Matter-Waves and Electron Diffraction

"The most incomprehensible thing about the world is that it is comprehensible."

– **Albert Einstein**

Day 16:
Questions?
Electron Diffraction
de Broglie Wavelength
The Wave Function
The Uncertainty Principle

Up Next:
Schrödinger Equation
Potentials and PE,

Possible Reading Quiz.

Which of the following is not correct:

a) $\Psi(x)$ can be used for photons and matter

b) $|\Psi(x)|^2$ tells us the probability of locating an object (is the probability density)

c) $\Psi(x)$ must be normalziable. (integral of $|\Psi(x)|^2$ over all space = 1)

or

d) all are true

Midterm II is in two weeks: Thurs 3/22
We will run 75min + 20min

Recently:

1. Complementarity and wave-particle duality
2. Matter-Wave Interference

If you're wrestling still:

a) that's good (if you do it the right way)
b) see videos on website
c) see the explanation (step—by-step) tab

Today:

1. Matter waves and electron interference
2. de Broglie wavelength.
3. Uncertainty Principle

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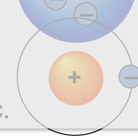
Models of the Atom

- Thomson – Plum Pudding
  - Why? Known that negative charges can be removed from a
  - Problem: just a random guess

- Rutherford – Solar System
  - Why? Scattering showed hard core.
  - Problem: electrons should spiral into nucleus in ~10^{-11} sec.



- Bohr – fixed energy levels
  - Why? Explains spectral lines.
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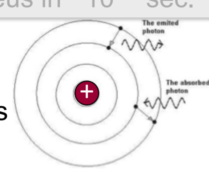

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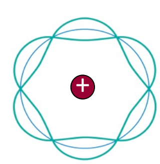


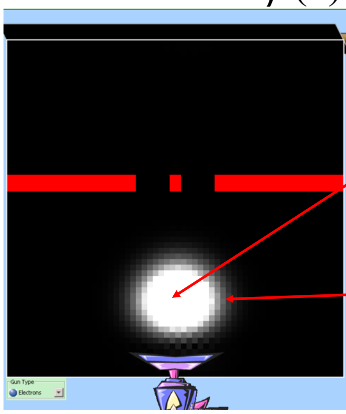
Same math for photons and matter waves:

- Describe massive particles with wave functions:

$$|\Psi\rangle = \Psi(x)$$

- Interpret (wave amplitude)^2 as a probability density:

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



Electron double slit experiment.
Display=Magnitude of wave function

Large Magnitude ($|\Psi|$)=
probability of detecting electron here is high

Small Magnitude ($|\Psi|$)=
probability of detecting electron here is low

http://phet.colorado.edu/en/simulation/quantum-wave-interference

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Double-Slit Experiment

$$\rho(r) = |\Psi(r)|^2 = \Psi^*(r)\Psi(\mathrm{r})$$

$$|\Psi(r)|^2 = \; {A_1}^2 + \; {A_2}^2 + 2\,A_1\,A_2\cos\big(k(r_2 - r_1)\big)$$

$$|\Psi(x)|^2 = \; {A_1}^2 + \; {A_2}^2 + 2\,A_1\,A_2\cos\left(\frac{2\pi}{\lambda}\left(\frac{d}{L}x\right)\right)$$

How do we connect this with what we observe?

$$|\Psi_1(r)|^2 = A_1\exp(-ikr_1)A_1\exp(ikr_1) = \; {A_1}^2$$

$$|\Psi_2(r)|^2 = A_2\exp(-ikr_2)A_2\exp(ikr_2) = \; {A_2}^2$$

Interpreting the math

If $|\Psi\rangle = |\Psi_1\rangle + |\Psi_2\rangle$, what is $|\Psi|^2$?

