Chapter 40

Wavefunctions and Uncertainty
Chapter 40. Wave Functions and Uncertainty

Topics:

• Waves, Particles, and the Double-Slit Experiment
• Connecting the Wave and Photon Views
• The Wave Function
• Normalization
• Wave Packets
• The Heisenberg Uncertainty Principle
Wave - Particle Duality

Electrons and Photons have both particle and wave aspects

Both exhibit interference - wave aspect

Both are detected as discrete chunks - particle aspect
FIGURE 40.1 The double-slit experiment with light.

Classical wave picture

Photons distribute themselves according to classical intensity
Diffraction of Matter

Electrons arrive one by one. Hitting the screen at discrete points. But over time a diffraction pattern is built up!

Puzzle: When it hits the screen it acts like a particle, but somehow it went through both slits.
FIGURE 40.1 The double-slit experiment with light.

Approaching wave fronts

Double slit

Screen

Crests overlap

Wave amplitude along the screen

Interference fringes

Photon arrival positions

Phytons distribute themselves according to classical intensity.
Photon’s and matter particle’s motion is described by a wave field that governs the probability of observing the particle at some point or with some property.

It’s weird.

To make predictions for measurements we need to make two steps.

1. Solve for the values of the wave field (wave function).

2. Use the wave function to calculate the probability of finding our particle somewhere. We can’t say for sure where it will be.

"God does not play dice with the universe." A. Einstein(1926)

So far as we know he does.
Probability First

The probability that outcome A occurs is \( P_A \).

What does this mean?

Let’s say you conduct an experiment \( N_{\text{tot}} \) times, and observe outcome A \( N_A \) times. Then:

\[
P_A = \lim_{N\to\infty} \frac{N_A}{N_{\text{tot}}}
\]

In other words, if you were to conduct the experiment an infinite number of times, \( P_A \) is the fraction of times outcome A occurs.

Certain qualifications need to be made: e.g. each try is independent of the others but otherwise each try is under the same conditions.
Comments:

\[ 0 \leq P_A \leq 1 \]

Probabilities are between zero and one

If A, B and C are exclusive outcomes

\[ P_{A \text{ or } B \text{ or } C} = P_A + P_B + P_C \]

If A, B and C are exclusive and the only possible outcomes

\[ P_{A \text{ or } B \text{ or } C} = P_A + P_B + P_C = 1 \]
Question

Is this true?

\[ P_{A \text{ or } B \text{ or } D} = P_A + P_B + P_D \]

A. Yes
B. No
C. Probably No
D. Maybe Yes
What is the probability that the dart hits right here?

45 in region A

35 in region B

20 in region C
What is the probability that the dart hits in this small area $\Delta A$?

$$P_{\Delta A} = \Delta A \, P(x, y)$$

Probability density function $P(x, y)$

Density of dots
One dimensional probability density

\[ P(x) \delta x \]

Is the probability that the value of the measured quantity \( x \) falls in the small interval \( \delta x \) centered at \( x \).
Some examples:

Your computer can generate “random” numbers \( x_1, x_2, \ldots \) that satisfy \( 0 < x_n < 1.0 \).

The chances of any particular value are equal.

What is the Probability Density Function (PDF) for \( x \)?

\[
P(x)
\]

Total Area under curve = 1

\[
\begin{array}{c}
0 \\
1
\end{array}
\]
In example 1, what is the probability a single random number number is generated that falls in the interval $\frac{1}{2} < x < \frac{2}{3}$? Call this outcome A.

$$P_A = \int_{\frac{1}{2}}^{\frac{2}{3}} P(x)\,dx = \left(\frac{2}{3} - \frac{1}{2}\right) = \frac{1}{6}$$
Example 2:

Students selected at random give different answers on exams.

A histogram of the exam scores for 120 students appears at right.

The underlying PDF might appear as the black curve.

\[
1 = \int_{0}^{100} P(x) dx
\]
Example 2:

What is the probability that a student (chosen at random) scores between 70 and 80?

\[
P_A = \int_{70}^{80} P(x) dx \approx 0.25
\]

Area under curve 20-100 = 1
Photons distribute themselves according to classical intensity
Interference of photons suggests the following heuristic approach.

