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

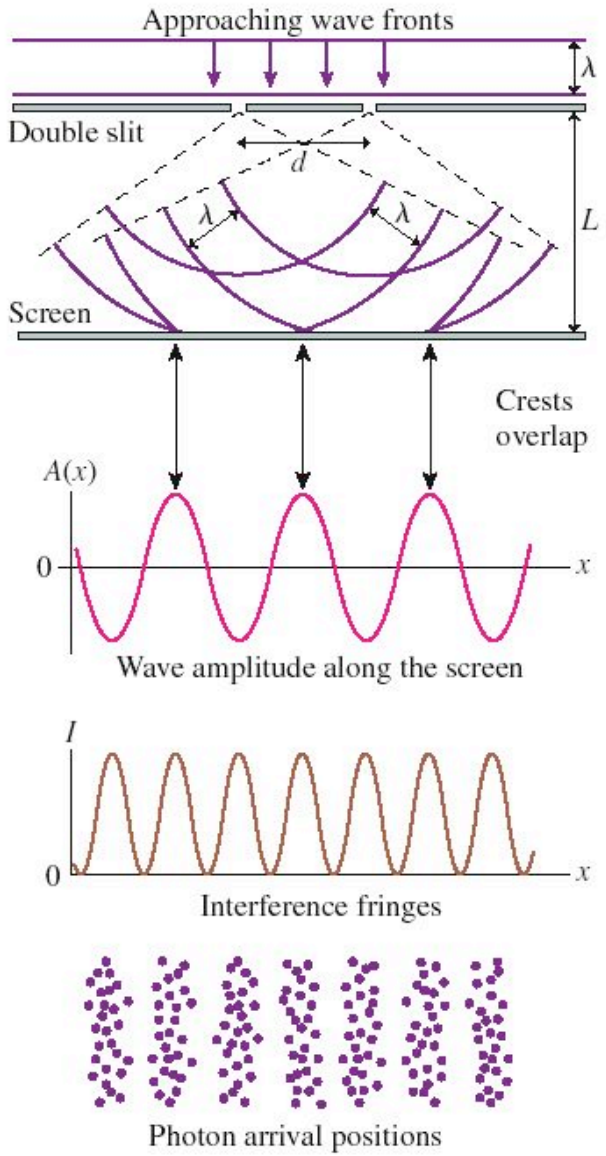
Wave - Particle Duality

Electrons and Photons have both particle and wave aspects

Both exhibit interference - wave aspect

Both are detected as discrete chunks - particle aspect

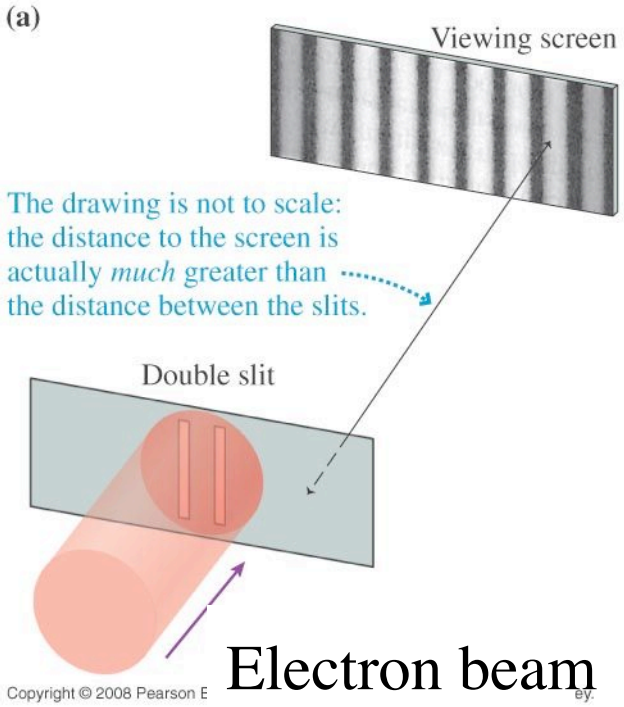
FIGURE 40.1 The double-slit experiment with light.



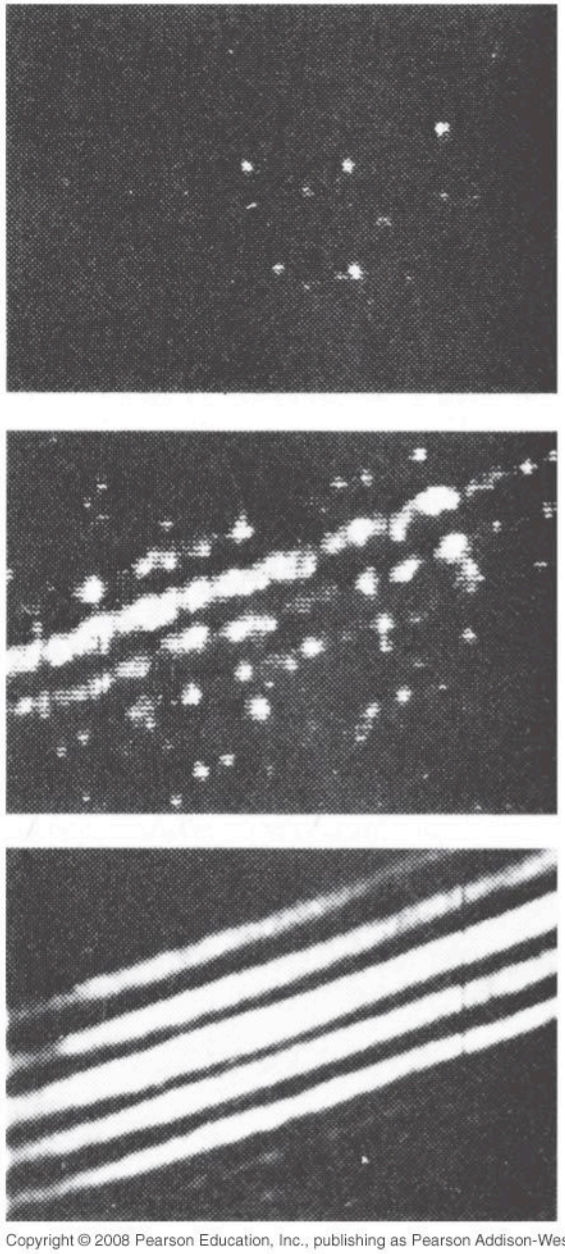
Classical wave picture

Photons distribute themselves according to classical intensity

Diffraction of Matter

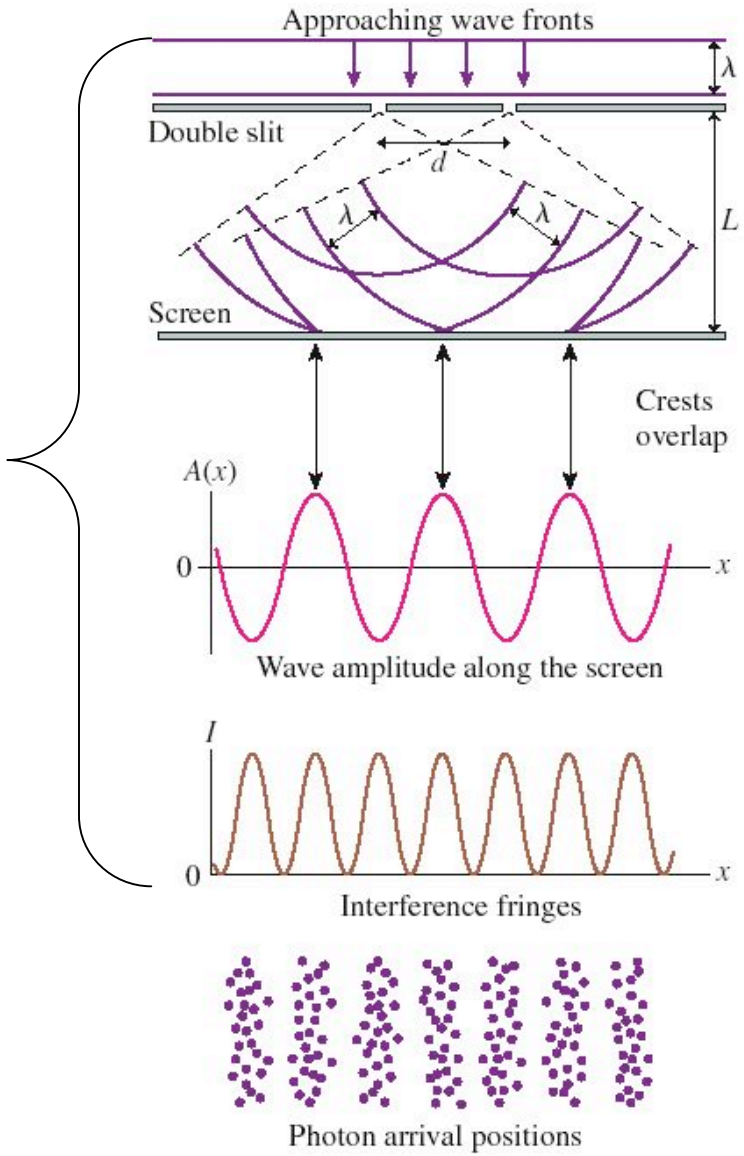


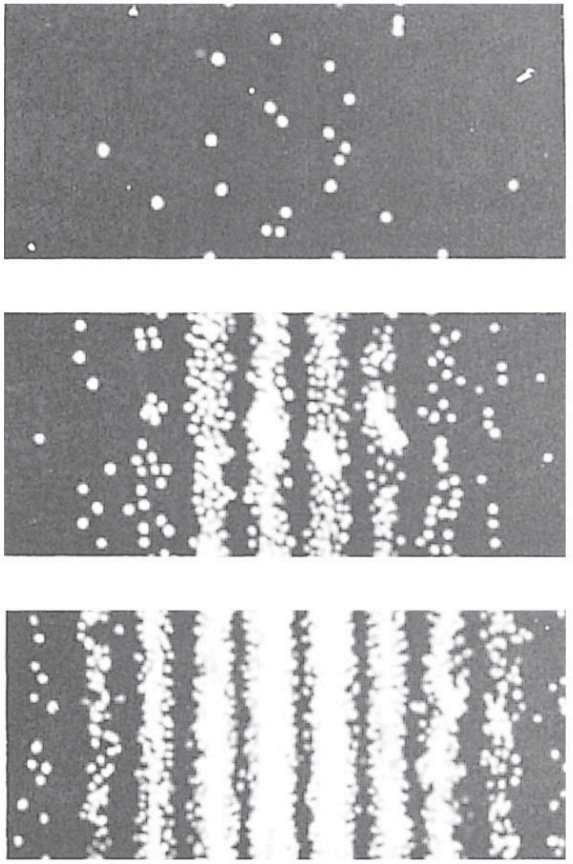
Electrons arrive one by one. Hitting the screen at discrete points. But over time a diffraction pattern is built up!