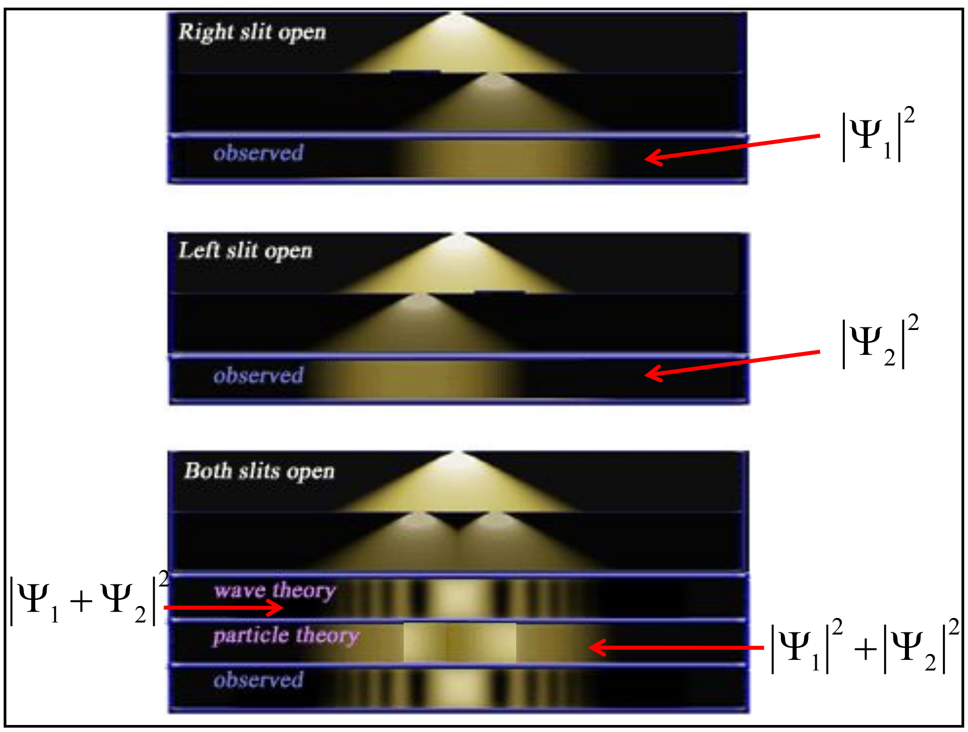
(note $<\Psi|\Psi> = |\Psi(r)|^2 = \Psi^*(r)\Psi(\mathrm{r})$)

a) $|\Psi|^2 = |\Psi_1|^2 + |\Psi_2|^2$

b) $|\Psi|^2 = |\Psi_1 + \Psi_2|^2$

c) a *and* b are the same

d) $|\Psi|^2 = |\Psi_1|^2 + |\Psi_2|^2 + \Psi_1^*\Psi_2 + \Psi_2^*\Psi_1$



Double-Slit Experiment

$$\rho(x) = |\Psi(x)|^2 = A_1{}^2 + A_2{}^2 + 2\,A_1\,A_2 \cos\left(\frac{2\pi}{\lambda}\left(\frac{d}{L}x\right)\right)$$

$|\Psi_1|^2$ $|\Psi_2|^2$ INTERFERENCE!

$$\rho_{1,2}(x) = |\Psi_1 + \Psi_2|^2$$

- In quantum mechanics, we add the individual amplitudes and square the sum to get the total probability (density).
- In classical physics, we added the individual probability densities to get the total.

Double-Slit Experiment

$$\rho(x) = |\Psi(x)|^2 = \Psi^*(x)\Psi(\mathrm{x})$$

$$|\Psi(x)|^2 = A_1{}^2 + A_2{}^2 + 2\,A_1\,A_2 \cos\left(\frac{2\pi}{\lambda}\left(\frac{d}{L}x\right)\right)$$

For a specific λ, $|\Psi(x)|^2$ describes where we find the interference maxima and minima of the fringe pattern.

What is the wavelength of an electron?

Matter Waves

As a doctoral student (1923), Louis de Broglie proposed that electrons might also behave like waves.

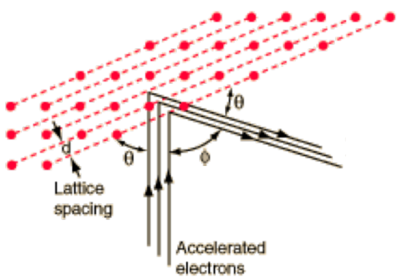
- Light, often thought of as a wave, had been shown to have particle-like properties.
- For ***photons***, we know how to relate momentum to wavelength:

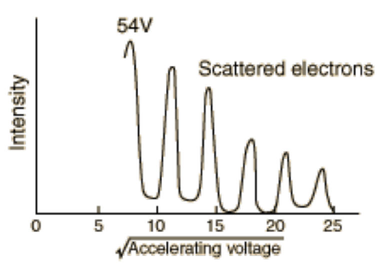
From the photoelectric effect: $E = hf = hc/\lambda$

From special relativity: $E = p_\gamma c$

Combined: $\lambda =$

Matter Waves



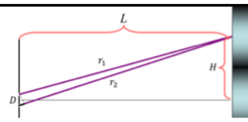


de Broglie wavelength:

$$\lambda = h/p$$

Confirmed experimentally by Davisson and Germer (1924).