1. First treat photons as waves and calculate the classical wave fields for a wave of frequency $\omega = 2\pi f$

   \[ E(x) \quad B(x) \]

2. Calculate the classical intensity

   \[ I(x) = \frac{1}{2} \sqrt{\frac{\varepsilon_0}{\mu_0}} |E(x)|^2 \]

3. Number of photons/second/area related to intensity

   \[ \frac{\text{# photons}}{\text{sec area}} = \frac{I(x)}{hf} \quad \text{Check units} \]

   Use Intensity to define $P(x)$ (PDF) for a single photon
What should we do for electrons?

We need to make up a wave equation for some quantity that we will square and say is the PDF

Requirements: \( \psi(x,t) \) satisfies a wave equation.

\[
|\psi(x,t)|^2 \quad \text{must act like a PDF}
\]

For wave like solutions

Momentum: \( p = h / \lambda = \hbar k \)

Energy: \( E = hf = \hbar \omega = \frac{p^2}{2m} + U(x) \)
Consider light waves as a guide

\[ \frac{\partial^2 E(x, t)}{\partial t^2} = c^2 \frac{\partial^2 E(x, t)}{\partial x^2} \]

Try a traveling wave solution

\[ E(x, t) = E_0 \cos(kx - \omega t) = \text{Re}[E_0 e^{i(kx - \omega t)}] \]

where \[ i = \sqrt{-1} \]

\[ \frac{\partial}{\partial t} e^{i(kx - \omega t)} = -i\omega e^{i(kx - \omega t)} \quad \frac{\partial}{\partial x} e^{i(kx - \omega t)} = ike^{i(kx - \omega t)} \]

Each time derivative becomes \(-i\omega\). Each x derivative becomes \(ik\)
\[ \frac{\partial^2 E(x,t)}{\partial t^2} = c^2 \frac{\partial^2 E(x,t)}{\partial x^2} \]

Try a traveling wave solution
\[ E(x,t) = E_0 \cos(kx - \omega t) = \text{Re}[E_0 e^{i(kx - \omega t)}] \quad i = \sqrt{-1} \]

Wave equation \(( -i\omega )^2 E_0 e^{i(kx - \omega t)} = c^2 (ik)^2 E_0 e^{i(kx - \omega t)}\)

After canceling common factors \(\omega^2 = c^2 k^2\)

If I say: \(E = \hbar \omega\) \(p = \hbar k\)

Then \(E = pc\) which describes photons but not particles.
To describe particles start with expression for particle energy.

\[ E = \frac{p^2}{2m} + U(x) \]

replace energy

\[ E = \hbar \omega = i\hbar \frac{\partial}{\partial t} \]

replace momentum

\[ p = \hbar k = -i\hbar \frac{\partial}{\partial x} \]

introduce wave function

\[ i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + U(x)\psi(x,t) \]

Schrodinger’s Equation
The wave function is complex.

\[ i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + U(x)\psi(x, t) \]

What is the PDF for finding a particle at \( x \)?

\[ P(x, t) = |\psi(x, t)|^2 \]

Step 1: solve Schrodinger equation for wave function

Step 2: probability density of finding particle at \( x \) is

\[ P(x, t) = |\psi(x, t)|^2 \]
Stationary States - Bohr Hypothesis

\[
i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + U(x)\psi(x,t)
\]

\[
\psi(x,t) = \hat{\psi}(x)e^{-iEt/\hbar} \quad \omega = \frac{E}{\hbar}
\]

Stationary State satisfies

\[
E\hat{\psi}(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \hat{\psi}(x,t) + U(x)\hat{\psi}(x,t)
\]

Note:

\[
|\psi(x,t)|^2 = |\hat{\psi}(x)e^{-iEt/\hbar}|^2 = |\hat{\psi}(x)|^2 = P(x)
\]

P(x) Independent of time
Corresponds to a particle in the potential

$$U = \frac{1}{2} k x^2$$

(b) Probability density

$$P(x) = |\psi(x)|^2$$

The particle has the maximum probability of being detected where $|\psi(x)|^2$ is a maximum.

The particle has zero probability of being detected where $|\psi(x)|^2 = 0.$
Normalization

• A photon or electron has to land somewhere on the detector after passing through an experimental apparatus.