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.





The particle-like dots arrange themselves into wave-like interference fringes.

Photons 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_{tot} times, and observe outcome A N_A times. Then:

$$P_A = \lim_{Ntot \to \infty} \frac{N_A}{N_{Tot}}$$

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:

$$0 \le P_A \le 1$$

Probabilities are between zero and one

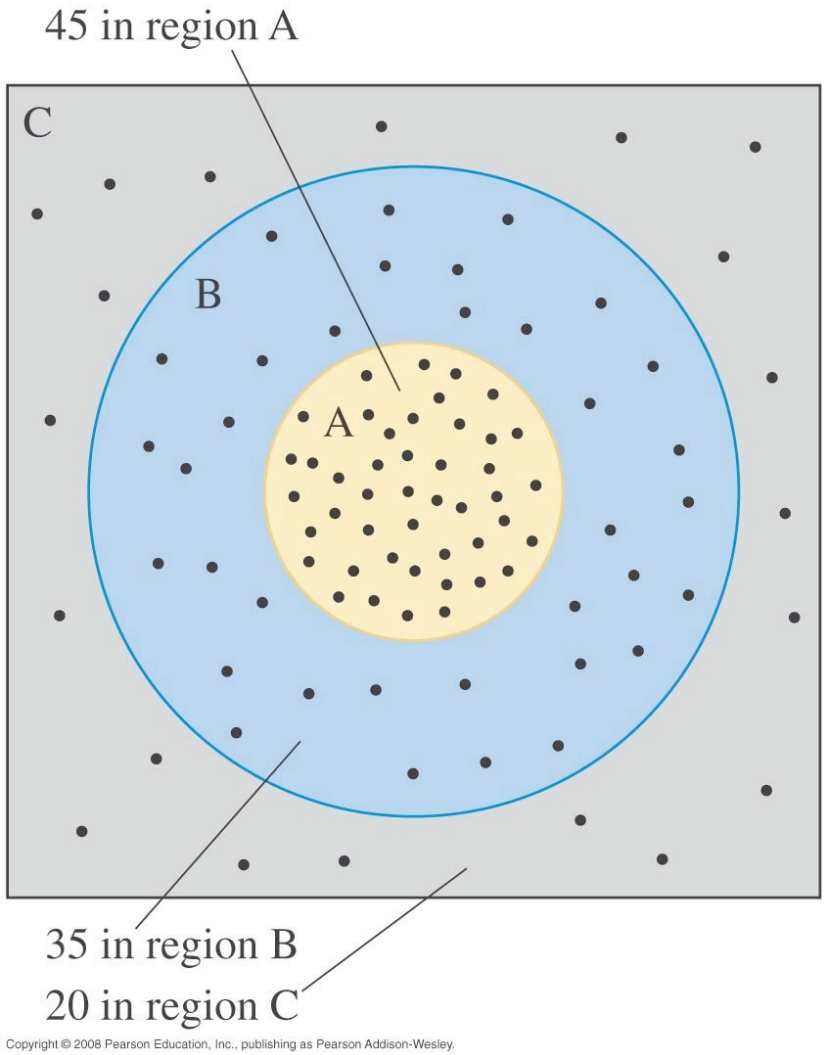
If A, B and C are exclusive outcomes

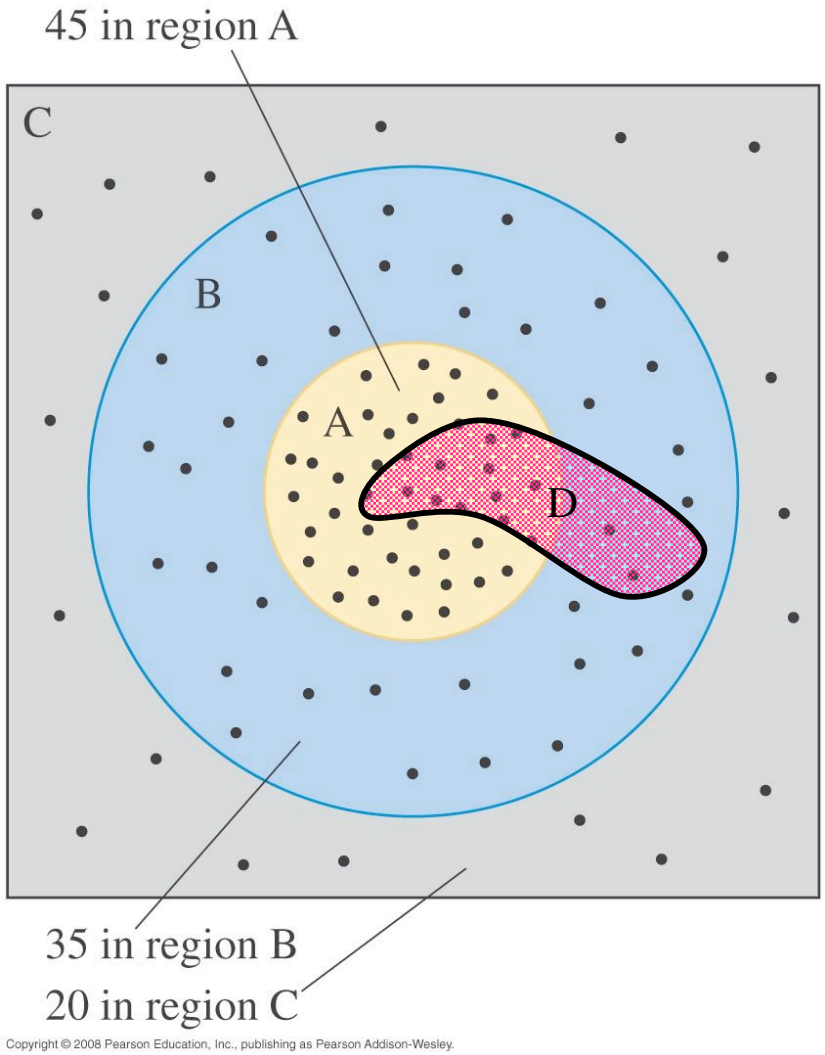
$$P_{A\ or\ B\ or\ C} = P_A + P_B + P_C$$