Matter Waves



de Broglie wavelength: $\lambda = h/p$

$$H = \frac{n\lambda L}{D}$$

In order to observe electron interference, it would be best to perform a double-slit experiment with:

A) Lower energy electron beam.
B) Higher energy electron beam.
C) It doesn't make any difference.

Matter Waves

de Broglie wavelength: $\lambda = h/p$

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In order to observe electron interference, it would be best to perform a double-slit experiment with:

A) Lower energy electron beam.
B) Higher energy electron beam.
C) It doesn't make any difference.

Lowering the energy will increase the wavelength of the electron.

Can typically make electron beams with energies from 25 – 1000 eV.

Matter Waves

de Broglie wavelength: $\lambda = h/p$ $\qquad H = \frac{n\lambda L}{D}$

$$h = 6.6\times10^{-34}\ \mathrm{J\cdot s}$$

For an electron beam of 25 eV, we expect Θ (the angle between the center and the first maximum) to be:

A) Θ << 1
B) Θ < 1
C) Θ > 1
D) Θ >> 1

Use $D = 5\times10^{-4}\ \mathrm{m}$

and remember: $\theta = \frac{\lambda}{D}$

& $E = \frac{p^2}{2m}$

m = 9.1 * 10^{-31} kg & 1.6 * 10^{-19} J/eV

Matter Waves

de Broglie wavelength: $\lambda = h/p$ $\qquad H = \frac{n\lambda L}{D}$

For an electron beam of 25 eV:

$$E = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mE}$$

$$\lambda = \frac{(6.6x10^{-34}\ \mathrm{J\cdot s})}{[2\times(9.1x10^{-31}\ \mathrm{kg})\times(25\ eV\times1.6x10^{-19} J/eV)]^{\frac{1}{2}}}$$

Matter Waves

de Broglie wavelength: $\lambda = h/p$ $H = \frac{n\lambda L}{D}$

For an electron beam of 25 eV: $h = 6.6\times10^{-34}\ \mathrm{J\cdot s}$

$$\lambda = h/p = \frac{6.6\times10^{-34}}{2.7\times10^{-24}} = 2.4\times10^{-10}\ m$$

H/ L= $\theta = \lambda/D = 4.9\times10^{-7}$ for $D = 5\times10^{-4}\ \mathrm{m}$

$$H = L\theta = (3m)(4.9\times10^{-7}) = 1.5\times10^{-6}m = 1.5\mu m$$

Too small to easily see!

Matter Waves

de Broglie wavelength: $\lambda = h/p$ $H = \frac{n\lambda L}{D}$

For an electron beam of 25 eV, how can we make the diffraction pattern more visible?

A) Make D much smaller.
B) Increase energy of electron beam.
C) Make D much bigger.
D) A & B
E) B & C

Matter Waves

de Broglie wavelength: $\lambda = h/p$ $\qquad h = 6.6\times10^{-34}\ \mathrm{J\cdot s}$

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E) B & C

25 eV is a lower bound on the energy of a decent electron beam.

Decreasing the distance between the slits will increase Θ.

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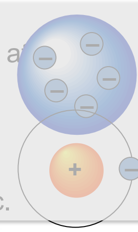

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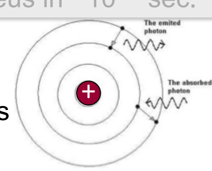

- deBroglie – electron standing waves
  - Why?...

Bohr model is a weird mix of classical physics and arbitrary rules…

- Why is angular momentum quantized yet Newton’s laws still work?
- Why don’t electrons radiate when they are in fixed orbitals yet Coulomb’s law still works?
- No way to know *a priori* which rules to keep and which to throw out…
- BUT IT WORKS (for certain things)!

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Summary: What things CAN’T the Bohr model explain?

