \quad E > U_o \]

Tell me \( E-U_o \) and I’ll calculate \( k_x \).
No restrictions on either \( E \) or \( k_x \)!
Probability of finding the particle at some $x_0$?

$$\Psi(x,t) = Ce^{i(k_x x - \omega t)}$$

$$P(x,t) = \Psi(x,t)\Psi^*(x,t) = CC^* \text{ (independent of } x \text{ and } t)$$

Physically troublesome since $\Psi$ cannot be readily normalized.