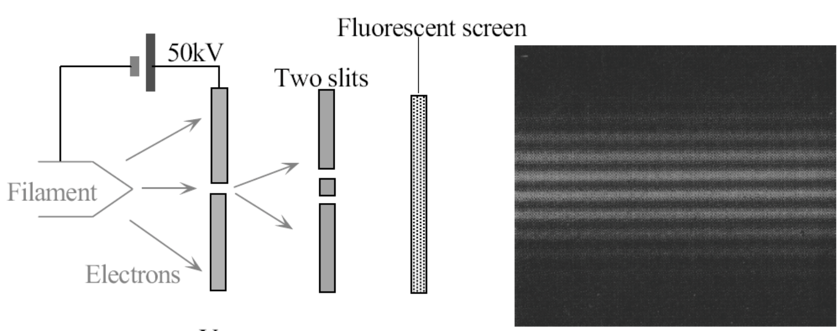
3.2 The electron as a wave



Electron diffraction fringes on the screen

From *Principles of Electronic Materials and Devices, Third Edition*, S.O. Kasap (© McGraw-Hill, 2005)

$m_{baseball} = 0.150kg$

$v = 50\ m/s$

$\lambda = h / mv = 6.63 * 10^{-34}\ Js / (0.150kg * 50\ m/s) =$

$= 8.8 * 10^{-35}\ m$

How does this compare to the ball's size?

- What about an electron?

  $m_{electron} = 9.11 * 10^{-31}\ kg$

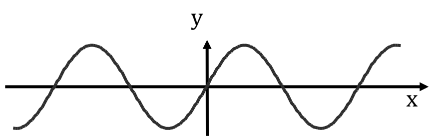
  $v = 0.1\ c = 3 * 10^{7}\ m/s$

  $\lambda = h / mv = 2.43 * 10^{-11}\ m$

How does this compare to the size of an atom?

Wave Equations

Vibrations on a string:



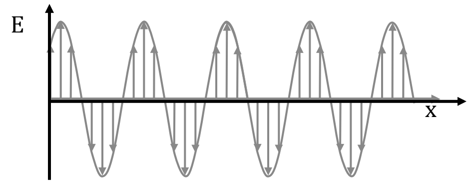
$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$$

v = speed of wave

Solutions: y(x,t)

Vertical displacement of String

Electromagnetic waves:



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

c = speed of light

Solutions: E(x,t)

Strength of Electric field

Matter waves (Schrödinger's equation):

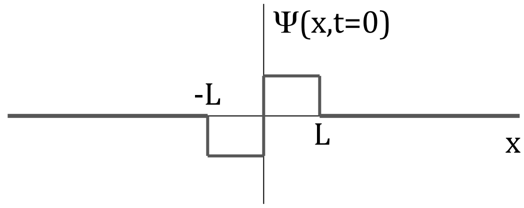
In 3-D:

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

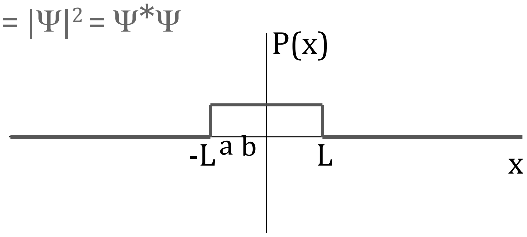
In 1-D:

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

Wave function = $\Psi(x,t)$



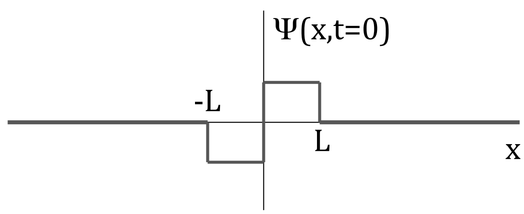
Probability *density* = $P(x,t=0) = |\Psi|^2 = \Psi^*\Psi$



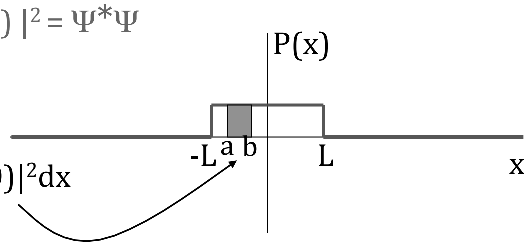
What is $\int_{-\infty}^{\infty} |\Psi(x,t=0)|^2 dx$?