- WHY is angular momentum quantized?
- WHY don’t electrons radiate when they are in fixed orbitals?
- How does electron know which level to jump to? (i.e. how to predict intensities of spectral lines)
- Can’t be generalized to more complex (multi-electron) atoms
- Shapes of molecular orbits and how bonds work
- Can’t explain doublet spectral lines

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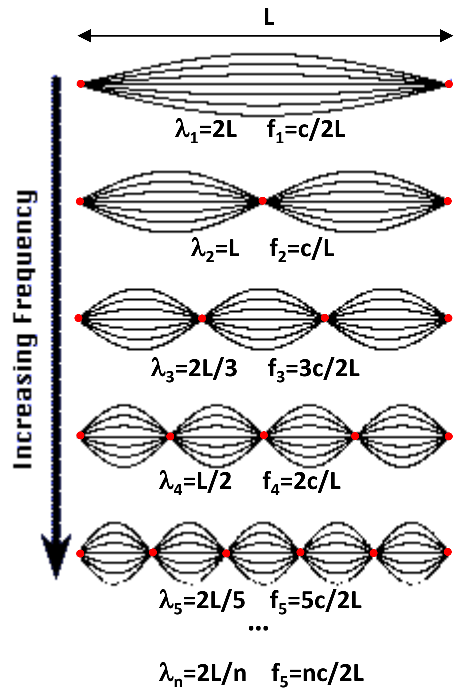
Elect. Waves

- Physicists at this time may have been confused about atoms, but they understood waves really well.
- They understood that for standing waves, boundary conditions mean that waves only have discrete modes.
- E.g. guitar strings

• = node = fixed point that doesn't move.



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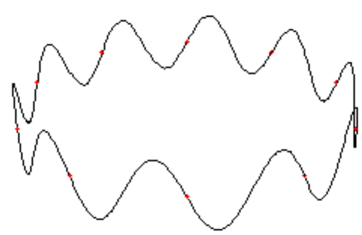
Standing Waves on a Ring

Just like standing wave on a string, but now the two ends of the string are joined. (sim)



What are the restrictions on the wavelength?

A. $r = \lambda$
B. $r = n\lambda$
C. $\pi r = n\lambda$
D. $2\pi r = n\lambda$
E. $2\pi r = \lambda/n$

$n = 1, 2, 3, \ldots$

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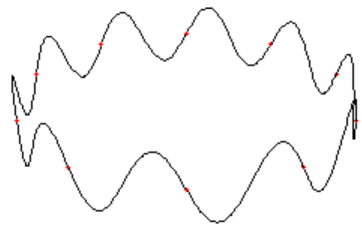
Standing Waves on a Ring

- Answer: D. $2\pi r = n\lambda$



- Circumference = $2\pi r$
- To get standing wave on ring:

  Circumference = $n\lambda$

  Must have integer number of wavelengths to get constructive, not destructive, interference.
- n = number of wavelengths

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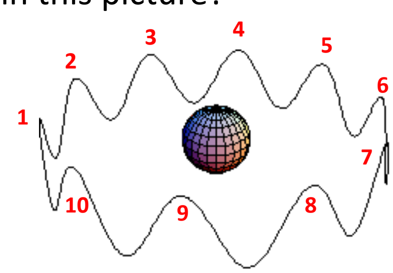
deBroglie Waves

What is n for electron wave in this picture?



A. 1
B. 5
C. 10
D. 20
E. Cannot determine from picture

Answer: C. 10

n = number of wavelengths.
It is **also** the number of the energy level $E_n = -13.6/n^2$.
So the wave above corresponds to
$E_{10} = -13.6/10^2 = -0.136\text{eV}$

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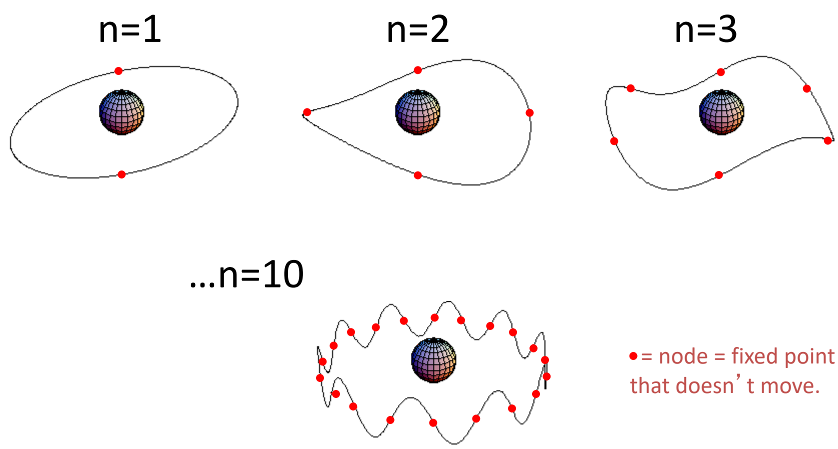
deBroglie Waves



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deBroglie Waves

Given the deBroglie wavelength (**λ=h/p**) and the condition for standing waves on a ring (**2πr = nλ**), what can you say about the angular momentum L of an electron if it is a deBroglie wave?

