

PHY 127 FS2023

Prof. Ben Kilminster

Lecture 5

March 24th, 2023

LECTURE 4 reminder

wave equation:

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

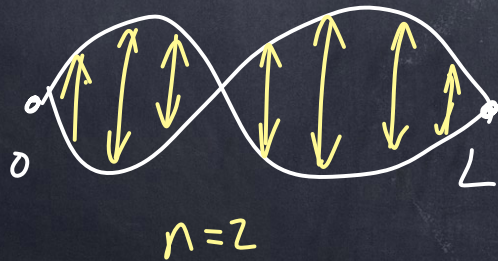
solutions:

$$\psi = A \sin(kx - \omega t)$$

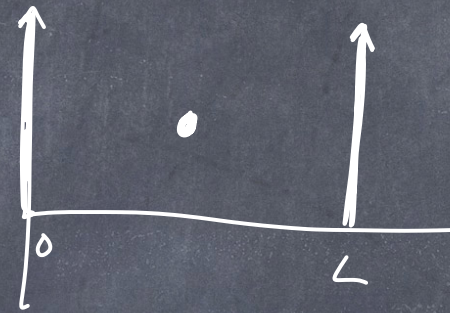
For a standing wave on a string:

$$\psi = A_n \sin \frac{n\pi x}{L}$$

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



"classical"
particle in a box:



Probability is equal for
it to be anywhere

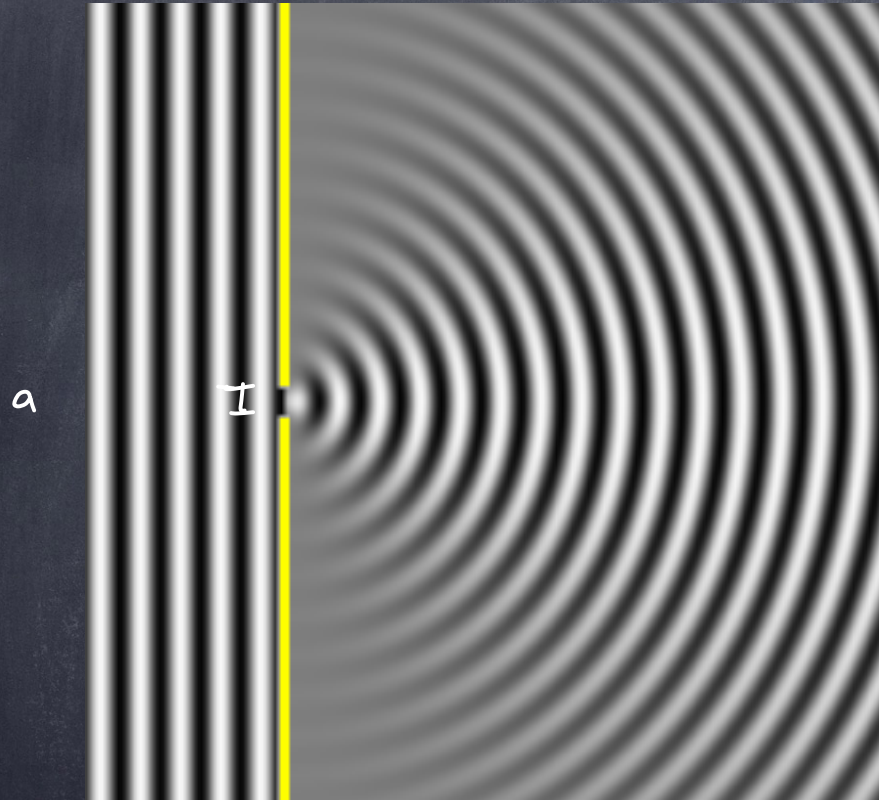
$$P(x) = \frac{1}{L}$$



A particle is a wave
with wavelength dependent
on its momentum p

$$\lambda = \frac{h}{p}$$

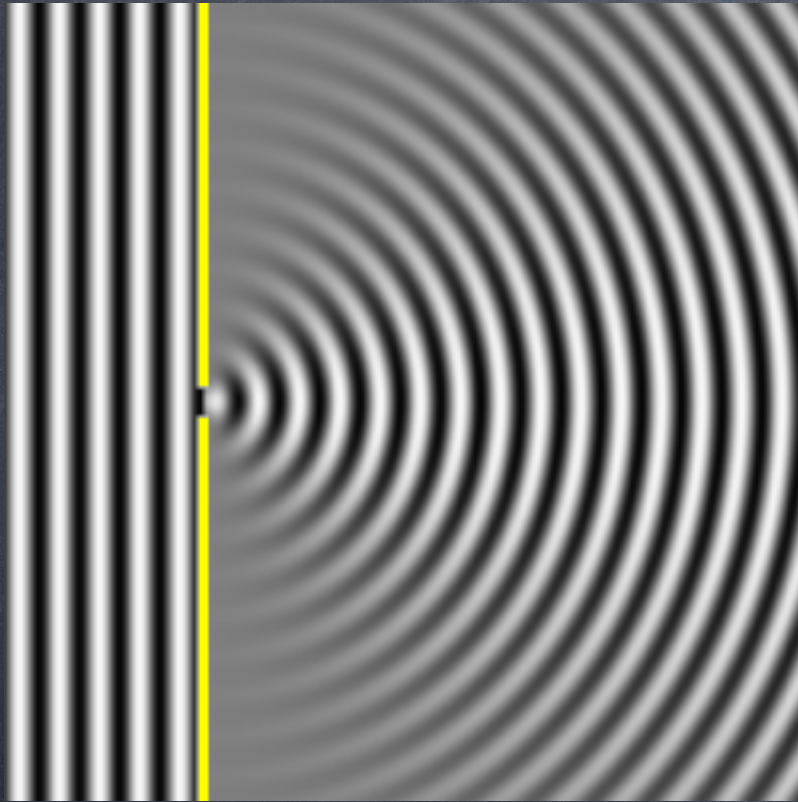
wave front



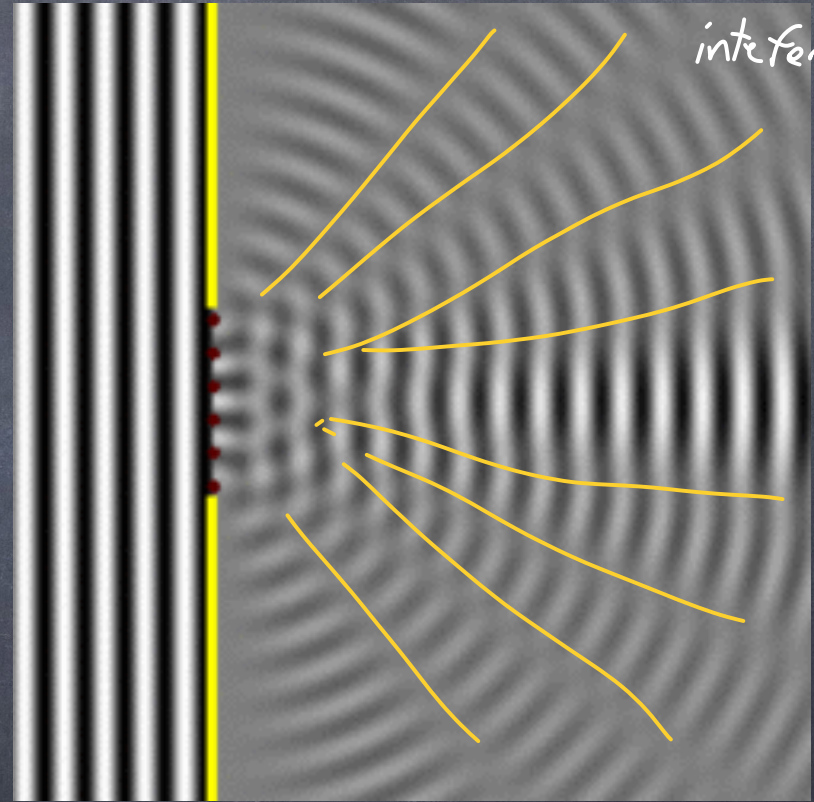
small hole, size a .

(videos on lecture notes web page)

Diffraction pattern:
from constructive + destructive
interference



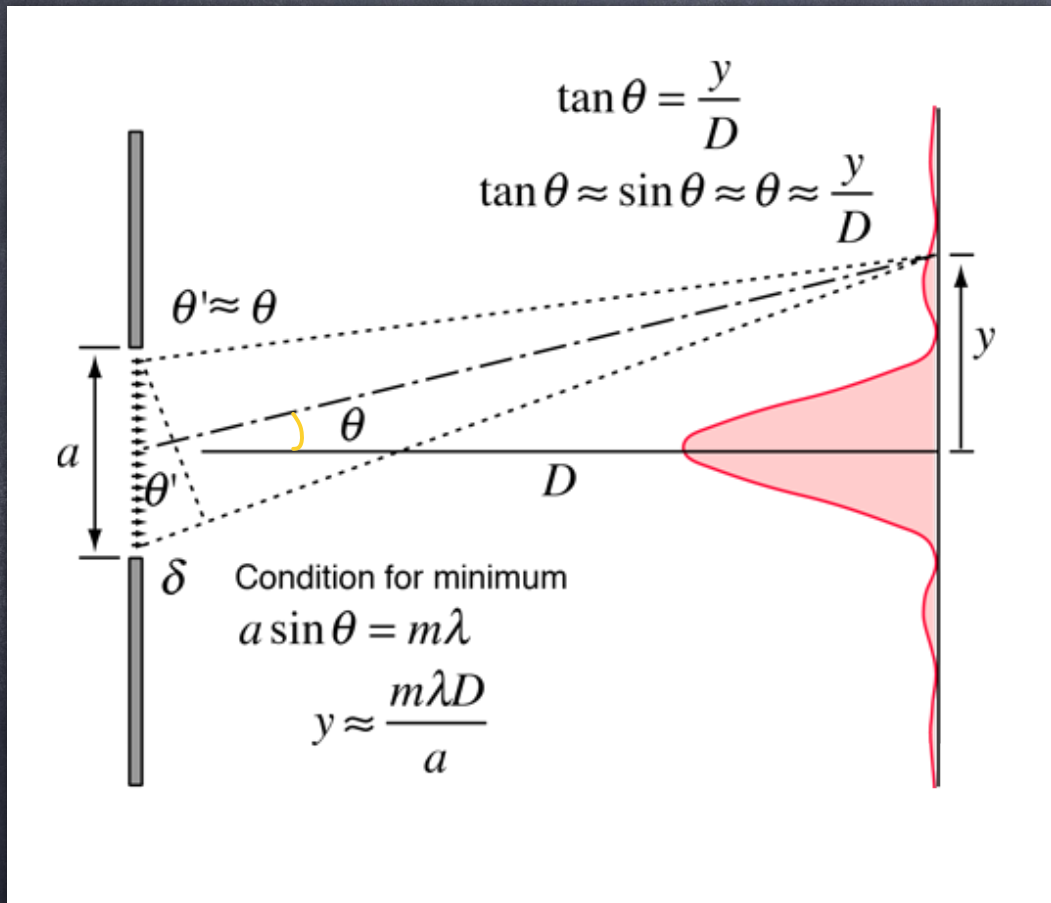
a



larger hole

Huygen's principle: every point on a wave front serves as a source of secondary spherical wavelets, little waves.

This is a diffraction pattern.



General rule:

$$a \sin \theta = m\lambda$$

$$m = 1, 2, 3, \dots$$

①

destructive interference
 \rightarrow dark spots

From geometry:

$$\tan \theta = \frac{y}{D}$$

For small angles

$$\tan \theta \sim \sin \theta$$

$$\rightarrow \sin \theta = \frac{y}{D}$$

②

① + ② : $\sin \theta = \frac{y}{D} = \frac{m\lambda}{a} \rightarrow$

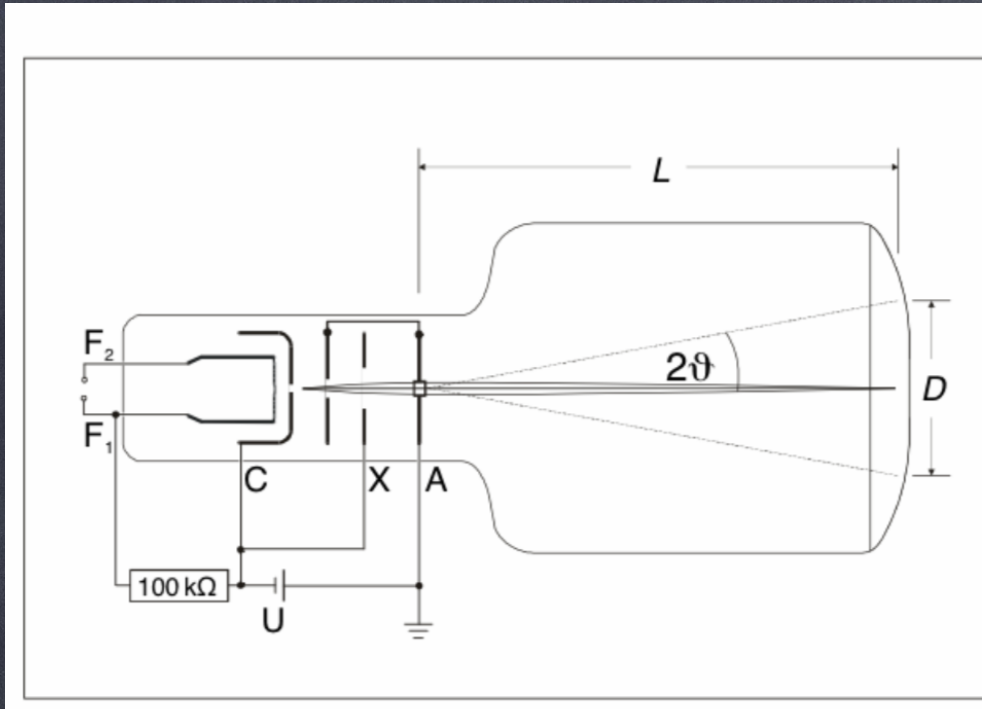
$$y = \frac{m\lambda D}{a}$$

$m = 1, 2, 3, \dots$

location of dark spots

circular diffraction with electrons

we accelerate electrons in an electric potential, U .