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

$$P_{A\ or\ B\ or\ C} = P_A + P_B + P_C = 1$$

Dart Board



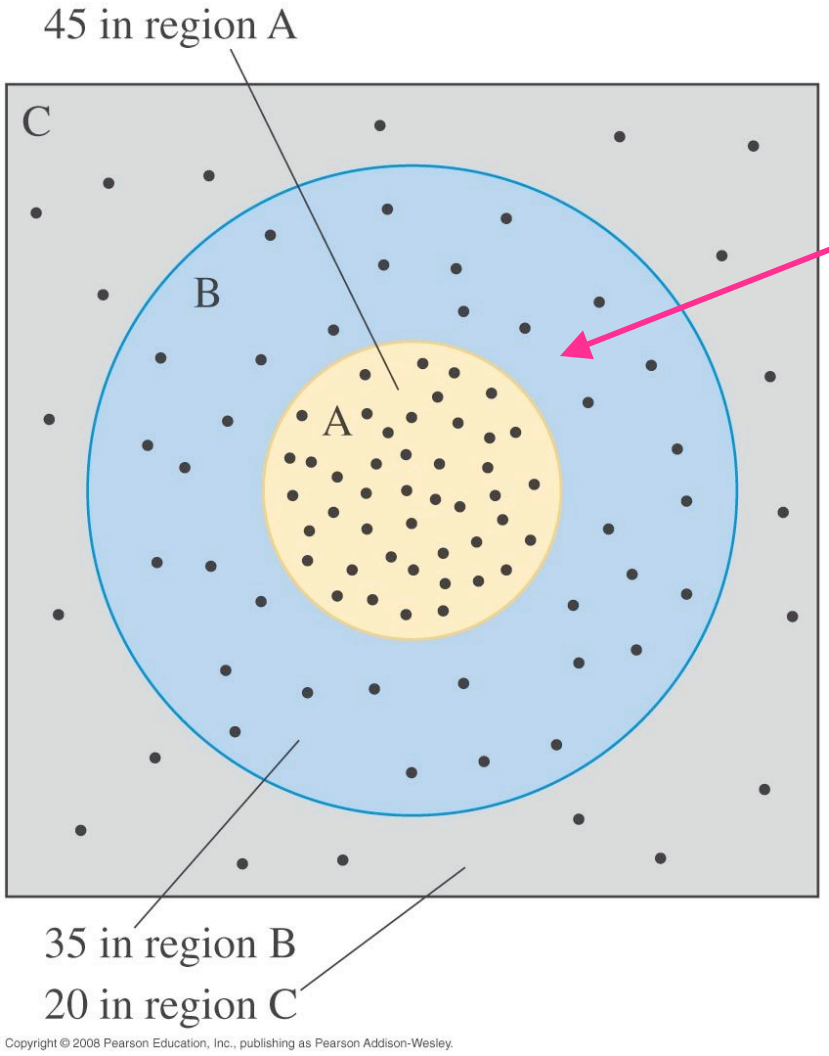


Question

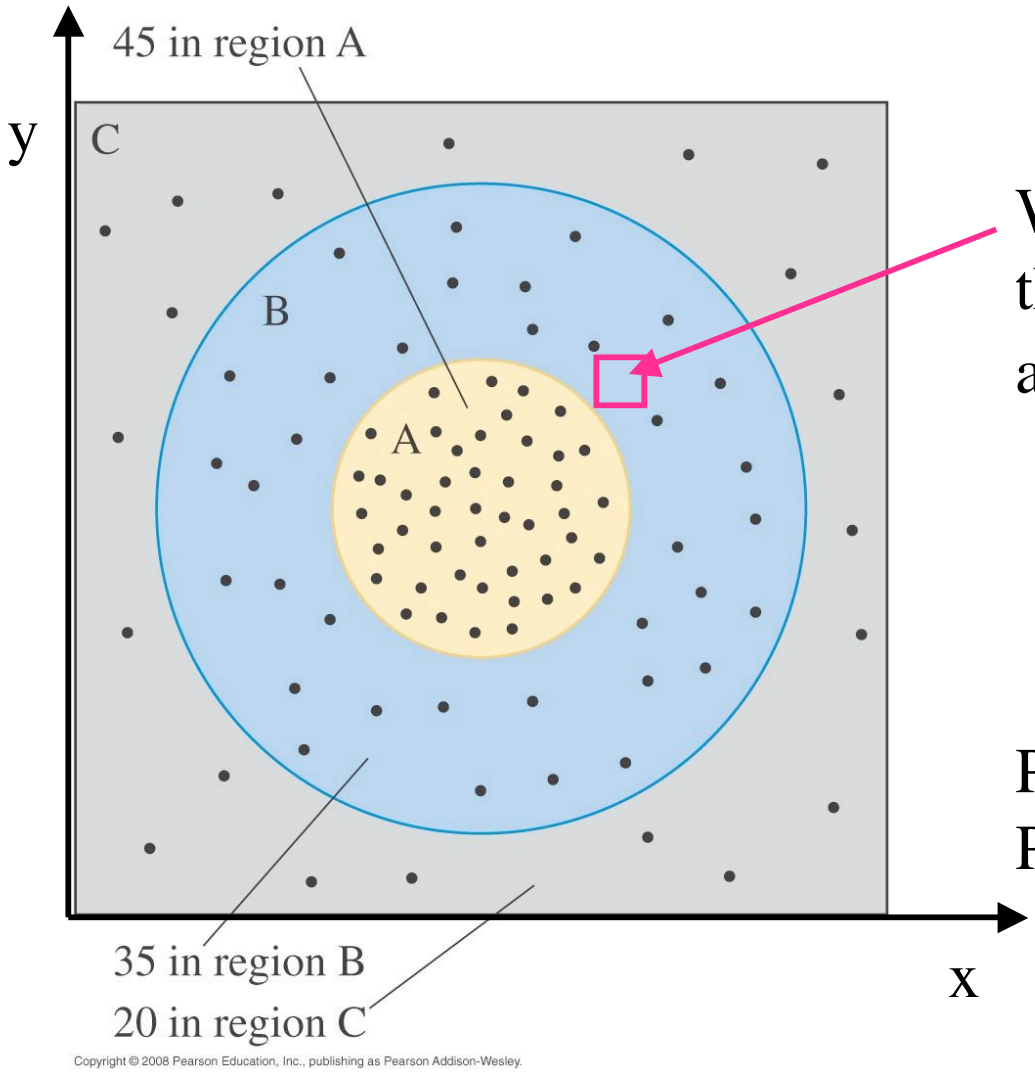
Is this true?

$$P_{A\ or\ B\ or\ D} = P_A + P_B + P_D$$

A. Yes
B. No
C. Probably No
D. Maybe Yes



What is the probability that the dart hits right here?

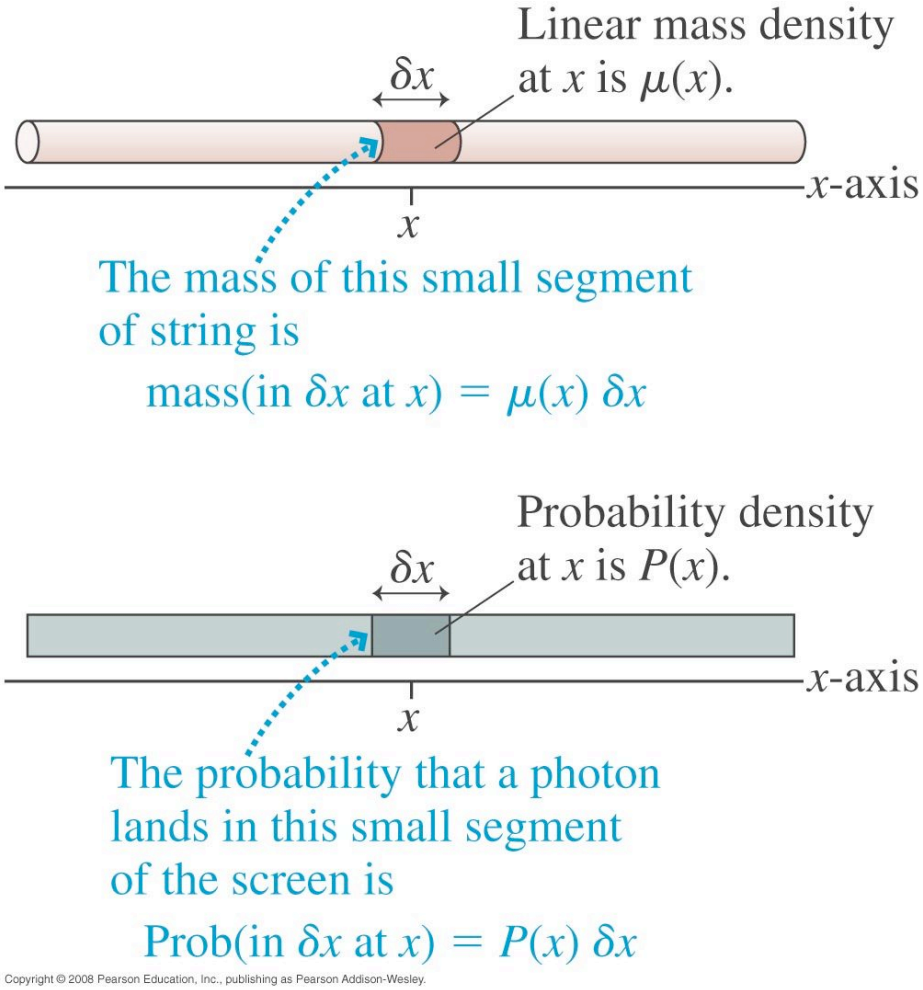


What is the probability that the dart hits in this small area ΔA?

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

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 δx centered at x.

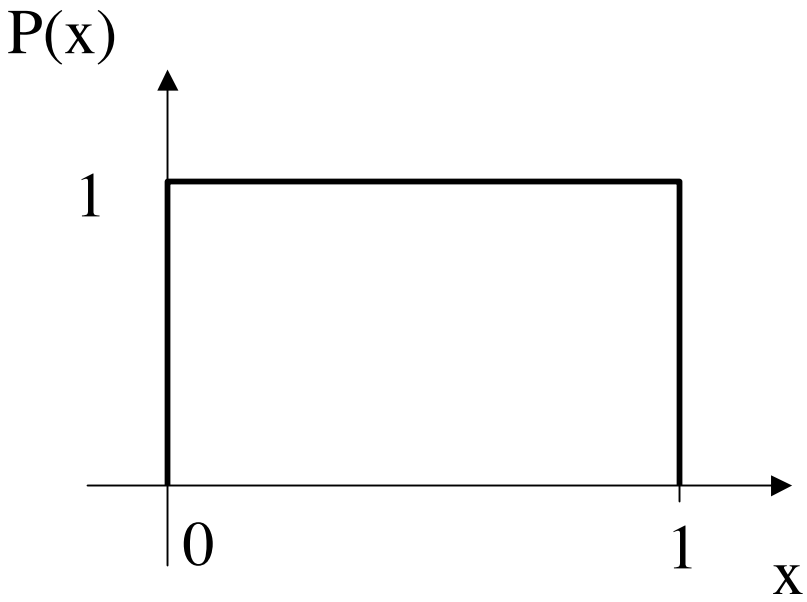
Some examples:

Your computer can generate "random" numbers x_1, x_2, … that satisfy $0 < x_n < 1.0$.

The chances of any particular value are equal.

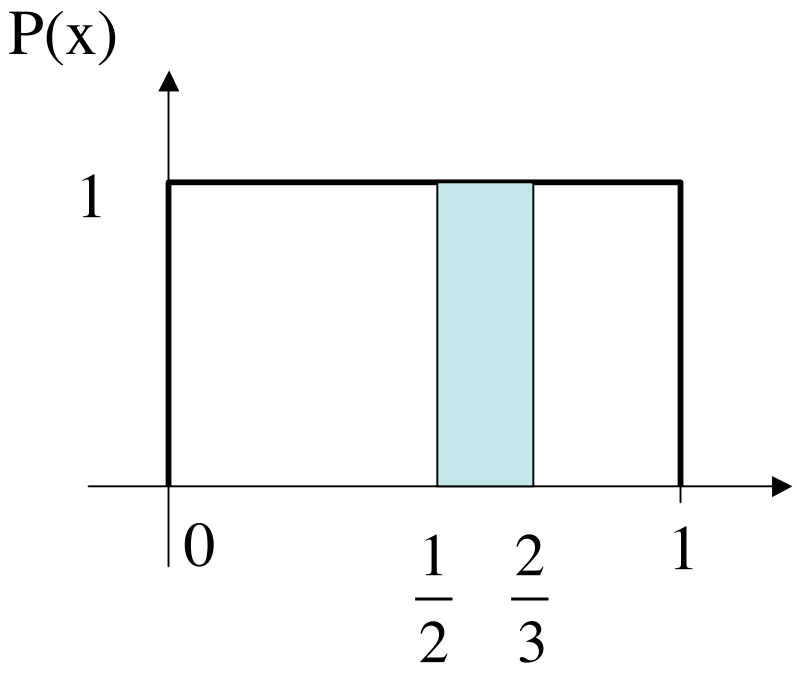
What is the Probability Density Function (PDF) for x?