L = angular momentum = p r

p = momentum = mv

A. $L = n\hbar/r$
B. $L = n\hbar$
C. $L = n\hbar/2$
D. $L = 2n\hbar/r$
E. $L = n\hbar/2r$

(Note: $\hbar = h/2\pi$)

$L = p\,r = (h/\lambda)\,r$
$\lambda = 2\pi\,r / n$
$L = h\,n\,r / (2\pi\,r)$
$= \hbar\,n$

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deBroglie Waves

- Substituting the deBroglie wavelength (λ=h/p) into the condition for standing waves ($2\pi r = n\lambda$), gives:

$$2\pi r = nh/p$$

- Or, rearranging:

$$pr = nh/2\pi$$

$$L = n\hbar$$

- deBroglie EXPLAINS quantization of angular momentum, and therefore EXPLAINS quantization of energy!

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deBroglie Waves

- This is a great story.
- But is it true?
- If so, why no observations of electron waves?
- What would you need to see to believe that this is actually true?
- Recall: Electron interference!

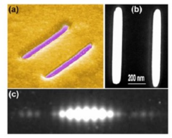

FIG. 2. (Color online) (a) SEM image of the two slits opened by FIB milling (yellow: gold, violet: silicon nitride). (b) TEM image of the transmittance of the slits, 83 nm wide, 420 nm spaced. (c) Fraunhofer electron diffraction pattern showing the two slit interference fringes superimposed to the intensity transmitted by each slit.

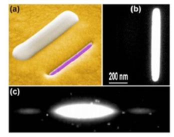

FIG. 3. (Color online) (a) SEM image of the two slits after the site-selective FIB deposition of Pt material (gray) blocking the left slit. (b) TEM image of the same area showing the still open right slit. (c) Fraunhofer electron diffraction pattern showing the typical single slit diffraction pattern.

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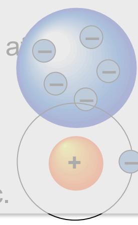

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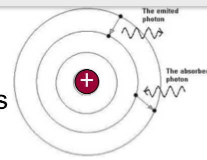

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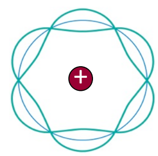
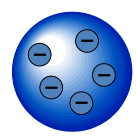


Models of the Atom



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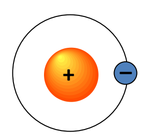

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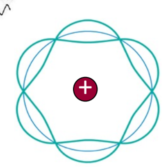
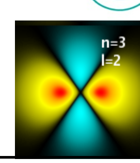


- Schrodinger – quantum wave functions
  - Why? Explains everything!
  - Problem: None (except that it's hard to understand)



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Matter waves:

- Describe massive particles with wave functions:

$$\left|\Psi\right\rangle = \Psi(x)$$

- Interpret (wave amplitude)^2 as a probability density:

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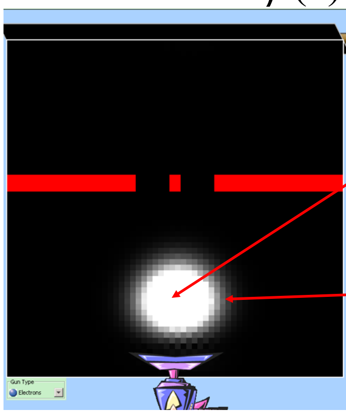

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What are these waves?

(students not responsible for the Matter Wave math yet)

EM Waves (light/photons)

- Amplitude E = electric field
- $|E|^2$ tells you the probability of detecting a photon.
- Maxwell's Equations:

$$\frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2}$$

- Solutions are sine/cosine waves:

$$E(x,t) = A\sin(kx - \omega t)$$

$$E(x,t) = A\cos(kx - \omega t)$$

Matter Waves (electrons/etc)

- Amplitude Ψ = matter field
- $|\Psi|^2$ tells you the probability of detecting a particle.
- Schrödinger Equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = i\hbar\frac{\partial \psi}{\partial t}$$

- Solutions are **complex** sine/cosine waves:

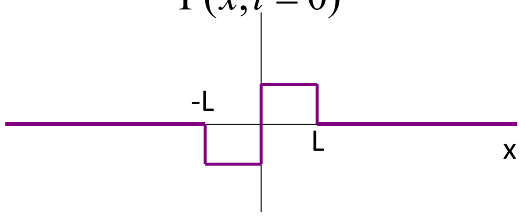
$$\Psi(x,t) = A\exp\left[i\left(kx - \omega t\right)\right]$$

$$= A\left[\cos(kx - \omega t) + i\sin(kx - \omega t)\right]$$

Matter Waves

- Describe a particle with a wave function. $|\Psi\rangle = \Psi(x,t)$
- Wave does **not** describe the path of the particle.
- Wave function contains information about the ***probability*** to find a particle at x, y, z & t.