• Consequently, the probability that it will be detected at some position is 100%.

• The statement that the photon or electron has to land somewhere on the $x$-axis is expressed mathematically as

$$\int_{-\infty}^{\infty} P(x) \, dx = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$$

• Any wave function must satisfy this normalization condition.
The value of the constant $a$ is

\[ P(x) = |\psi(x)|^2 \]

A. $a = 0.5 \text{ mm}^{-1/2}$.
B. $a = 1.0 \text{ mm}^{-1/2}$.
C. $a = 2.0 \text{ mm}^{-1/2}$.
D. $a = 1.0 \text{ mm}^{-1}$.
E. $a = 2.0 \text{ mm}^{-1}$.
A property of the Schrödinger equation is that if initially
\[ \int_{-\infty}^{\infty} P(x) \, dx = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1 \]
Then it will be true for all time.
The figure shows the detection of photons in an optical experiment. Rank in order, from largest to smallest, the square of the amplitude function of the electromagnetic wave at positions A, B, C, and D.

A. D > C > B > A
B. A > B > C > D
C. A > B = D > C
D. C > B = D > A
This is the wave function of a neutron. At what value of $x$ is the neutron most likely to be found?

A. $x = 0$
B. $x = x_A$
C. $x = x_B$
D. $x = x_C$
Uncertainty Relation

There are certain pairs of variables we can not predict simultaneously with arbitrary accuracy.

Energy and Time

Momentum and Position

Uncertainty relations:

\[ \Delta E \Delta t > h \]

\[ \Delta p \Delta x > h \]
How to remember which variables go together

Traveling Wave \[ \psi(x, t) = \psi_0 e^{i(kx - \omega t)} \]

Pairs: \( k \) and \( x \) \hspace{1cm} \( \omega \) and \( t \)

Remember
\[ p = \hbar k = -i\hbar \frac{\partial}{\partial x} \hspace{1cm} E = \hbar \omega = i\hbar \frac{\partial}{\partial t} \]

Momentum is derivative wrt \( x \) \hspace{1cm} Energy is derivative wrt \( t \)
Wavefunctions with a single value of momentum or energy

\[ \psi(x, t) = \psi_0 e^{i(kx - \omega t)} \]

Probability density is constant in space and time

\[ P \propto |\psi(x, t)|^2 = |\psi_0 e^{i(kx - \omega t)}|^2 = |\psi_0|^2 = \text{const.} \]

So, if momentum has a definite value, PDF in constant x.

If energy has definite value, PDF is constant in time.
Example of a wave function that is not extended in time.

A Pulse of duration $\Delta t$ has a spread in Frequency values $\Delta f$.

$$\Delta f = \frac{1}{\Delta t}$$
A sum (superposition) on many sine waves can give you a pulse.

The mathematical statement that a time dependent pulse can be represented as a sum of sinusoidal waves with different frequencies is a branch of mathematics known as Fourier analysis.

Very important in Physics and Engineering.
Jean Baptiste Joseph Fourier (21 March 1768 ñ 16 May 1830) wikimedia commons
A sum of two waves gives beats. (I hate beets!)

\[ \cos\left(\frac{\omega + \Delta \omega}{2} t\right) + \cos\left(\frac{\omega - \Delta \omega}{2} t\right) = 2 \cos(\omega t) \cos(\Delta \omega t) \]

Displacement

rapid oscillations
given by \( \omega \), average frequency.

Duration \( \Delta t \) given by
variation in
frequency, \( \Delta \omega \)

\[ \Delta \omega \Delta t = \pi \]
Wave Packets

Suppose a single non-repeating wave packet of duration \( t \) is created by the superposition of many waves that span a range of frequencies \( \Delta f \).

Fourier analysis shows that for any wave packet

\[
\Delta f \Delta t \approx 1
\]

We have not given a precise definition of \( \Delta t \) and \( \Delta f \) for a general wave packet.