Total Area under curve = 1



In example 1, what is the probability a single random number number is generated that falls in the interval 1/2 < x < 2/3 ? Call this outcome A.

$$P_A = \int_{1/2}^{2/3} P(x)dx = (\frac{2}{3} - \frac{1}{2}) = \frac{1}{6}$$

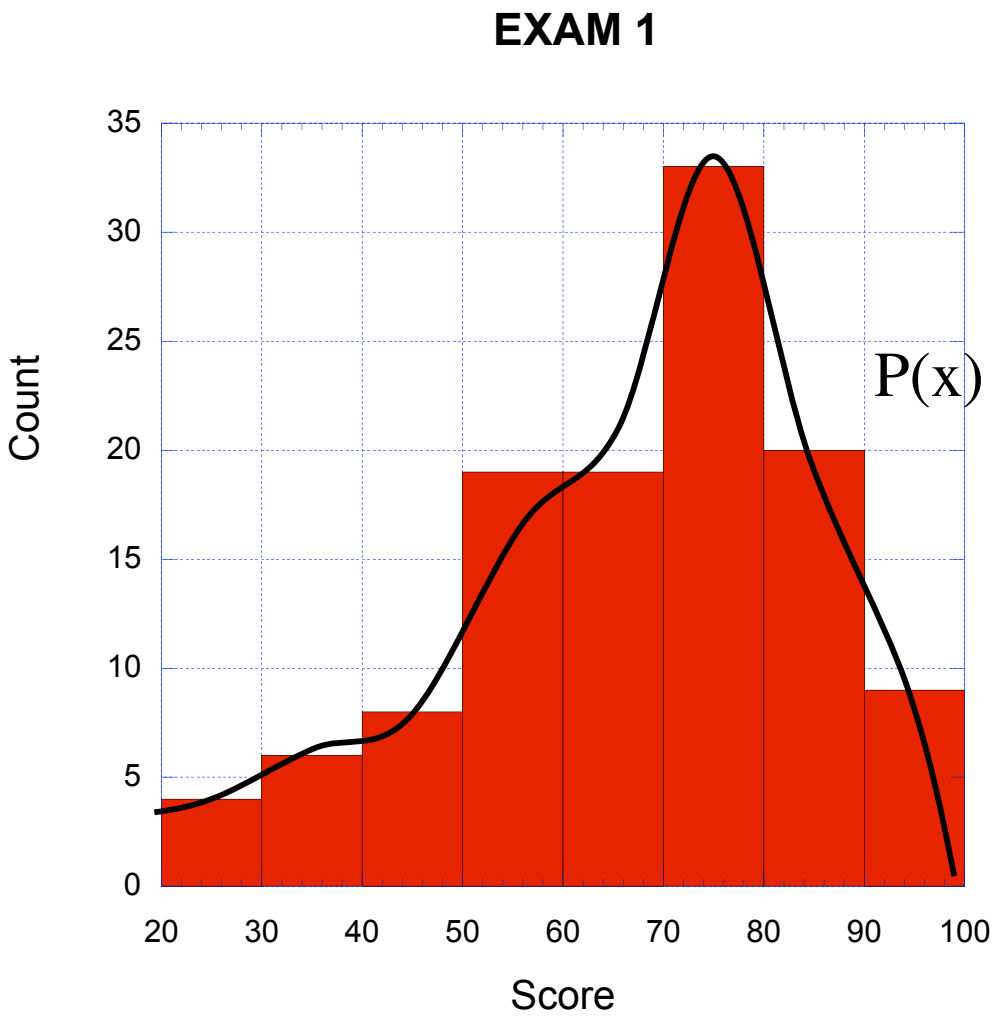


Example 2:

Students selected at random give different answers on exams.

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

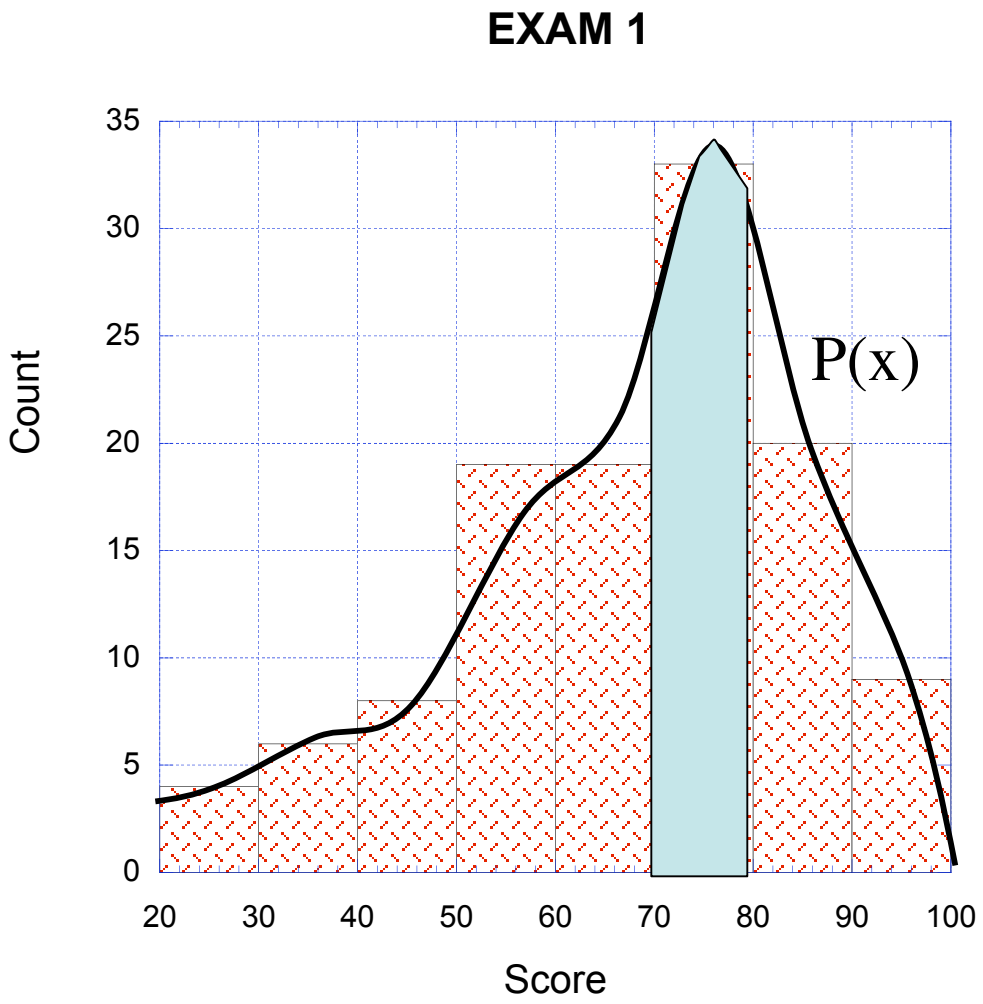
The underlying PDF might appear as the black curve.



$$1 = \int_0^{100} P(x)dx$$

Example 2:

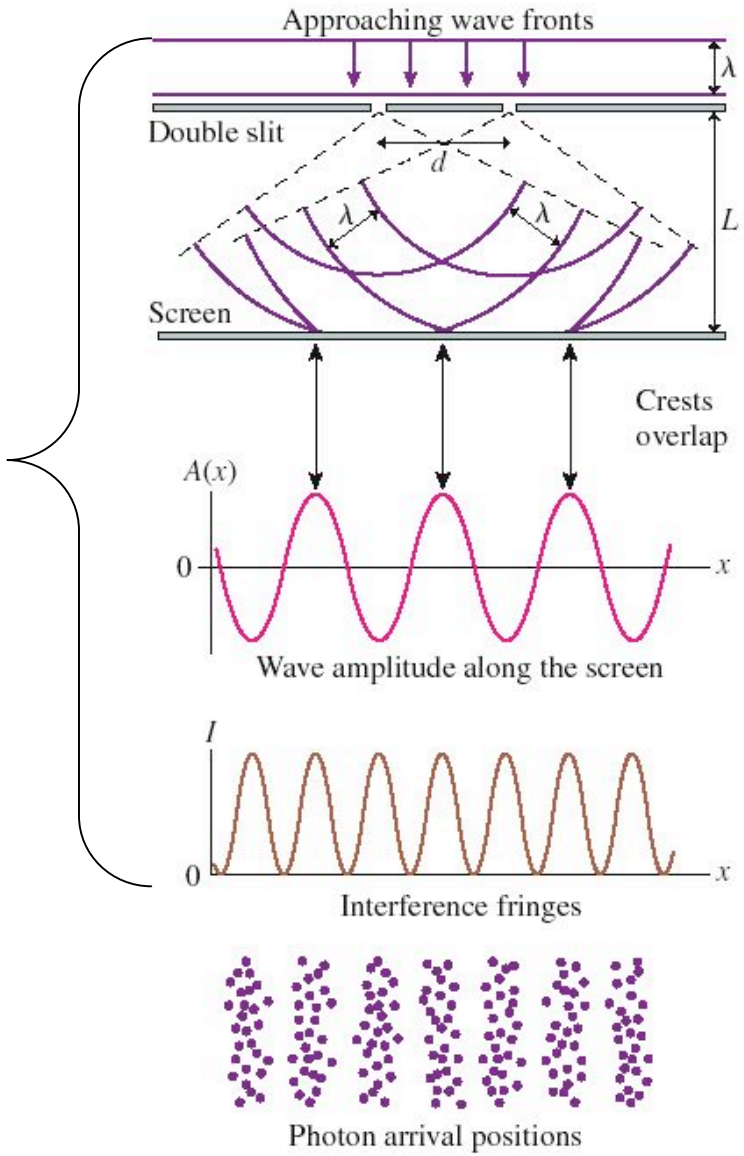
What is the probability that a student (chosen at random) scores between 70 and 80?