$$\underbrace{eU}_{\text{potential energy}} = \underbrace{\frac{1}{2}mv^2}_{\text{kinetic energy}}$$

$$v = \sqrt{\frac{zeU}{m}} \quad p = mv = \sqrt{2emU}$$

The wavelength of the electrons is

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2emU}}$$

$$eU = \frac{1}{2}mv^2$$

$$v^2 = \frac{zeU}{m} \quad v = \sqrt{\frac{zeU}{m}} \quad p = mv = m\sqrt{\frac{zeU}{m}} = \sqrt{\frac{zeUm^2}{m}}$$

Q: why does
 $v = \frac{\omega}{k}$?

A: start with:
 $v = \lambda \nu$

Since

$$\omega = 2\pi\nu \Rightarrow \nu = \frac{\omega}{2\pi}$$
$$k = \frac{2\pi}{\lambda} \Rightarrow \lambda = \frac{2\pi}{k}$$

↓

$$\left(\frac{2\pi}{k}\right) \left(\frac{\omega}{2\pi}\right) = \frac{\omega}{k} = v$$

graphite target

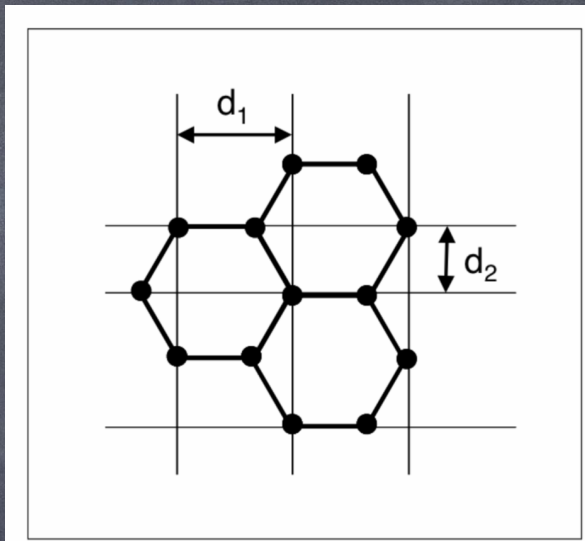
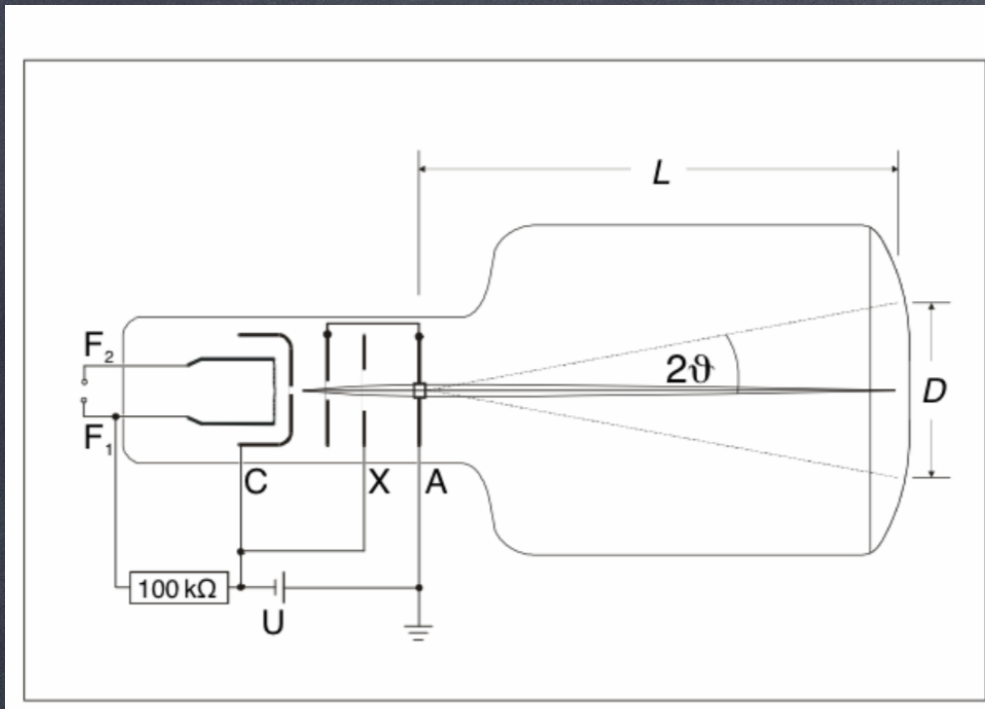
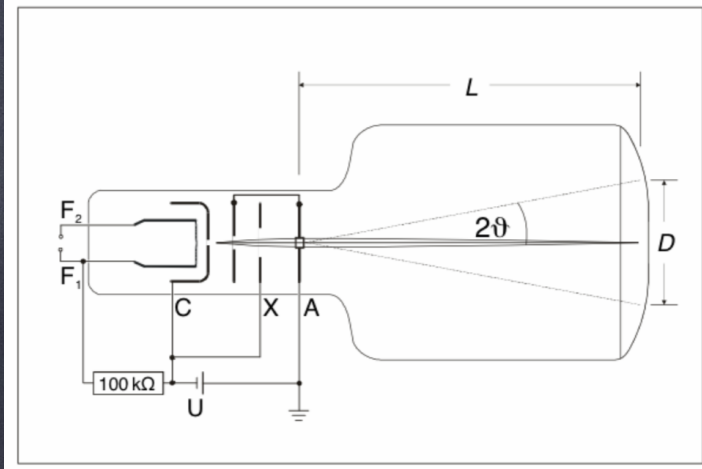


Fig. 3 Lattice plane spacings in graphite:
 $d_1 = 2.13 \cdot 10^{-10}$ m
 $d_2 = 1.23 \cdot 10^{-10}$ m

lattice spacings d_1, d_2



condition for diffraction:

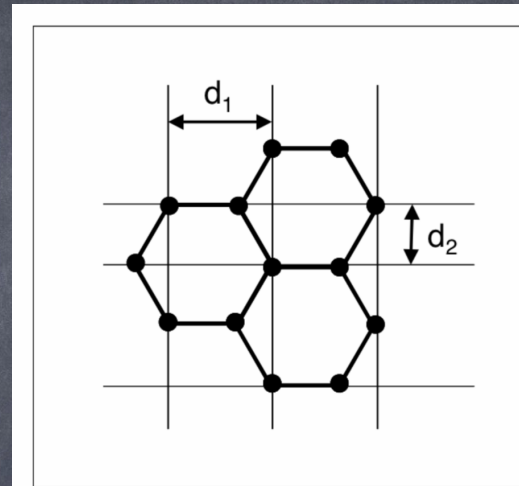


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 $d_1 = 2.13 \cdot 10^{-10} \text{ m}$
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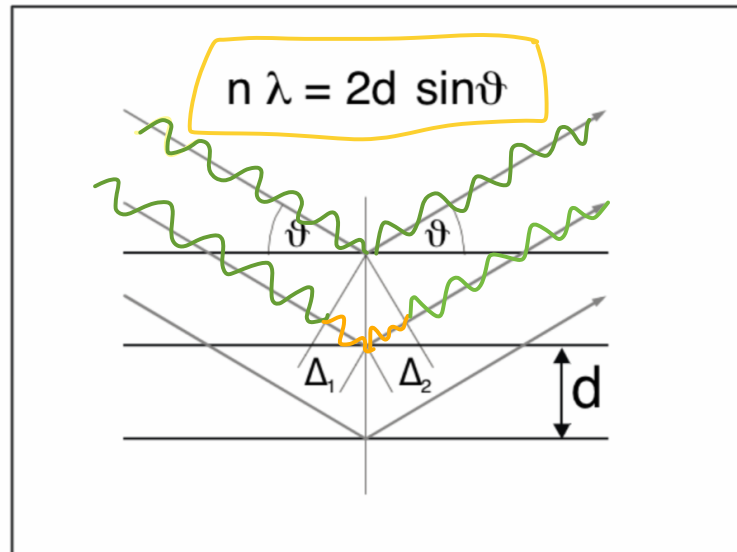
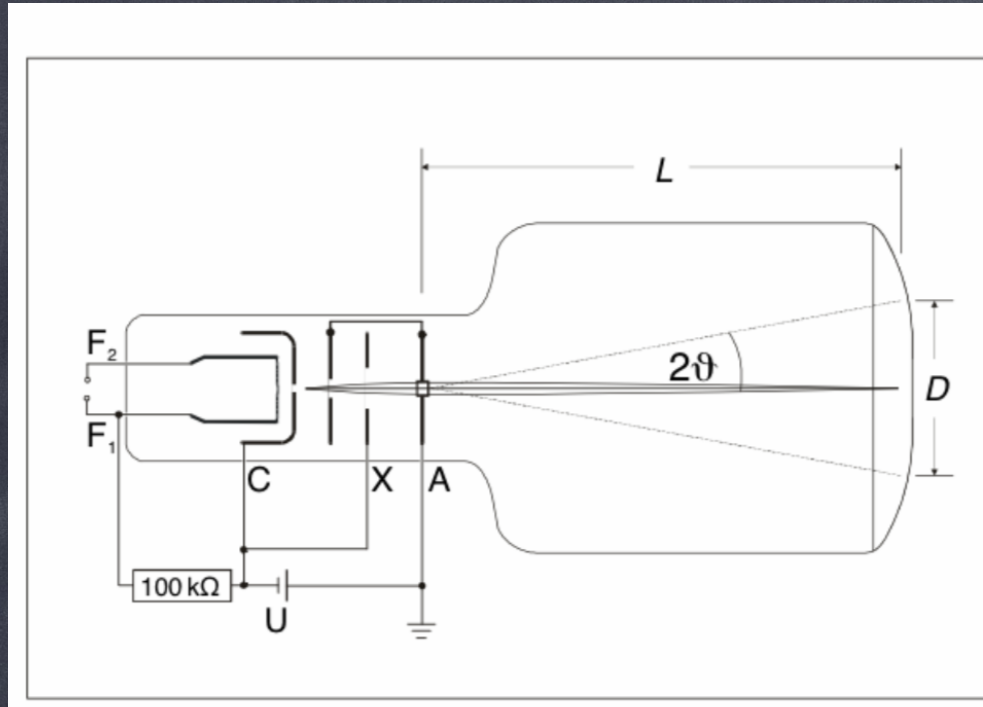


Fig. 2: Schematic representation of the Bragg condition.

we will get an interference pattern because the wave has different path lengths depending on which plane it scatters off



by geometry :

$$\tan(2\theta) = \frac{D}{2L} = \frac{D}{2L}$$

small-angle approximations

$$\tan(2\theta) \sim \sin(2\theta) \sim 2\sin\theta$$

$$2\sin\theta \cong \frac{D}{2L} \text{ (a)}$$

we have $n\lambda = 2d\sin\theta$

$$2\sin\theta = \frac{n\lambda}{d} \text{ (b)}$$

set (a) = (b) $\rightarrow \frac{D}{2L} = \frac{n\lambda}{d}$

$$D = \frac{n\lambda 2L}{d} \quad n=1, 2, 3, \dots$$

This tells us where we will see the bright rings

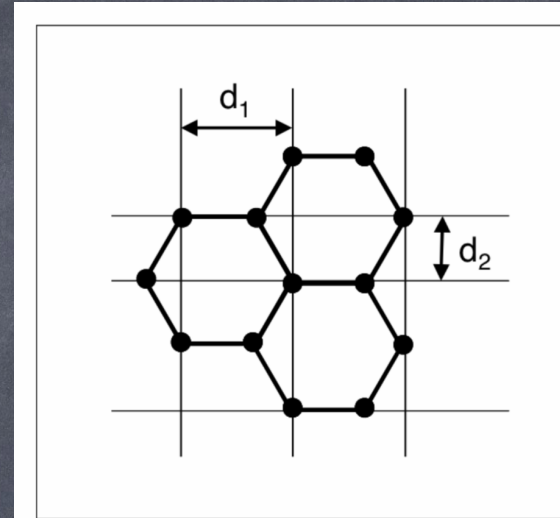
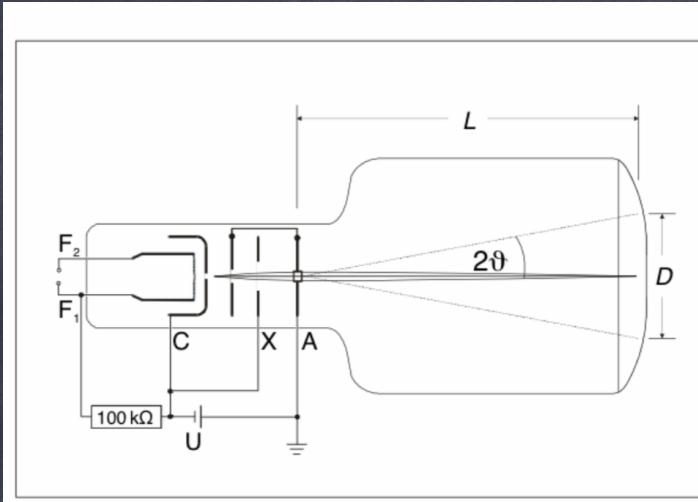