A. 1
B. ½
C. 2L
D. ???

Wave function = $\Psi(x,t)$

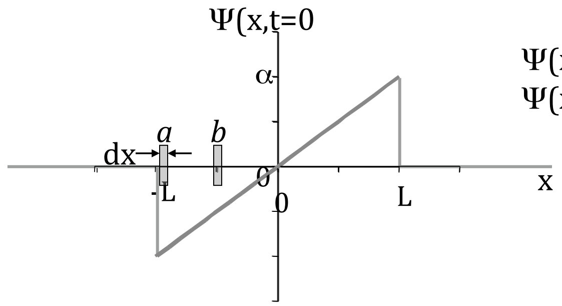


Probability *density* = $|\Psi(x,t=0)|^2 = \Psi^*\Psi$



Probability of electron being between a and b $= \int_{a}^{b} |\Psi(x,t=0)|^2 dx$

An electron is described by the following wave function:

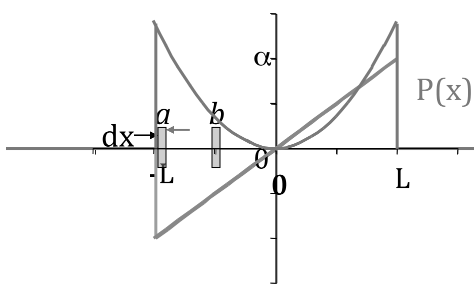


$\Psi(x,t=0)=\alpha x/L$ from -L to L
$\Psi(x,t=0)=0$ elsewhere

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

A. (probability at *a*) > *2**(probability at *b*)
B. (probability at *a*) = *2**(probability at *b)*
C. (probability at *a*) < *2**(probability at *b)*

$\Psi(x,t=0)=\alpha x/L$ from -L to L



Probability density

$$|\Psi(x,t=0)|^2= \frac{\alpha^2 x^2}{L^2}$$

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

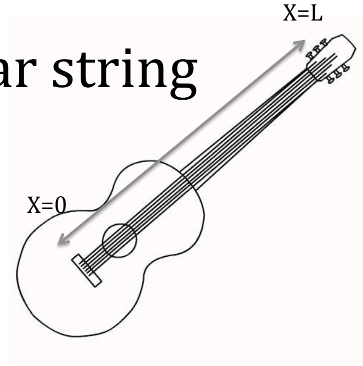
A. (probability at *a*) > *2**(probability at *b*)
B. (probability at *a*) = *2**(probability at *b)*
C. (probability at *a*) < *2**(probability at

Probability density is what we detect!!

What is the easiest way to solve a differential equation?

Guess the solution!
(Make sure it works and apply appropriate boundary conditions)

Example: a guitar string



$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$$

Functional form of solution?
y(x,t) = Acos(kx+wt) + Bcos(kx-wt)

Boundary conditions?
y(x,t) = 0 at x=0 and L

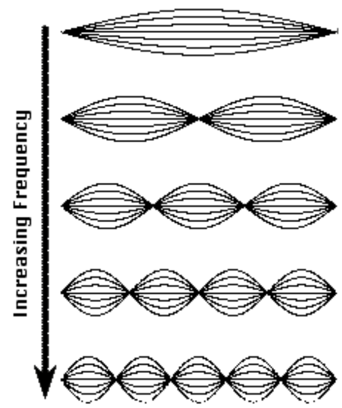
Trig. identities

At x=0: y(x,t) = Acos(wt)+Bcos(wt) = 0 → B=-A

y(x,t) =Acos(kx+wt) - Acos(kx-wt) = 2Asin(kx)sin(wt)

At x=L:
$y = 2A\sin(kL)\sin(\omega t) = 0$
→ $A\sin(kL) = 0$ for any t
→ $kL = n\pi$ (n=1,2,3, …)
→ $k = n\pi/L$

$\lambda = 2\pi/k$ $\lambda = 2L/n$



$$y(x,t) = 2A\sin(n\pi x/L)\sin(\omega t)$$

Quantization of k …
quantization of λ and ω

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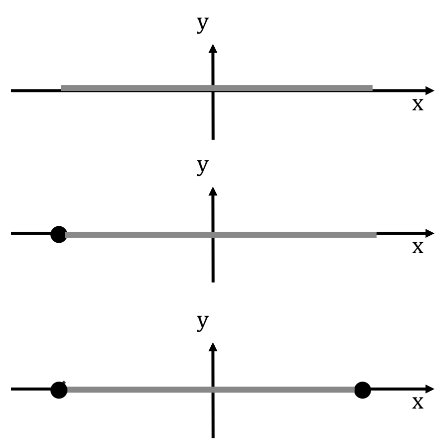
Three strings:

Case I: no fixed ends

Case II: one fixed end

Case III, two fixed end:



For which of these cases, do you expect to have only certain frequencies or wavelengths allowed? That is, for which cases will the allowed frequencies be quantized?

