# PHY 127 FS2024

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Lecture 5

March 21st, 2024

## LECTURE 4 reminder

wave equation:

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

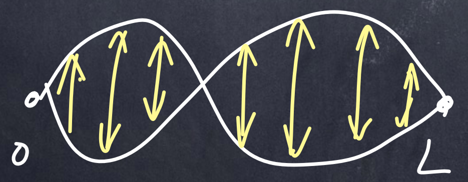
solutions:

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

For a standing wave on a string:

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

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

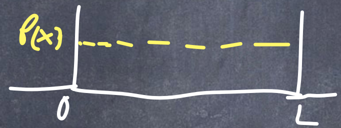



$n=2$

"classical" particle in a box:


Probability is equal for it to be anywhere

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

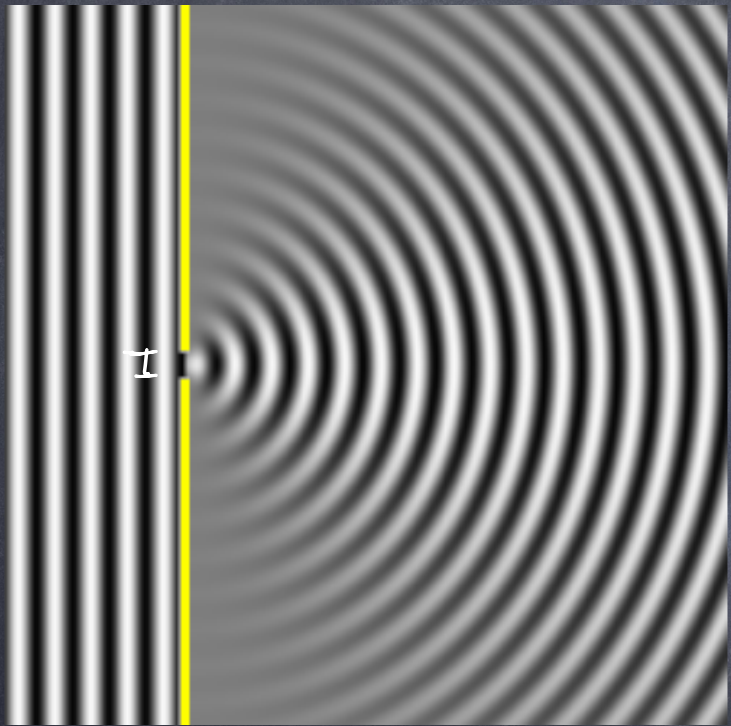



A particle is a wave with wavelength dependent on its momentum $p$

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

wave front

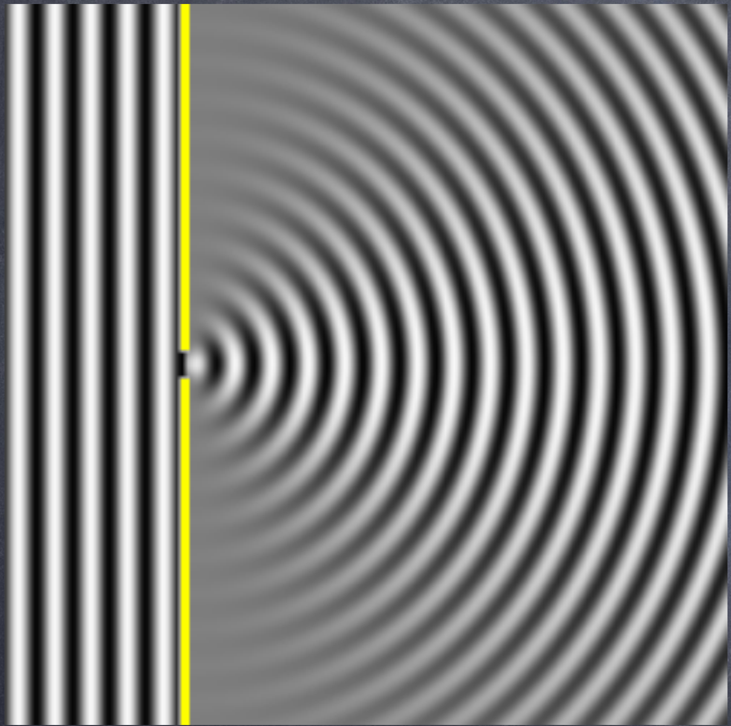
a

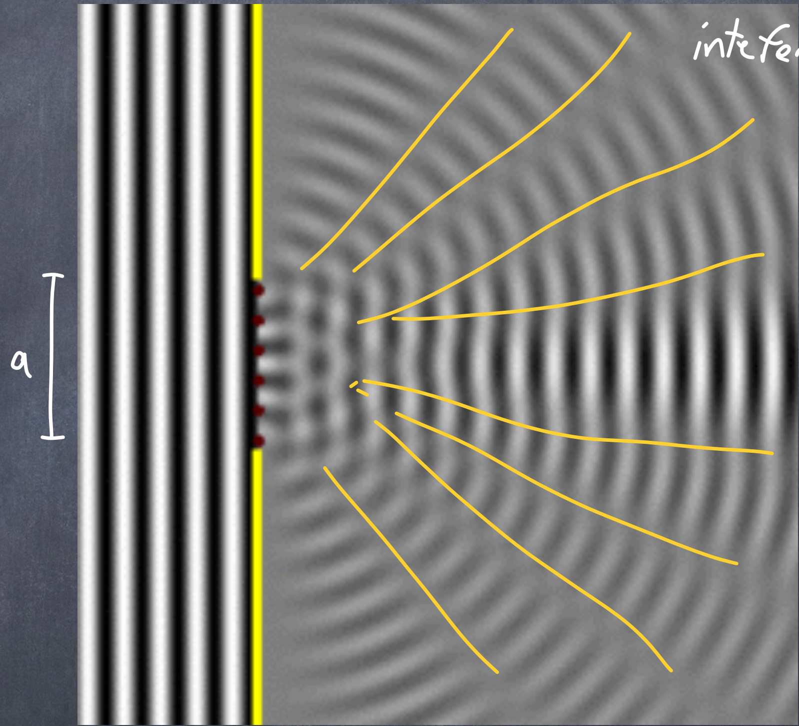


small hole, size a.

(videos on lecture notes web page)