$\Psi(x,t=0)$



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

In general:

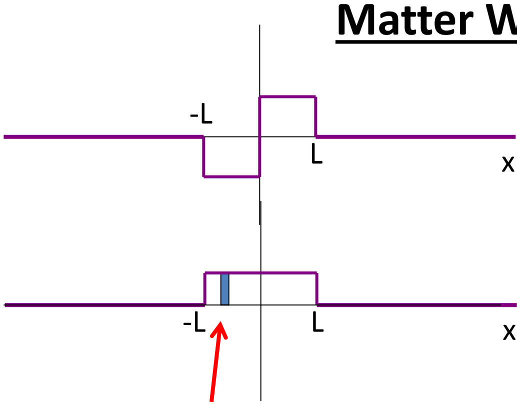
$\Psi(x,y,z,t)$

$\Psi(r,\theta,\phi,t)$

Simplified:

$\Psi(x,t)$ & $\Psi(x)$

Matter Waves



Wavefunction

$\Psi(x,t=0)$

Probability Density

$\rho(x,t=0) = |\Psi(x,t=0)|^2$

Probability of finding particle in the interval dx is $\rho(x)dx$

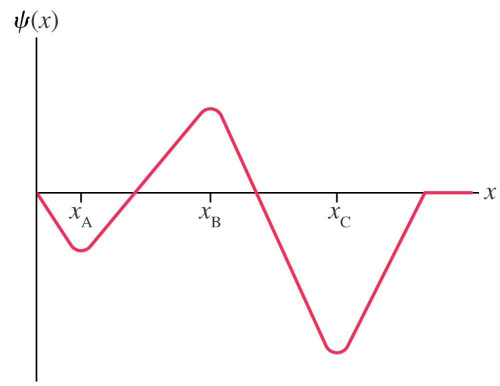
$$P[-\infty < x < +\infty] = \int_{-\infty}^{\infty} \rho(x)dx = \int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = 1$$

Normalized wave functions

Matter Waves

Below is a wave function for a neutron. At what value of x is the neutron most likely to be found?

A) X_A B) X_B C) X_C D) There is no one most likely place



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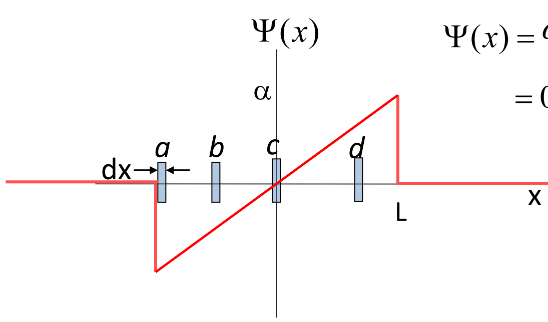
An electron is described by the following wave function:

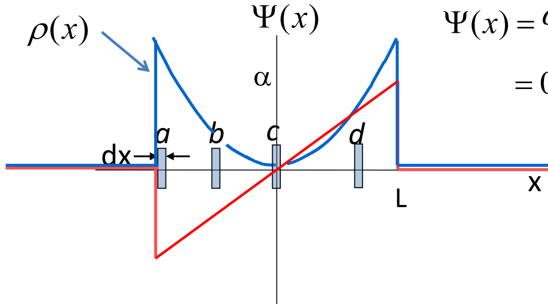


$$\Psi(x) = \alpha x / L \text{ from } x = -L \text{ to } x = +L$$
$$= 0 \text{ elsewhere}$$

How do the probabilities of finding the electron near (within dx) of *a,b,c,* and *d* compare?