A. I only B. II only C. III only D. more than one

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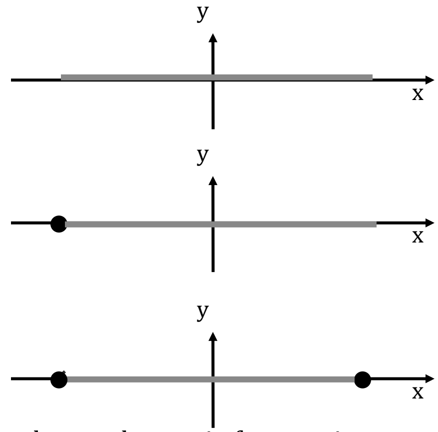
Three strings:

Case I: no fixed ends

Case II: one fixed end

Case III, two fixed end:



For which of these cases, do you expect to have only certain frequencies or wavelengths allowed… that is for which cases will the allowed frequencies be quantized.

a. I only b. II only c. III only d. more than one

Quantization came in when applied 2nd boundary condition, bound on both sides

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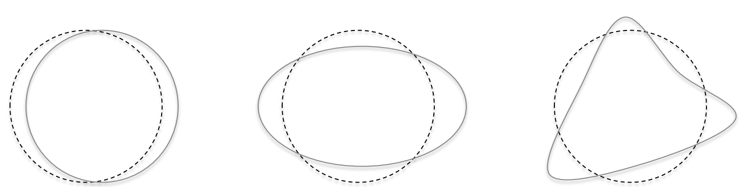
If the electron is a wave wrapped around a circle:



$2\pi r = 1\ \lambda$ $2\pi r = 2\ \lambda$ $2\pi r = 3\ \lambda$

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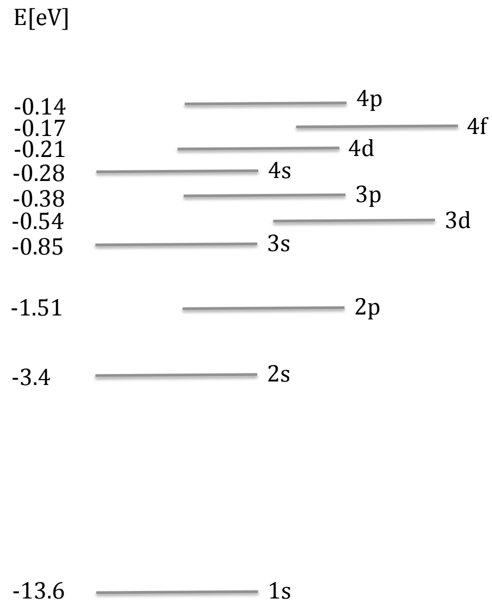
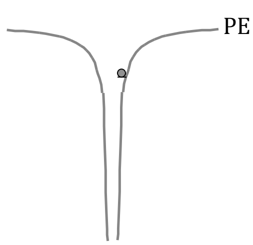
Hydrogen energy levels



**Note: not to scale

Electron bound
in atom (by potential energy)

Free electron



Only certain energies allowed
(Quantized energies)

Any energy allowed

QUESTION:

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

We want to calculate electron waves in a physical situation. The first step is:

A. figure out what general solutions will be by plugging in trial solutions and seeing if can solve.

B. figure out what the forces will be on the electron in that physical situation.

C. figure out what the boundary conditions must be on the electron wave.

D. figure out what potential energy is at different x and t for the physical situation.

The Schrodinger equation for electron wave in 1 D $\Psi(x,t)$

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

D. figure out what potential energy is at different x and t for the physical situation.

The potential energy V(x,t) completely determines the situation, and how the electron will behave!

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

In most physical situations, no time dependence in V!

$\Psi(x,t) = \psi(x)\,\Phi(t)$

$\Phi(t) = \exp(-iEt/h)$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

Time-independent Schrödinger equation

Steps for solving the Schrodinger equation for electron wave in 1 D

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

1. Figure out what V(x) is for situation given.
2. Guess or look up functional form of solution.
3. Check solution.
4. Figure out what boundary conditions must be to make sense physically.
5. Figure out values of constants to meet boundary conditions and normalization $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$
6. Multiply by time dependence $\Phi(t) = \exp(-iEt/\hbar)$ to have full solution.

The free electron:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

What is V(x)?

A. 0
B. = constant
C. $-ke^2/r$
D. I don't know

The free electron:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

What is V(x)?

A. 0
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