The quantity \( \Delta t \) is “about how long the wave packet lasts,” while \( \Delta f \) is “about the range of frequencies needing to be superimposed to produce this wave packet.”
The same considerations apply to the spatial dependence of a wave packet.

\[ \Delta k \Delta x = \pi \]

\[ p = \hbar k = h / \lambda \]

\[ \Delta p = \hbar \Delta k \approx h / \Delta x \]
EXAMPLE 40.4 Creating radio-frequency pulses

QUESTION:

EXAMPLE 40.4 Creating radio-frequency pulses
A short-wave radio station broadcasts at a frequency of 10,000 MHz. What is the range of frequencies of the waves that must be superimposed to broadcast a radio-wave pulse lasting 0.800 μs?
EXAMPLE 40.4 Creating radio-frequency pulses

**MODEL**  A pulse of radio waves is an electromagnetic wave packet, hence it must satisfy the relationship $\Delta f \Delta t \approx 1$. 
EXAMPLE 40.4 Creating radio-frequency pulses

VISUALIZE FIGURE 40.15 shows the pulse.

FIGURE 40.15 A pulse of radio waves.

\[ T = 0.100 \, \mu s \]

\[ \Delta t = 0.800 \, \mu s \]
EXAMPLE 40.4 Creating radio-frequency pulses

**SOLVE** The period of a 10.000 MHz oscillation is 0.100 μs. A pulse 0.800 μs in duration is 8 oscillations of the wave. Although the station broadcasts at a nominal frequency of 10.000 MHz, this pulse is not a pure 10.000 MHz oscillation. Instead, the pulse has been created by the superposition of many waves whose frequencies span

\[
\Delta f \approx \frac{1}{\Delta t} = \frac{1}{0.800 \times 10^{-6} \text{ s}} = 1.250 \times 10^6 \text{ Hz} = 1.250 \text{ MHz}
\]

This range of frequencies will be centered at the 10.000 MHz broadcast frequency, so the waves that must be superimposed to create this pulse span the frequency range

\[9.375 \text{ MHz} \leq f \leq 10.625 \text{ MHz}\]
FIGURE 40.16 Two wave packets with different $\Delta t$.

(a) This wave packet has a large frequency uncertainty $\Delta f$.

(b) This wave packet has a small frequency uncertainty $\Delta f$.

These two wave packets have the same average frequency $f$, but different spreads in frequency $\Delta f$. 
What minimum bandwidth must a medium have to transmit a 100-ns-long pulse?

A. 100 MHz  
B. 0.1 MHz  
C. 1 MHz  
D. 10 MHz  
E. 1000 MHz
Which of these particles, A or B, can you locate more precisely?

A. A  
B. B  
C. Both can be located with same precision.
The Heisenberg Uncertainty Principle

• The quantity $\Delta x$ is the length or spatial extent of a wave packet.

$\Delta p_x$ is a small range of momenta corresponding to the small range of frequencies within the wave packet.

• Any matter wave must obey the condition

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$  \hspace{1cm} \text{(Heisenberg uncertainty principle)}

This statement about the relationship between the position and momentum of a particle was proposed by Heisenberg in 1926. Physicists often just call it the \textbf{uncertainty principle}. 
EXAMPLE 40.5 The uncertainty of a dust particle

QUESTION:

A 1.0-μm-diameter dust particle (m ≈ 10^{-15} \text{ kg}) is confined within a 10-μm-long box. Can we know with certainty if the particle is at rest? If not, within what range is its velocity likely to be found?
EXAMPLE 40.5 The uncertainty of a dust particle

**MODEL** All matter is subject to the Heisenberg uncertainty principle.
EXAMPLE 40.5 The uncertainty of a dust particle

**SOLVE** If we know *for sure* that the particle is at rest, then $p_x = 0$ with no uncertainty. That is, $\Delta p_x = 0$. But then, according to the uncertainty principle, the uncertainty in our knowledge of the particle’s position would have to be $\Delta x \to \infty$. In other words, we would have no knowledge at all about the particle’s position—it could be anywhere! But that is not the case. We know the particle is *somewhere* in the box, so the uncertainty in our knowledge of its position is at most $\Delta x = L = 10 \, \mu\text{m}$. With a finite $\Delta x$, the uncertainty $\Delta p_x$ *cannot* be zero. We cannot know with certainty if the particle is at rest inside the box. No matter how hard we try to bring the particle to rest, the uncertainty in our knowledge of the particle’s momentum will be $\Delta p_x \approx \hbar/(2\Delta x) = \hbar/2L$. 
EXAMPLE 40.5 The uncertainty of a dust particle