Fig. 3 Lattice plane spacings in graphite:
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 $d_2 = 1.23 \cdot 10^{-10} \text{ m}$

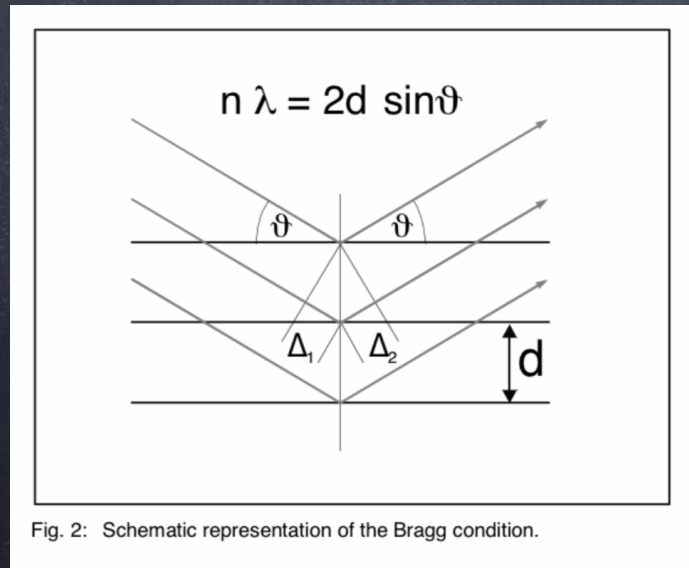


Fig. 2: Schematic representation of the Bragg condition.

$$D = \frac{2L\lambda}{d}$$

$$D_1 = \frac{2\lambda L}{d_1}$$

$$D_2 = \frac{2\lambda L}{d_2}$$

for $n=1$

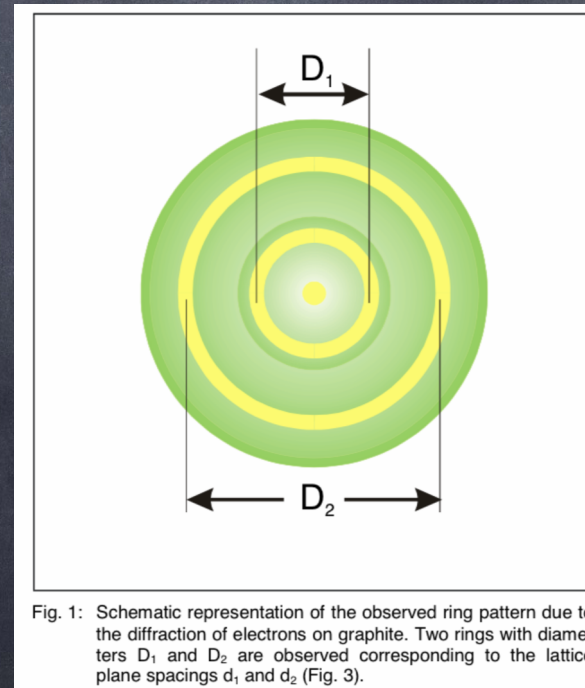


Fig. 1: Schematic representation of the observed ring pattern due to the diffraction of electrons on graphite. Two rings with diameters D_1 and D_2 are observed corresponding to the lattice plane spacings d_1 and d_2 (Fig. 3).

Note:
 diffraction allows us to measure atomic & molecular structure similar to x-ray crystallography

If an electron is a wave, what does it look like?

A wave with a singular angular frequency
($\omega = 2\pi\nu$)
and a wave number ($k = \frac{2\pi}{\lambda}$) looks like this:



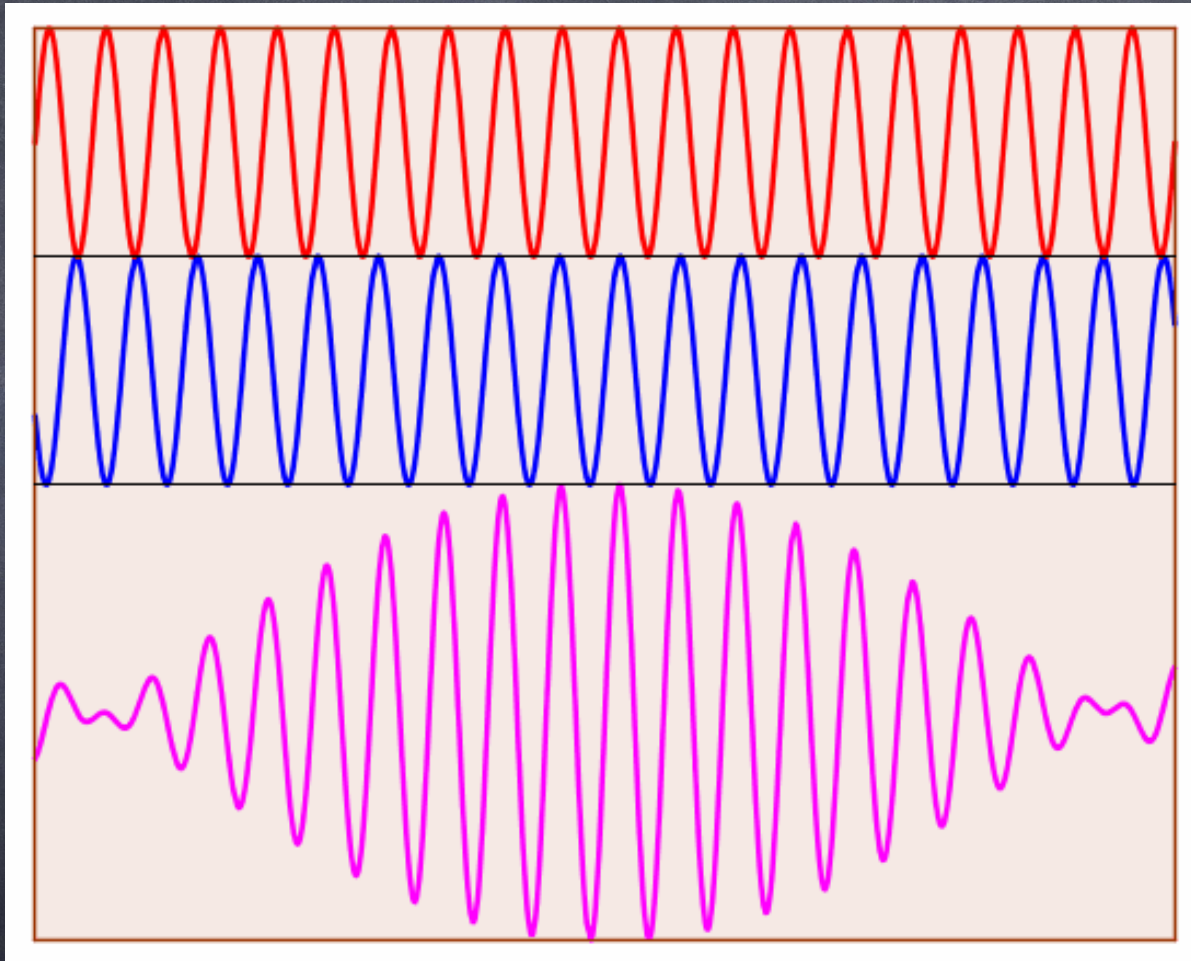
perfect sine wave with an exact $\omega + k$

It has no beginning or end in space.
we can't define where it is.