A) d > c > b > a
B) a = b = c = d
C) d > b > a > c
D) a > d > b > c

An electron is described by the following wave function:



$$\Psi(x) = \alpha x / L \text{ from } x = -L \text{ to } x = +L$$
$$= 0 \text{ elsewhere}$$

$$\rho(x) = |\Psi(x)|^2 = \frac{\alpha^2 x^2}{L^2}$$

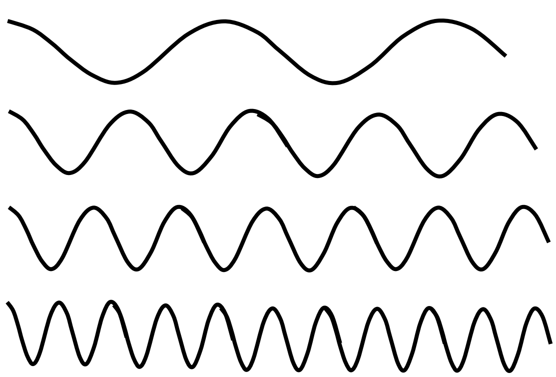
How do the probabilities of finding the electron near (within dx) of *a,b,c,* and *d* compare?

A) d > c > b > a
B) a = b = c = d
C) d > b > a > c
D) a > d > b > c

Plane Waves

Plane waves (sines, cosines, complex exponentials) extend forever in space:

$$\Psi_1(x,t) = \exp\left[i\left(k_1 x - \omega_1 t\right)\right]$$
$$\Psi_2(x,t) = \exp\left[i\left(k_2 x - \omega_2 t\right)\right]$$
$$\Psi_3(x,t) = \exp\left[i\left(k_3 x - \omega_3 t\right)\right]$$
$$\Psi_4(x,t) = \exp\left[i\left(k_4 x - \omega_4 t\right)\right]$$



Different *k*'s correspond to different energies, since

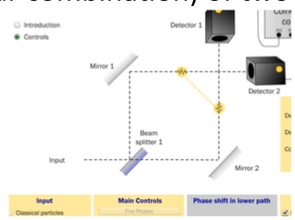
$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} \qquad k = \frac{2\pi}{\lambda} \qquad \hbar = \frac{h}{2\pi}$$

Superposition

If $\Psi_1(x,t)$ and $\Psi_2(x,t)$ are solutions to a wave equation,

then so is $\Psi(x,t) = \Psi_1(x,t) + \Psi_2(x,t)$

Superposition (linear combination) of two waves

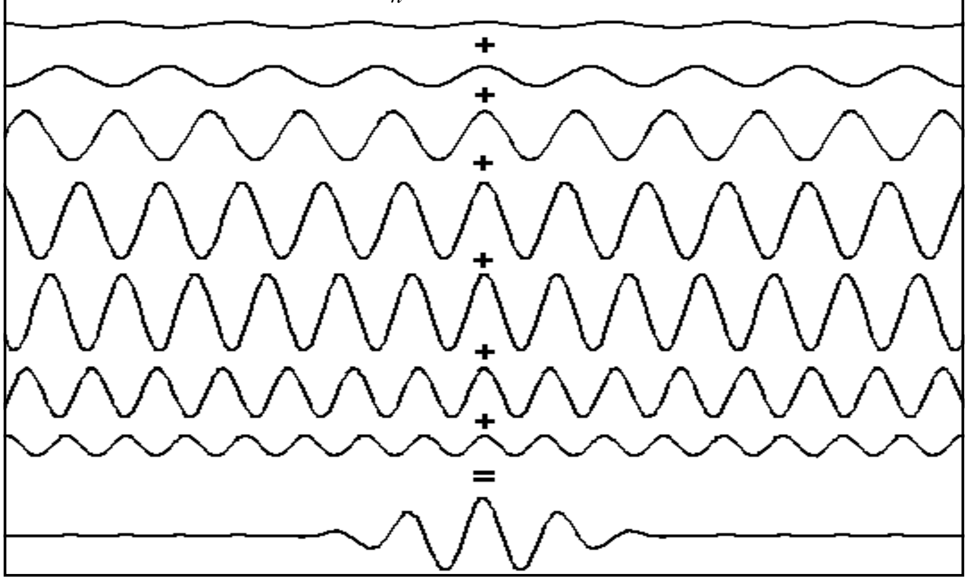


We can construct a **"wave packet"** by combining many plane waves of different energies (different k's).

http://phet.colorado.edu/en/simulation/fourier

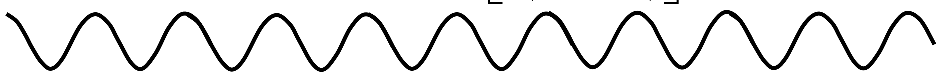
Superposition

$$\Psi(x,t) = \sum_n A_n \exp\left[i\left(k_n x - \omega_n t\right)\right]$$



Plane Waves vs. Wave Packets

$$\Psi(x,t) = A\exp\left[i\left(kx - \omega t\right)\right]$$



$$\Psi(x,t) = \sum_n A_n \exp\left[i\left(k_n x - \omega_n t\right)\right]$$

Which one looks more like a particle?