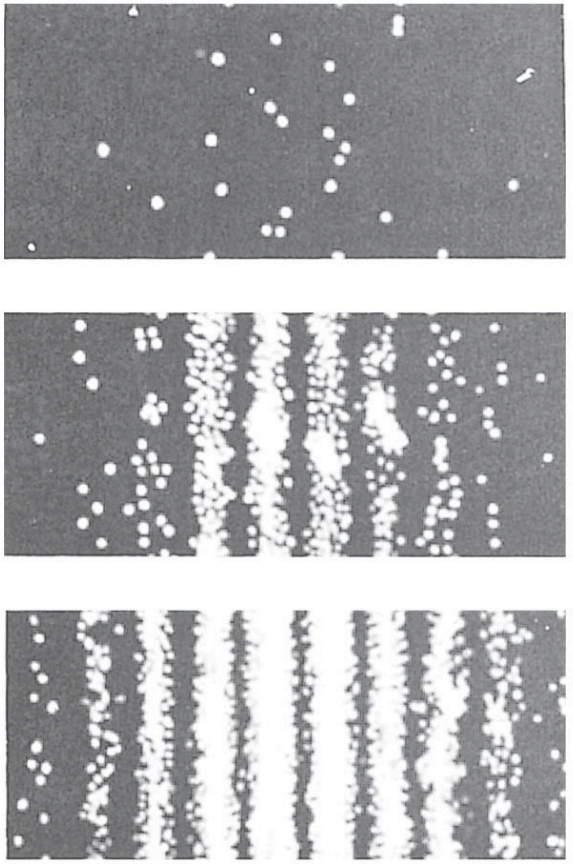


$$P_A = \int_{70}^{80} P(x)dx \simeq .25$$

Area under curve 20-100 = 1

FIGURE 40.1 The double-slit experiment with light.





The particle-like dots arrange themselves into wave-like interference fringes.

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) B(x)

2. Calculate the classical intensity

$$I(x)=\frac{1}{2}\sqrt{\frac{\varepsilon_0}{\mu_0}}\left|E(x)\right|^2$$

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

$$\frac{\#\ photons}{\sec\ area}=\frac{I(x)}{hf}$$

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.

$|\psi(x,t)|^2$ 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

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

where $i = \sqrt{-1}$

$$\frac{\partial}{\partial t} e^{i(kx-\omega t)} = -i\omega e^{i(kx-\omega t)} \qquad \frac{\partial}{\partial x} e^{i(kx-\omega t)} = ike^{i(kx-\omega t)}$$

Each time derivative becomes -iω. 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

$$E(x,t) = E_0 \cos\left(kx - \omega t\right) = \mathrm{Re}[E_0 e^{i(kx-\omega t)}] \qquad i = \sqrt{-1}$$

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

After canceling common factors $\quad \omega^2 = c^2 k^2$

If I say: $\quad E = \hbar\omega \qquad p = \hbar k$

Then $\quad E = pc$ 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 ?

$$P(x,t) = \left|\psi(x,t)\right|^2$$

Step 1: solve Schrodinger equation for wave function

Step 2: probability density of finding particle at x is

$$P(x,t) = \left|\psi(x,t)\right|^2$$

Stationary States - Bohr Hypothesis

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

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

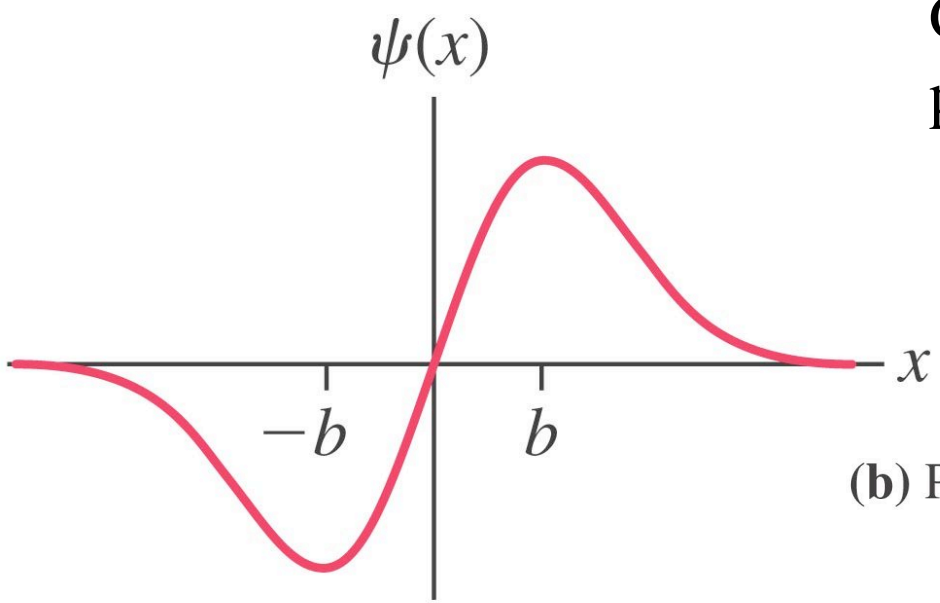
Stationary State satisfies

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

Note: $$\left|\psi(x,t)\right|^2 = \left|\hat{\psi}(x)e^{-iEt/\hbar}\right|^2 = \left|\hat{\psi}(x)\right|^2 = P(x)$$

P(x) Independent of time

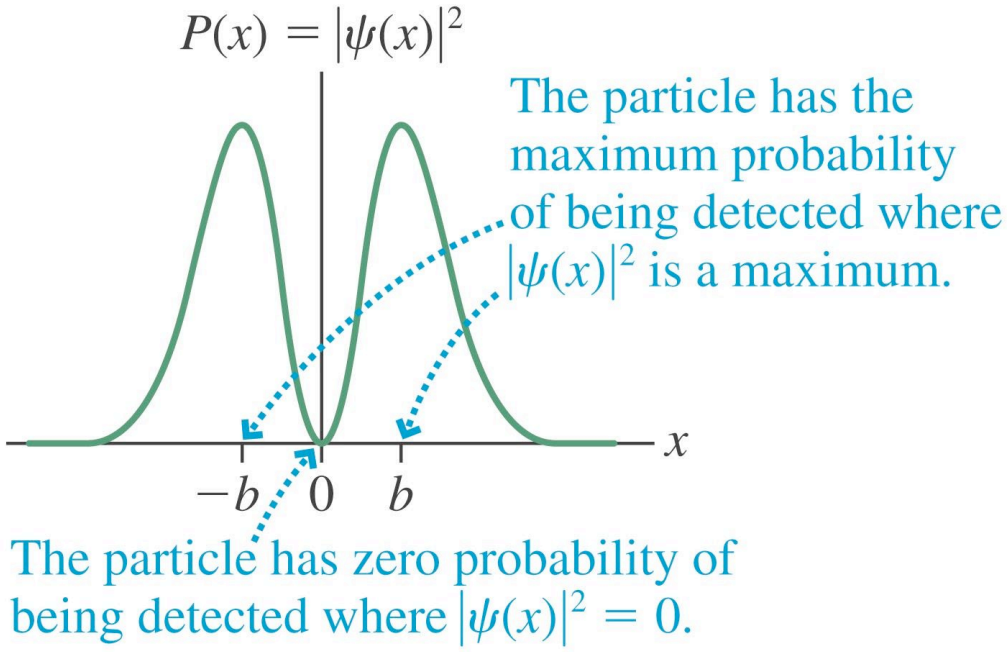
(a) Wave function



Corresponds to a particle in the potential

$$U = \frac{1}{2}kx^2$$

(b) Probability density



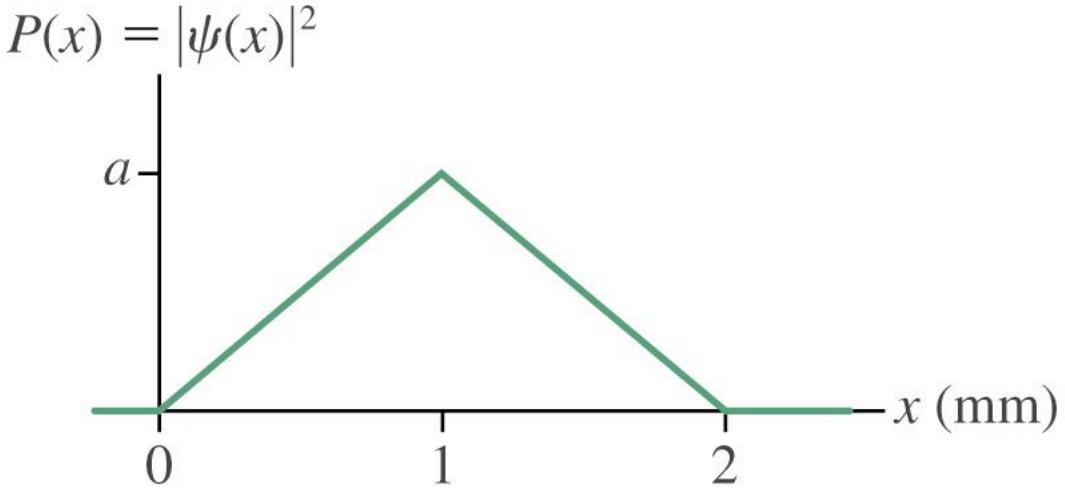
Normalization

- 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

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

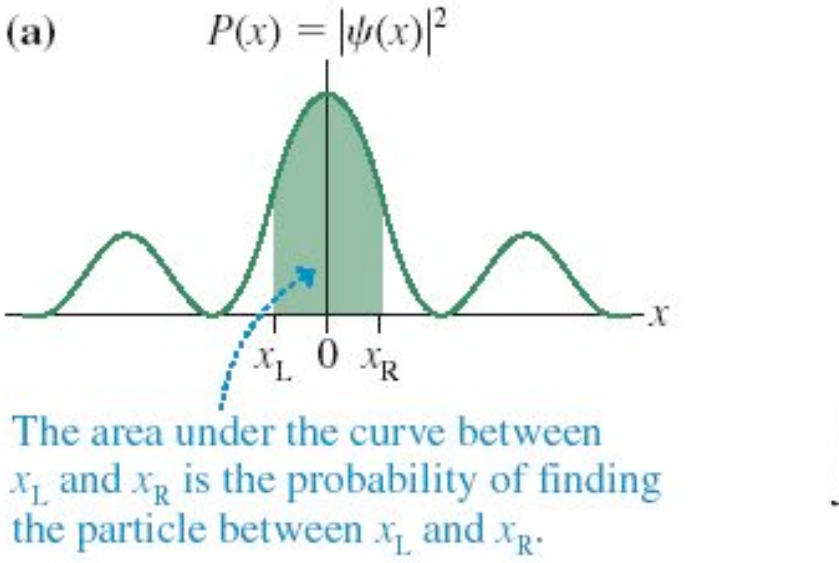
- Any wave function must satisfy this **normalization condition.**

The value of the constant *a* is



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. $a = 2.0\ \text{mm}^{-1}$.