To represent a localized position of a wave, we need a group of waves, called a "wave packet".

(video on lecture notes web page)

Two waves
of
slightly
different
 $\omega + k$

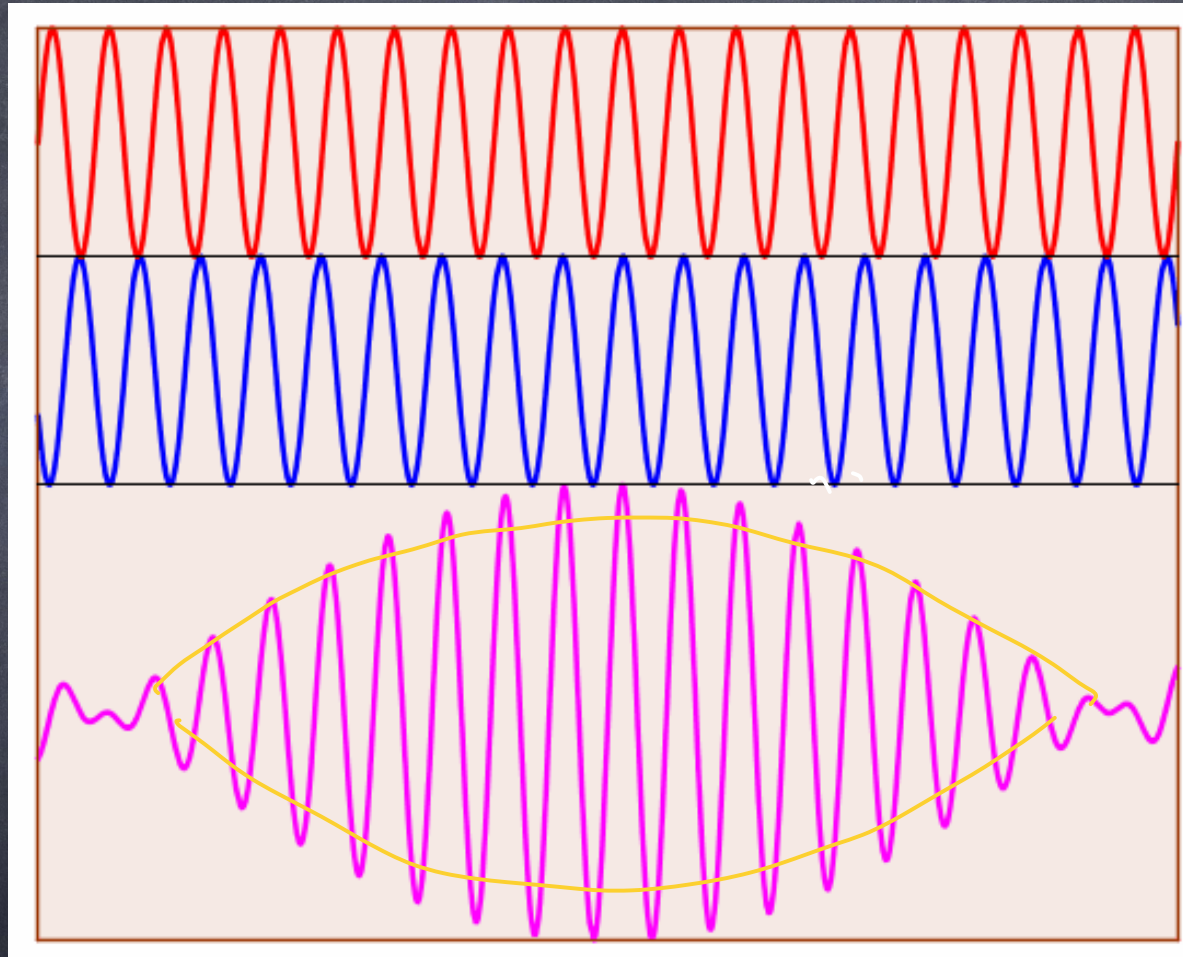


combination

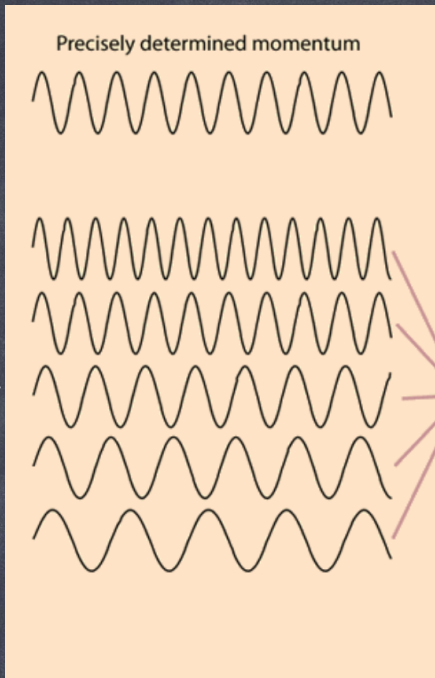
(video on lecture notes web page)

Two waves
of
slightly
different
 $\omega + k$

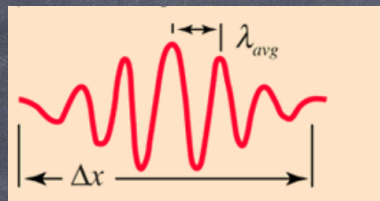
combination



wave packet is the envelope
of the added waves.



wave packet represents the location of a particle



Δx : location range of ptcl.

Each individual wave has its own

$\lambda_i \rightarrow$ own ω_i, k_i

$$V_i = \frac{\omega_i}{k_i}$$

$$\Delta \lambda = \lambda_n - \lambda_1 \Rightarrow \Delta k = \frac{2\pi}{\Delta \lambda}$$

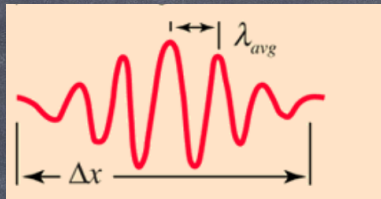
The wave packet has a range of $\Delta k + \Delta \omega$

The wave packet has its own velocity, $V_g = \frac{\Delta \omega}{\Delta k}$

The average of the individual waves has a velocity $V_p = \text{phase velocity} = \frac{\omega_{avg}}{k_{avg}}$

ω
group velocity

Precisely determined momentum



$$p = \frac{h}{\lambda}$$

↓

Precisely determined momentum

A sine wave of wavelength λ implies that the momentum is precisely known. But the wavefunction and the probability of finding the particle $\Psi^* \Psi$ is spread over all of space!