We’ve assumed the most accurate measurements possible so that the $\Delta$ in Heisenberg’s uncertainty principle becomes $\approx$. Consequently the range of possible velocities is

$$\Delta v_x = \frac{\Delta p_x}{m} \approx \frac{h}{2mL} \approx 3.0 \times 10^{-14} \text{ m/s}$$

This range of possible velocities will be centered on $v_x = 0 \text{ m/s}$ if we have done our best to have the particle be at rest. Thus all we can know with certainty is that the particle’s velocity is somewhere within the interval $-1.5 \times 10^{-14} \text{ m/s} \leq v \leq 1.5 \times 10^{-14} \text{ m/s}$. 
EXAMPLE 40.5 The uncertainty of a dust particle

**ASSESS** For practical purposes you might consider this to be a satisfactory definition of “at rest.” After all, a particle moving with a speed of $1.5 \times 10^{-14}$ m/s would need $6 \times 10^{10}$ s to move a mere 1 mm. That is about 2000 years! Nonetheless, we can’t know if the particle is “really” at rest.
EXAMPLE 40.6 The uncertainty of an electron

QUESTION:

What range of velocities might an electron have if confined to a 0.10-nm-wide region, about the size of an atom?
EXAMPLE 40.6 The uncertainty of an electron

**MODEL** Electrons are subject to the Heisenberg uncertainty principle.
EXAMPLE 40.6 The uncertainty of an electron

**SOLVE** The analysis is the same as in Example 40.5. If we know that the electron’s position is located within an interval $\Delta x \approx 0.1$ nm, then the best we can know is that its velocity is within the range

$$\Delta v_x = \frac{\Delta p_x}{m} \approx \frac{h}{2mL} \approx 4 \times 10^6 \text{ m/s}$$

Because the average velocity is zero, the best we can say is that the electron’s velocity is somewhere in the interval $-2 \times 10^6 \text{ m/s} \leq v \leq 2 \times 10^6 \text{ m/s}$. It is simply not possible to know the electron’s velocity any more precisely than this.
EXAMPLE 40.6 The uncertainty of an electron

**ASSESS** Unlike the situation in Example 40.5, where $\Delta v$ was so small as to be of no practical consequence, our uncertainty about the electron’s velocity is enormous—about 1% of the speed of light!
General Principles

Wave Functions and the Probability Density

We cannot predict the exact trajectory of an atomic-level particle such as an electron. The best we can do is to predict the probability that a particle will be found in some region of space. The probability is determined by the particle’s wave function $\psi(x)$.

- $\psi(x)$ is a continuous, wave-like (i.e., oscillatory) function.
- The probability that a particle will be found in the narrow interval $\delta x$ at position $x$ is
  $\text{Prob(in } \delta x \text{ at } x) = |\psi(x)|^2 \delta x$
- $|\psi(x)|^2$ is the probability density $P(x)$.
- For the probability interpretation of $\psi(x)$ to make sense, the wave function must satisfy the normalization condition:
  \[
  \int_{-\infty}^{\infty} P(x)dx = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1
  \]
  That is, it is certain that the particle is somewhere on the x-axis.
- For an extended interval
  \[
  \text{Prob}(x_L \leq x \leq x_R) = \int_{x_L}^{x_R} |\psi(x)|^2 dx = \text{area under the curve}
  \]
Heisenberg Uncertainty Principle

A particle with wave-like characteristics does not have a precise value of position $x$ or a precise value of momentum $p_x$. Both are uncertain. The position uncertainty $\Delta x$ and momentum uncertainty $\Delta p_x$ are related by $\Delta x \Delta p_x \geq \hbar/2$. The more you try to pin down the value of one, the less precisely the other can be known.
Important Concepts

The **probability** that a particle is found in region \( A \) is

\[
P_A = \lim_{N_{\text{tot}} \to \infty} \frac{N_A}{N_{\text{tot}}}
\]

If the probability is known, the expected number of \( A \) outcomes in \( N \) trials is \( N_A = N P_A \).
A wave packet of duration $\Delta t$ can be created by the superposition of many waves spanning the frequency range $\Delta f$. These are related by

$$\Delta f \Delta t \approx 1$$