FIGURE 40.8 The area under the probability density curve is a probability.

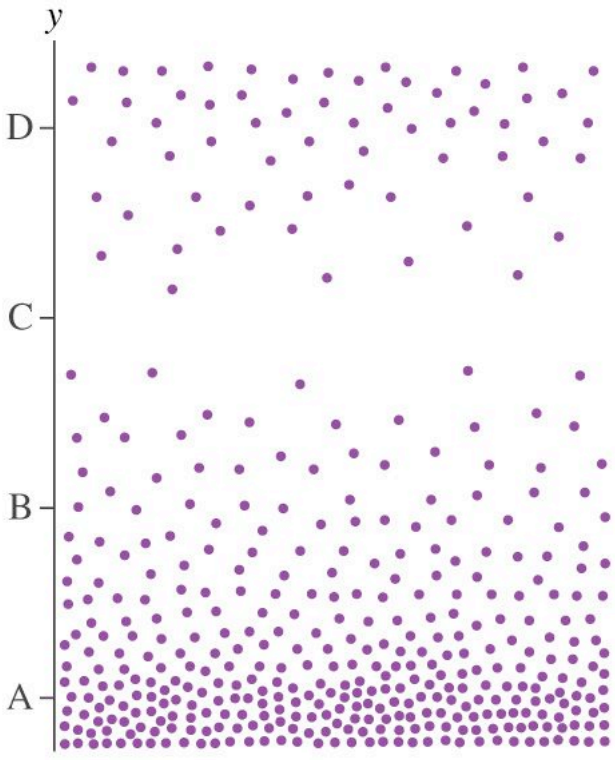


A property of the Schrodinger equation is that if initially

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

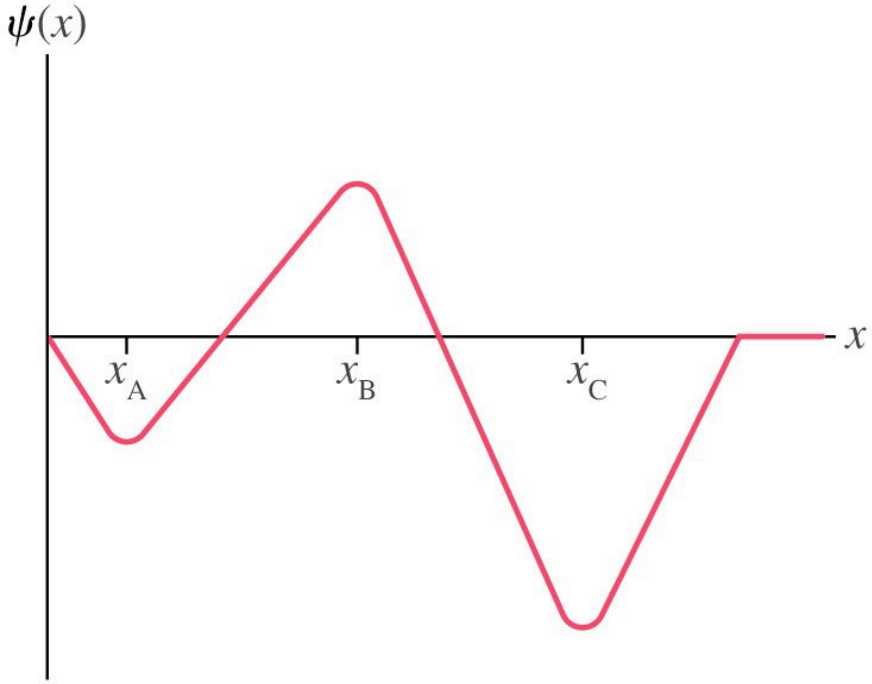
Then it will be true for all time.

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 ω and t

Remember $p = \hbar k = -i\hbar \frac{\partial}{\partial x}$ $E = \hbar\omega = i\hbar \frac{\partial}{\partial t}$

Momentum is derivative wrt x

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 is constant in space and time

$$P \propto \left|\psi(x,t)\right|^2 = \left|\psi_0 e^{i(kx-\omega t)}\right|^2 = \left|\psi_0\right|^2 = const.$$

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 Δt has a spread in Frequency values Δf.

$$\Delta f = 1 / \Delta t$$

FIGURE 40.12 History graph of a wave packet with duration Δt.

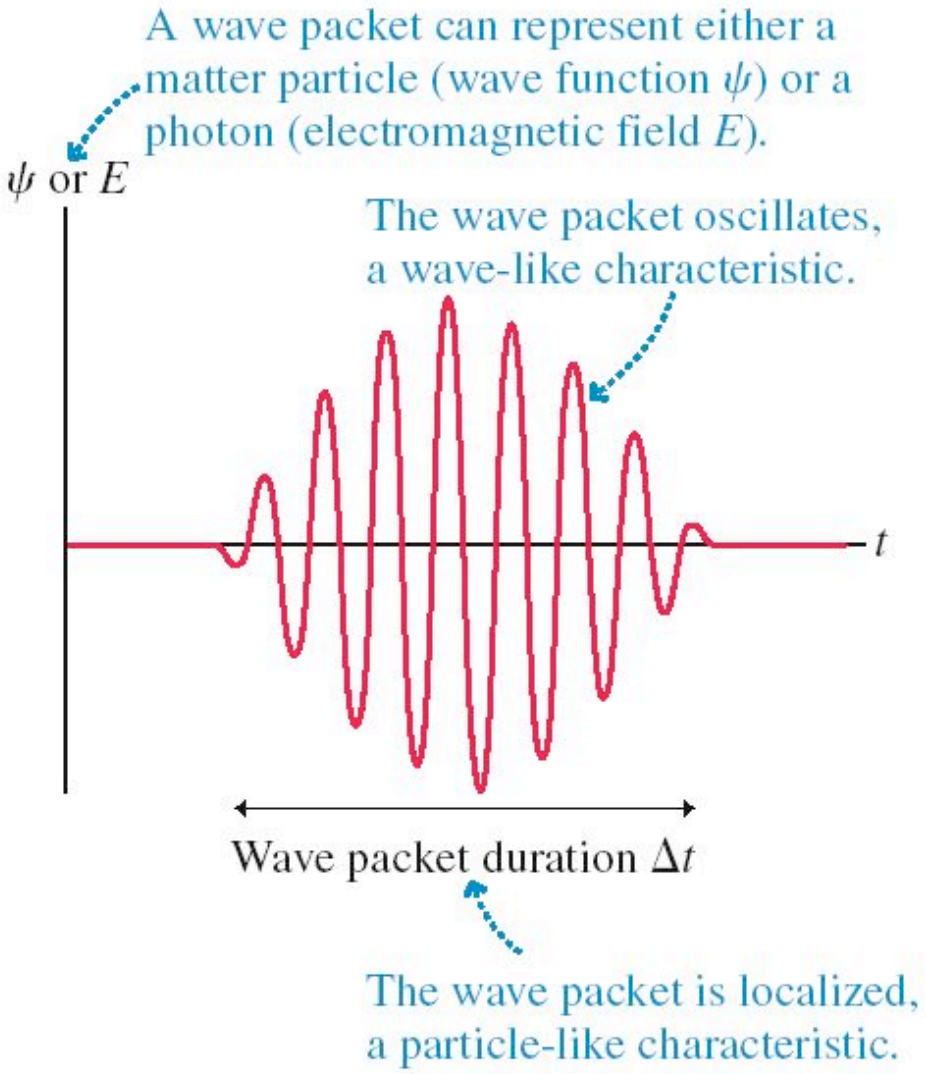
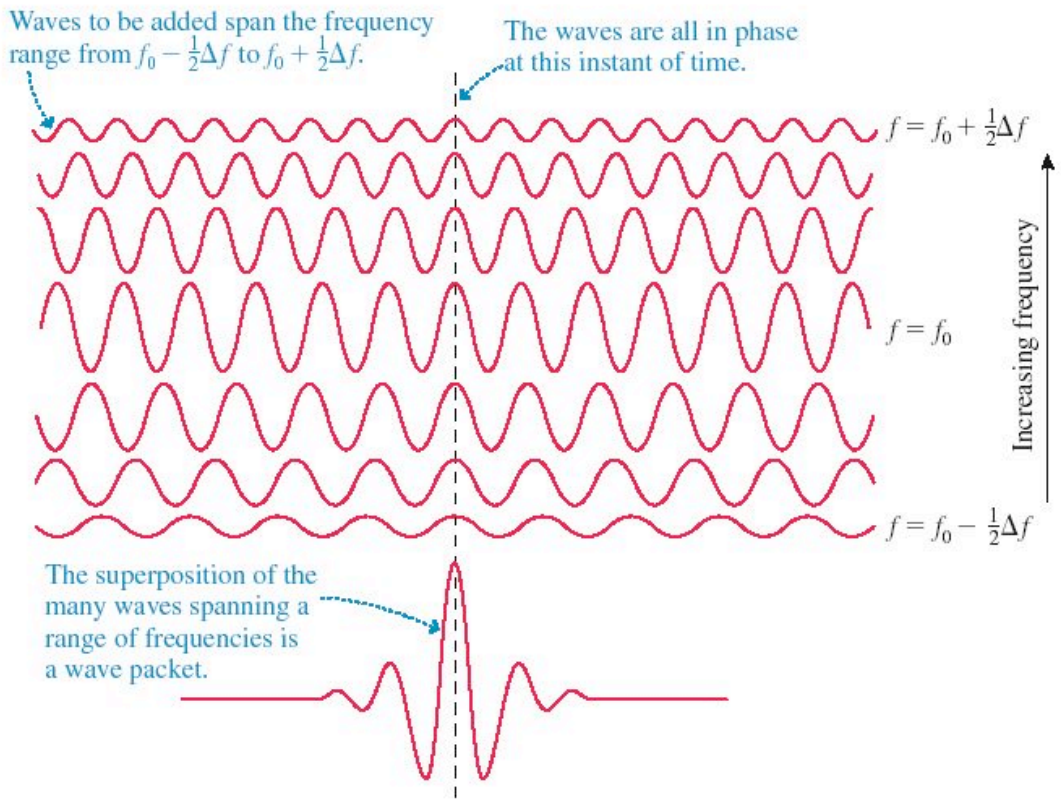


FIGURE 40.14 A single wave packet is the superposition of many component waves of similar wavelength and frequency.