$p = \frac{h}{\lambda}$

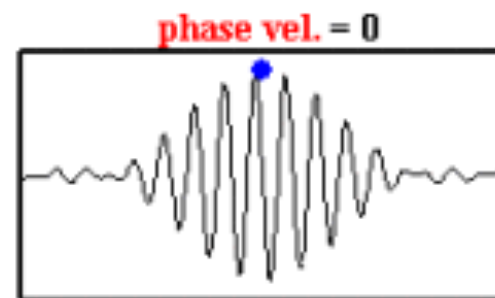
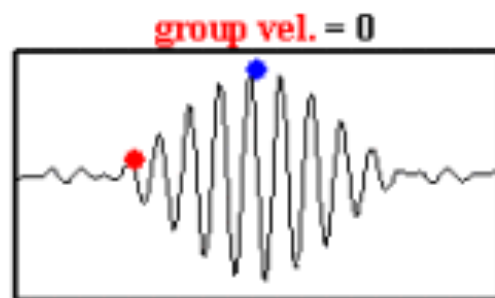
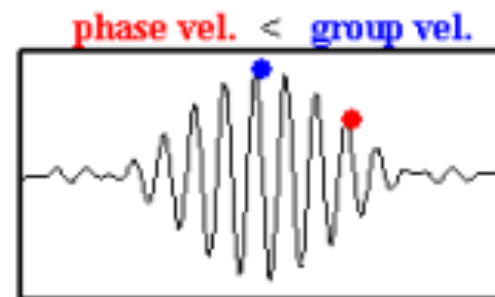
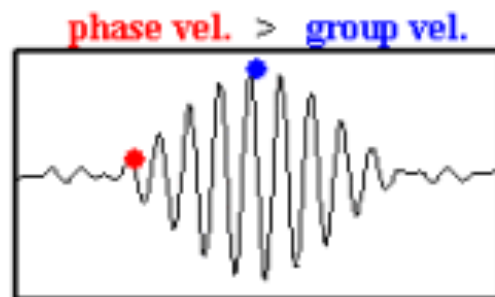
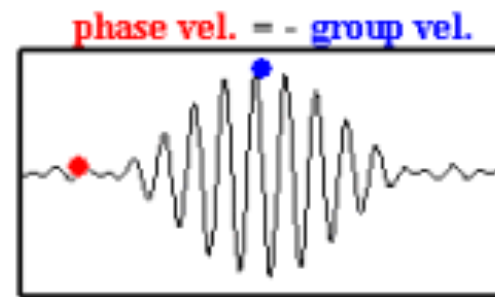
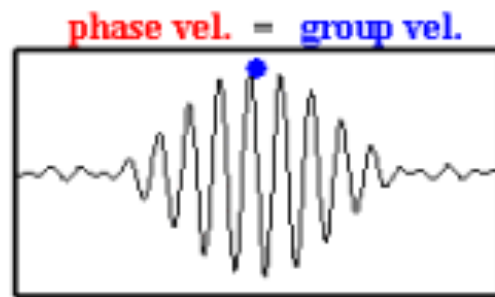
p precise
x unknown

Adding several waves of different wavelength together will produce an interference pattern which begins to localize the wave.

But that process spreads the momentum values and makes it more uncertain. This is an inherent and inescapable increase in the uncertainty Δp when Δx is decreased.

$\Delta x \Delta p > \frac{\hbar}{2}$

(video on lecture notes web page)



isvr

A general property of waves is that

$$\Delta k \Delta x \sim 1$$

Δk : range of wave numbers

$$\Delta \omega \Delta t \sim 1$$

Δx : location, or size of wave packet.

we can multiply these equations by \hbar : Planck constant, $\frac{h}{2\pi} = \hbar$

$$p = \frac{h}{\lambda} = \hbar k \quad E = \hbar \omega = \hbar \nu$$

$$\Delta p \Delta x \sim \hbar$$
$$\Delta E \Delta t \sim \hbar$$

These relations provide a fundamental concept. Since particles are waves, they must obey the rules of waves, and therefore, we can't know both the p & x simultaneously. Likewise, we can't know E & t simultaneously.

This is expressed as:

$$\Delta p \Delta x \geq \frac{\hbar}{2}$$
$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Heisenberg's uncertainty principle (s).

Δt : time available for measurement

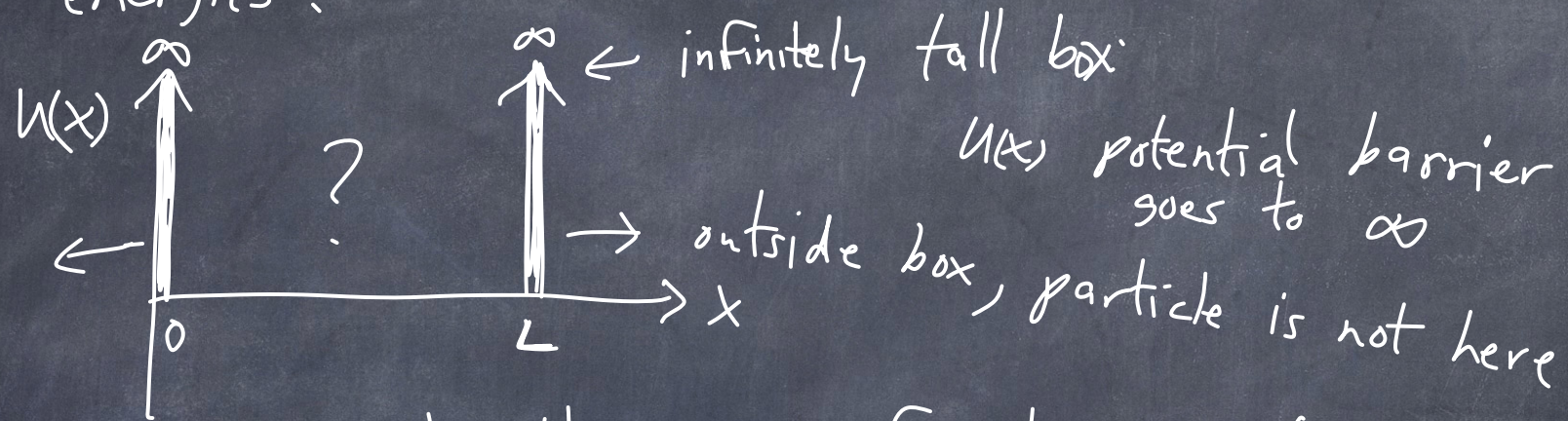
ΔE : uncertainty in measured energy

Δp : uncertainty in ^{measured} momentum

Δx : uncertainty in position:

If you know x exactly, then you know p exactly, so $\Delta p = 0$. Then $\Delta x \sim \infty$

Let's go back to our electron in a 1-D box.
 What is the wave function? What are the allowed energies? Where is it?



we write the wave function as $\Psi = \Psi(x)$

$P(x) = \Psi^2(x)$ is the probability of finding the particle at some x .