Plane Waves vs. Wave Packets

$$\Psi(x,t) = A\exp\left[i\left(kx - \omega t\right)\right]$$

$$\Psi(x,t) = \sum_n A_n \exp\left[i\left(k_n x - \omega_n t\right)\right]$$

For which wave is the position (x) and momentum (p) most well-defined?

A) x most well-defined for plane wave, p most well-defined for wave packet.

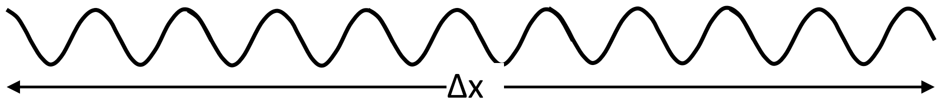
B) p most well-defined for plane wave, x most well-defined for wave packet.

C) p most well-defined for plane wave, x equally well-defined for both.

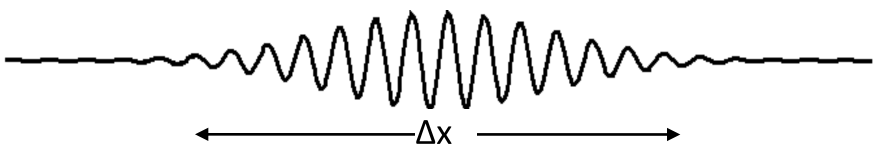
D) x most well-defined for wave packet, p equally well-defined for both.

E) p and x are equally well-defined for both.

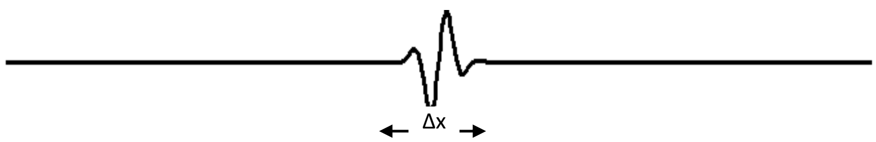
Uncertainty Principle



small Δp – only one wavelength



medium Δp – wave packet made of several waves



large Δp – wave packet made of lots of waves

Uncertainty Principle

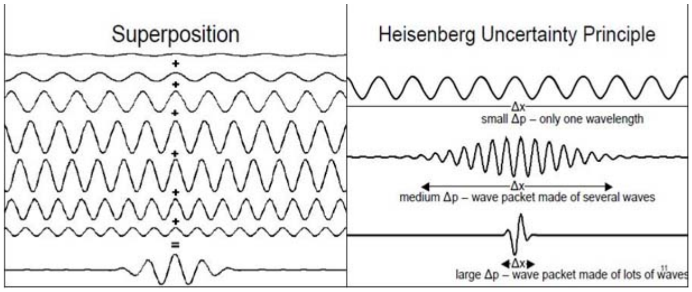
In math: $\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$

In words:
The position and momentum of a particle cannot **both** be determined with complete precision. The more precisely one is determined, the less precisely the other is determined.

What do Δx (uncertainty in position) and Δp (uncertainty in momentum) mean?

Uncertainty Principle

A <u>Wave</u> Interpretation:



- Wave packets are constructed from a series of plane waves.
- The more spatially localized the wave packet, the less uncertainty in position.
- With less uncertainty in position comes a greater uncertainty in momentum.

Matter Waves (Summary)

- Electrons and other particles have wave properties (interference) [observation]
- When not being observed, electrons are spread out in space (delocalized waves) [NF interpretation from inference!]
- When being observed, electrons are found in one place (localized particles) [observation]
- Particles are described by wave functions: $|\Psi\rangle = \Psi(x,t)$ (probabilistic, not deterministic) [calculation / observation]
- Physically, what we measure is $\rho(x,t) = |\Psi(x,t)|^2$ (probability density for finding a particle in a particular place at a particular time) [observation]
- Simultaneous measurements of x & p are constrained by the Uncertainty Principle: $\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$ [calculation / observation]