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

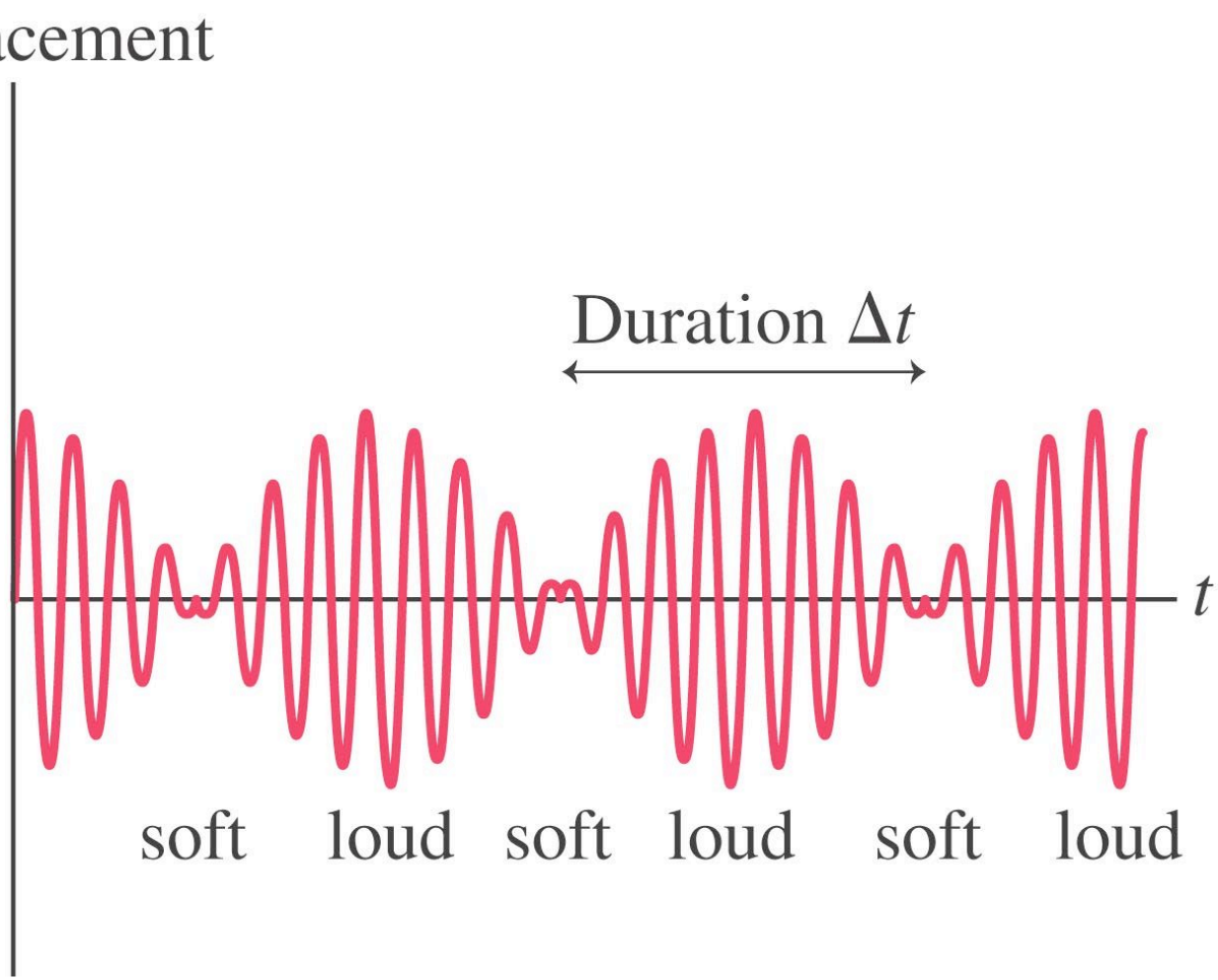
A sum of two waves gives beats. (I hate beets!)

$$\cos\left[(\omega + \Delta\omega/2)t\right] + \cos\left[(\omega - \Delta\omega/2)t\right] = 2\cos\left[\omega t\right]\cos\left[\Delta\omega t\right]$$

rapid oscillations given by ω, average frequency.

Duration Δt given by variation in frequency, Δω

$$\Delta\omega\Delta t = \pi$$



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 Δf.

Fourier analysis shows that for *any* wave packet

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

We have not given a precise definition of Δt and Δf for a general wave packet.

The quantity Δt is "about how long the wave packet lasts," while Δf is "about the range of frequencies needing to be superimposed to produce this wave packet."

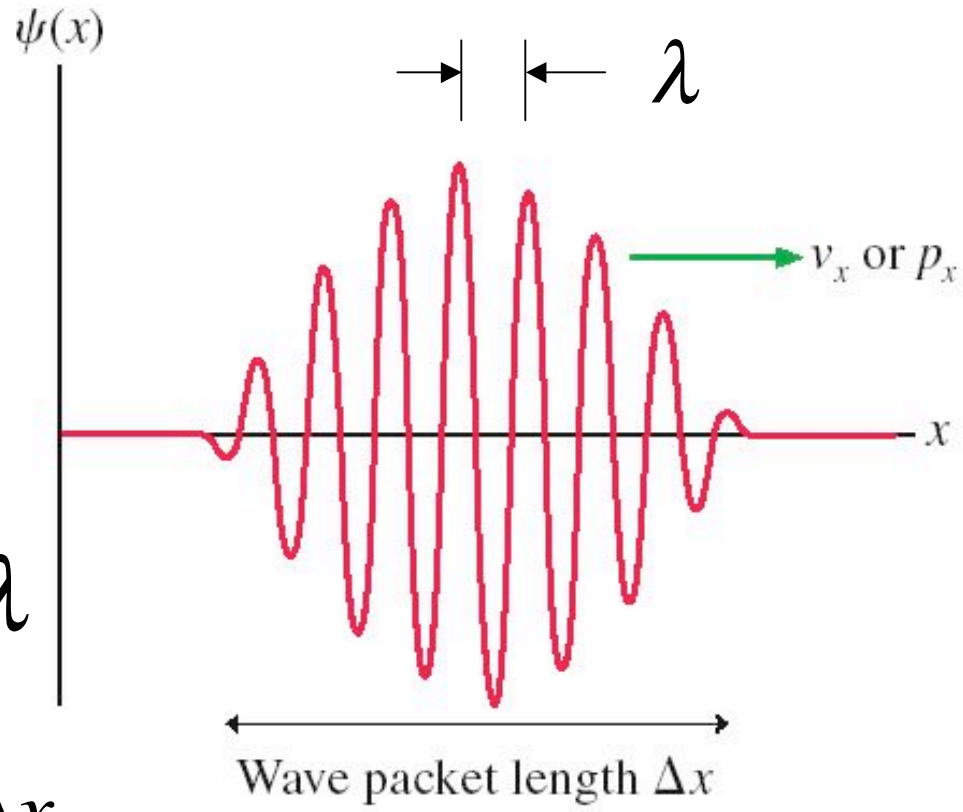
The same considerations apply to the spatial dependence of a wave packet.

$$\Delta k \Delta x = \pi$$

$$p = \hbar k = h / \lambda$$

$$\Delta p = \hbar \Delta k \simeq h / \Delta x$$

FIGURE 40.17 A snapshot graph of a wave packet.



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?

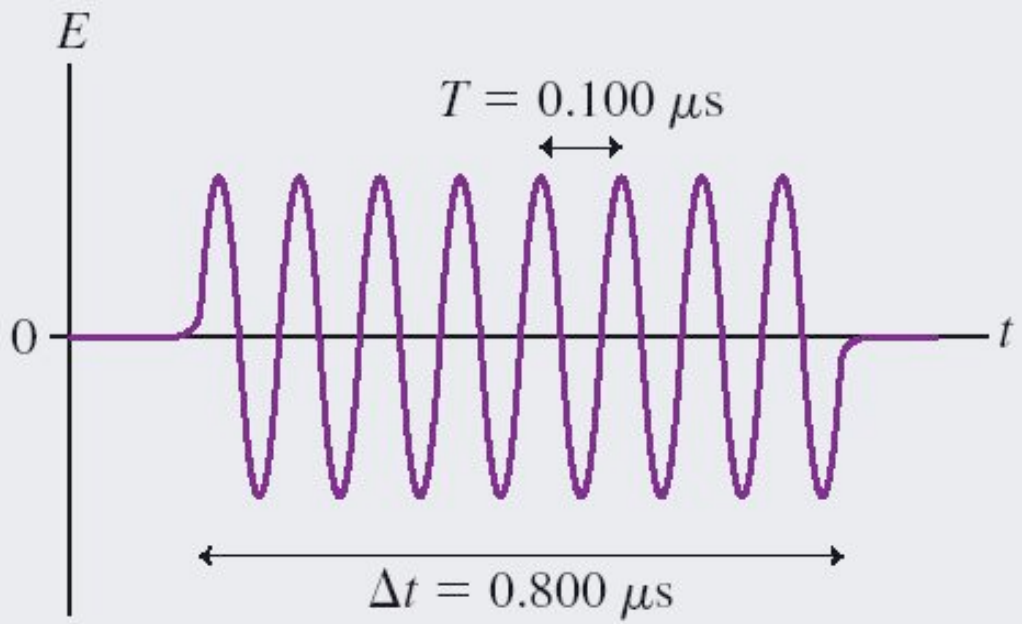
EXAMPLE 40.4 Creating radio-frequency pulses

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.