Boundary conditions: $\Psi(x=0) = 0$ $\Psi(x=L) = 0$

$$\int_{-\infty}^{\infty} P(x) dx = 1$$

The energy of the particle is $E = K + U$
(kinetic) (potential)

The wave equation for quantum mechanics is:

Schroedinger
wave
equation.
(time-independent)

$$\underbrace{\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}}_{\text{Kinetic energy, } K} \Psi(x) + \underbrace{U(x)}_{\text{potential energy, } U} \Psi(x) = \underbrace{E}_{\text{total energy}} \Psi(x)$$

↑
wave function

Inside the box, $U(x) = 0$, the particle has no potential energy.

we can simplify the above to:

$$\frac{\partial^2 \Psi(x)}{\partial x^2} = \frac{-2mE}{\hbar^2} \Psi(x)$$

Now, let's call $k^2 = \frac{2mE}{\hbar^2}$

this is a constant K , not Kinetic energy

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} = E \Psi(x) \quad \textcircled{a}$$

→ then $E = \frac{k^2 \hbar^2}{2m} \quad \textcircled{1}$

and write \textcircled{a} as

$$\frac{\partial^2 \Psi(x)}{\partial x^2} = -k^2 \Psi(x) \quad \textcircled{b}$$

To solve this, we need a ^{wave} function whose 2nd derivative is $-k^2$ times the function.

guess: IF $\Psi(x) = A \sin kx$

$$\frac{\partial \Psi(x)}{\partial x} = Ak \cos kx$$

$$\frac{\partial^2 \Psi(x)}{\partial x^2} = -Ak^2 \sin kx$$

we can see that $\frac{\partial^2 \Psi(x)}{\partial x^2} = -k^2 \Psi(x)$

Also, $\Psi(x) = B \cos kx$, it would also work. (B also a constant)

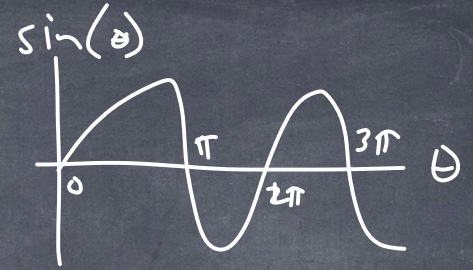
So the general solution, $\Psi(x) = A \sin kx + B \cos kx$

we know that $\Psi(x=0) = 0$ $\Psi(x=L) = 0$

$$\Psi(x=0) = 0 = \underbrace{A \sin k(0)}_0 + \underbrace{B \cos k(0)}_1 = B$$

so this means B must be zero!

$\Psi(x=L) = 0 = A \sin kL$
when does this happen?



It happens when $kL = n\pi$ where $n = \text{integer}$
we get that $k = \frac{n\pi}{L}$ for $n = 0, 1, 2, 3, \dots$
 $n = 0, 1, 2, 3, \dots$

From ①, $E = \frac{k^2 \hbar^2}{2m} = \frac{\left(\frac{n\pi}{L}\right)^2 \hbar^2}{2m}$ $n = 0, 1, 2, \dots$

$E = \frac{n^2 \hbar^2 \pi^2}{2m L^2}$ since we know $\hbar = \frac{h}{2\pi}$

$$E_n = \frac{n^2 h^2}{8m L^2}, n = 1, 2, 3, \dots$$

The allowed energy levels of an electron in a 1-D box.

for $n=1$, $E_1 = \frac{h^2}{8mL^2}$ and $E_n = n^2 E_1$
 for $n=1, 2, \dots$

The energy is quantized.

$$\Psi(x) = A \sin kx = A_n \sin\left(\frac{n\pi x}{L}\right) \quad \text{for } n=1, 2, \dots$$

what is A_n ?

A_n : constant for each n

we use $\int_0^L \Psi^2(x) dx = 1$

must be true.

$$\int_0^L \left[A_n \sin\left(\frac{n\pi x}{L}\right) \right]^2 dx = 1$$

To solve, substitution of $\frac{n\pi x}{L} = \theta$

$$\frac{n\pi dx}{L} = d\theta$$

when $x=L$, $\theta = n\pi$

$$A_n^2 \frac{L}{n\pi} \int_0^{n\pi} \sin^2 \theta d\theta = 1$$

For this integral:

$$\int_a^b \sin^2 x \, dx = \frac{1}{2} \left(x - \frac{1}{2} \sin 2x \right) \Big|_a^b$$

For our case:

$$A_n^2 \frac{L}{n\pi} \left[\frac{\theta}{2} - \frac{\sin 2\theta}{4} \right]_0^{n\pi} = A_n^2 \frac{L}{n\pi} \cdot n\pi = 1$$

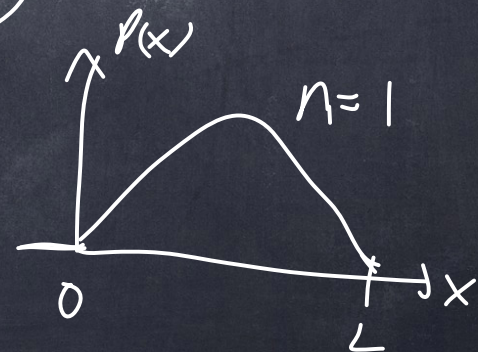
we find that $A_n = \sqrt{\frac{2}{L}}$ (independent of n)

So the solution is $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ for $n=1, 2, 3, \dots$
 n : are the quantum numbers

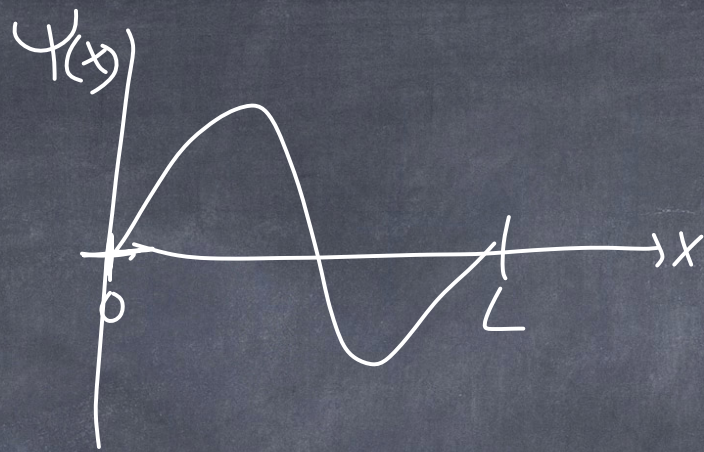
If $n=1$, then $\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$



$$P(x) = \psi_1^2(x)$$



For $n=2$



The classical limit $n \rightarrow$ large number