EXAMPLE 40.4 Creating radio-frequency pulses

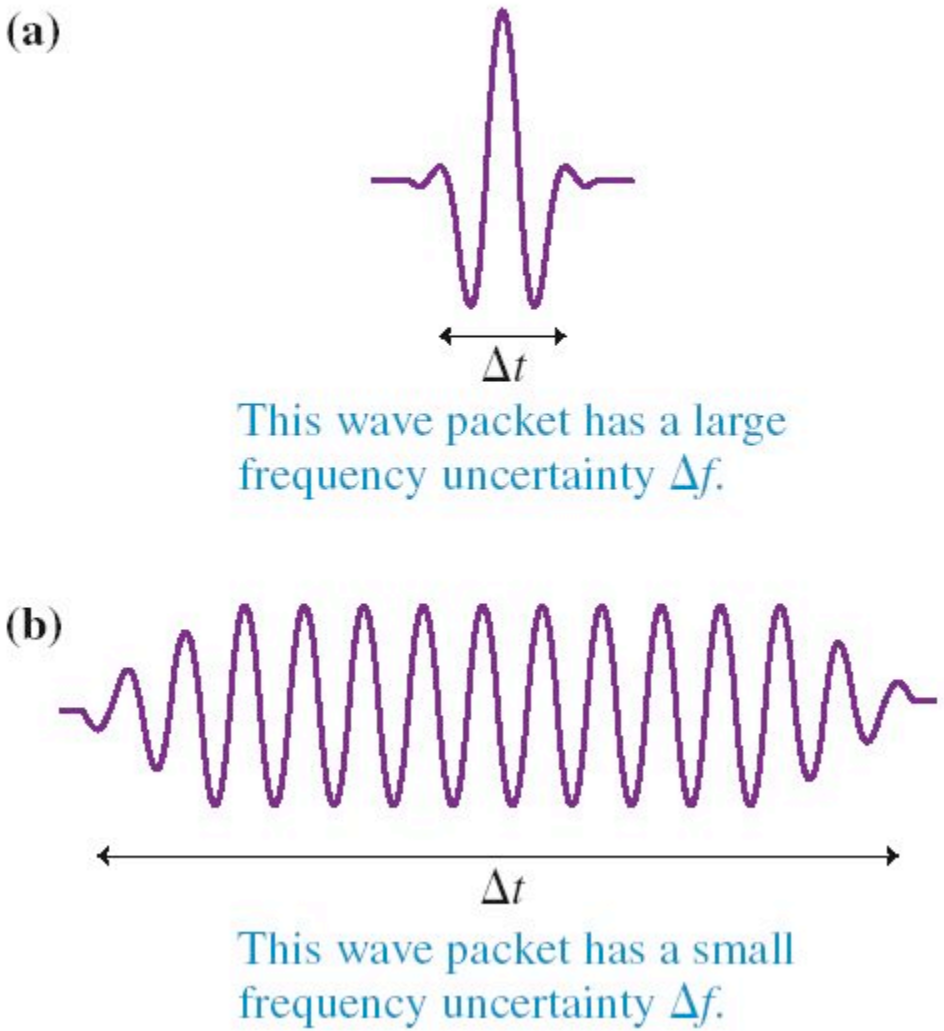
SOLVE The period of a 10.000 MHz oscillation is 0.100 μs. A pulse 0.800 μs in duration is 8 oscillations of the wave. Although the station broadcasts at a nominal frequency of 10.000 MHz, this pulse is not a pure 10.000 MHz oscillation. Instead, the pulse has been created by the superposition of many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

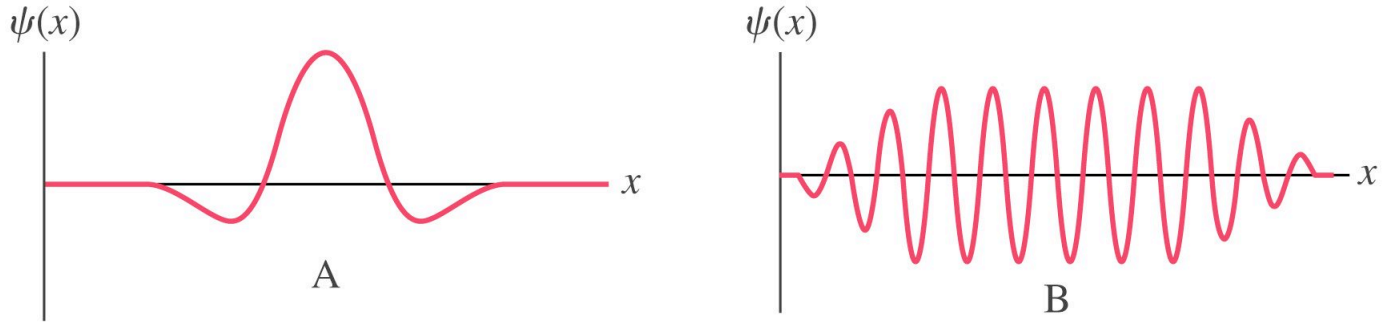


These two wave packets have the same average frequency f, but different spreads in frequency Δf.

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 Δx is the length or spatial extent of a wave packet.

Δp_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

$$\Delta x \Delta p_x \geq \frac{h}{2} \qquad \text{(Heisenberg uncertainty principle)}$$

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 **uncertainty principle.**

EXAMPLE 40.5 The uncertainty of a dust particle

QUESTION:

EXAMPLE 40.5 The uncertainty of a dust particle

A 1.0-μm-diameter dust particle ($m \approx 10^{-15}$ 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 Δx, the uncertainty Δp_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 $\Delta p_x \approx h/(2\Delta x) = h/2L$.

EXAMPLE 40.5 The uncertainty of a dust particle

We've assumed the most accurate measurements possible so that the $\geq$ 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 $v_x = 0$ 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 1.5×10^{-14} m/s would need 6×10^{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:

EXAMPLE 40.6 The uncertainty of an electron

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 -2×10^6 m/s $\leq v \leq 2 \times 10^6$ 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 Δv 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 $\psi(x)$.

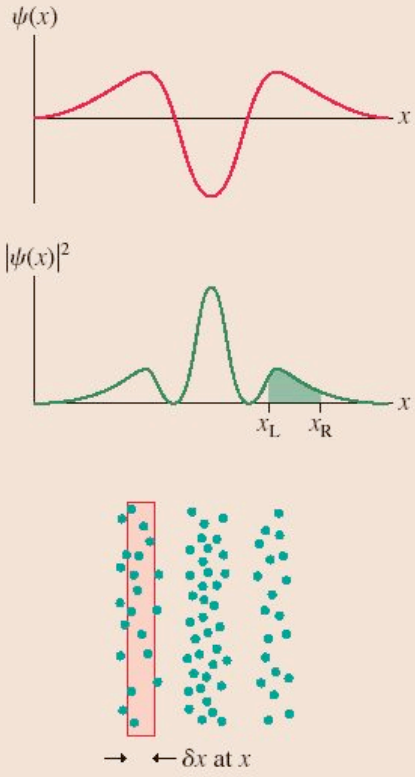
- $\psi(x)$ is a continuous, wave-like (i.e., oscillatory) function.
- The probability that a particle will be found in the narrow interval δx at position x is

$$\text{Prob(in } \delta x \text{ at } x) = |\psi(x)|^2 \delta x$$

- $|\psi(x)|^2$ 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

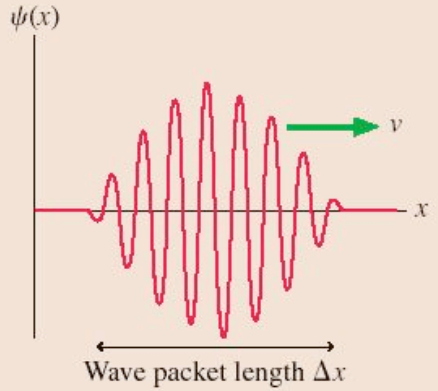
$$\text{Prob}(x_L \le x \le x_R) = \int_{x_L}^{x_R} |\psi(x)|^2 dx = \text{area under the curve}$$



General Principles

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 Δx and momentum uncertainty Δp_x are related by $\Delta x \Delta p_x \geq h/2$. The more you try to pin down the value of one, the less precisely the other can be known.

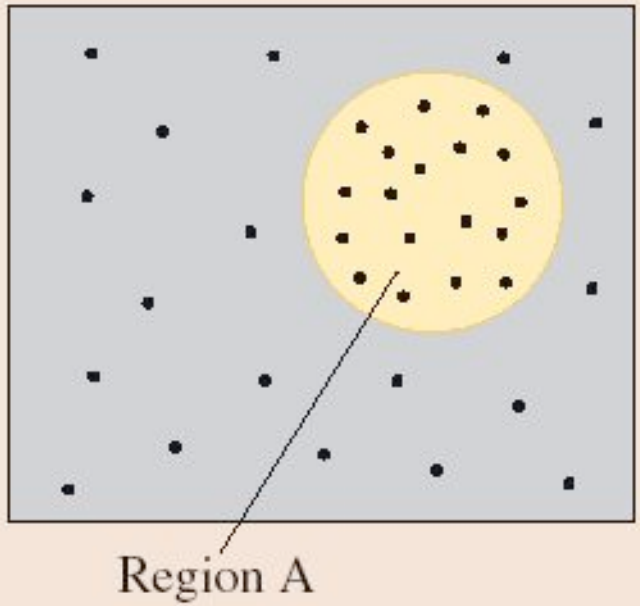


Important Concepts

The probability that a particle is found in region A is

$$P_A = \lim_{N_{tot} \to \infty} \frac{N_A}{N_{tot}}$$

If the probability is known, the expected number of A outcomes in N trials is $N_A = NP_A$.



Important Concepts

A wave packet of duration Δt can be created by the superposition of many waves spanning the frequency range Δf. These are related by

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