Diffraction pattern: from constructive + destructive interference

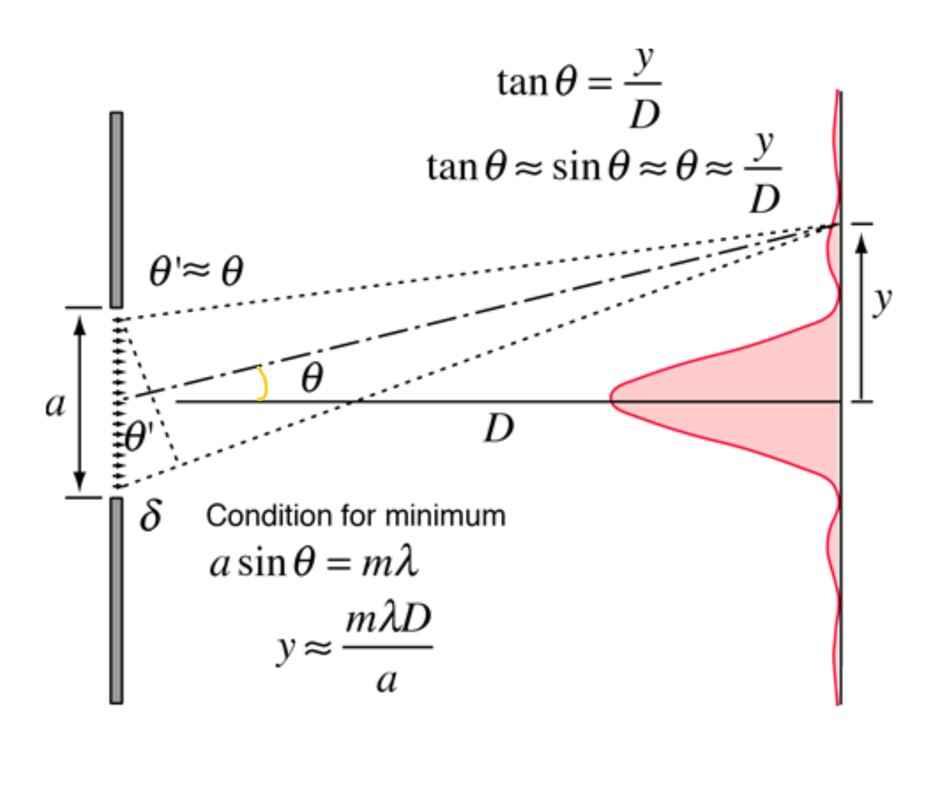





larger hole

Huygen's principle: every point on a wave front serves as a source of secondary spherical $\underbrace{\text{wavelets}}_{\text{little waves.}}$

This is a diffraction pattern.




General rule:

$$\boxed{a\sin\theta = m\lambda \quad m = 1, 2, 3, \ldots} \quad (1)$$

destructive interference
$\rightarrow$ dark spots

from geometry:

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

For small angles

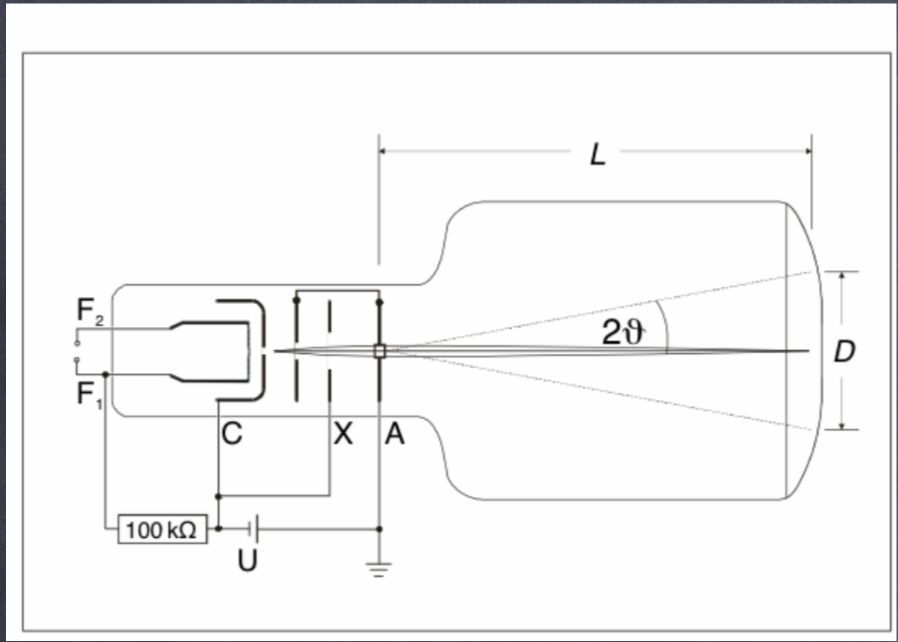
$$\tan\theta \sim \sin\theta$$

$$\rightarrow \boxed{\sin\theta = \frac{y}{D}} \quad (2)$$

(1) + (2):

$$\sin\theta = \frac{y}{D} = \frac{m\lambda}{a} \rightarrow \boxed{y = \frac{m\lambda D}{a}} \quad m = 1, 2, 3, \ldots$$

location of dark spots




## circular diffraction with electrons

we accelerate electrons in an electric potential, $U$.

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

$$v = \sqrt{\frac{2eU}{m}} \qquad p = mv = \sqrt{2emU}$$

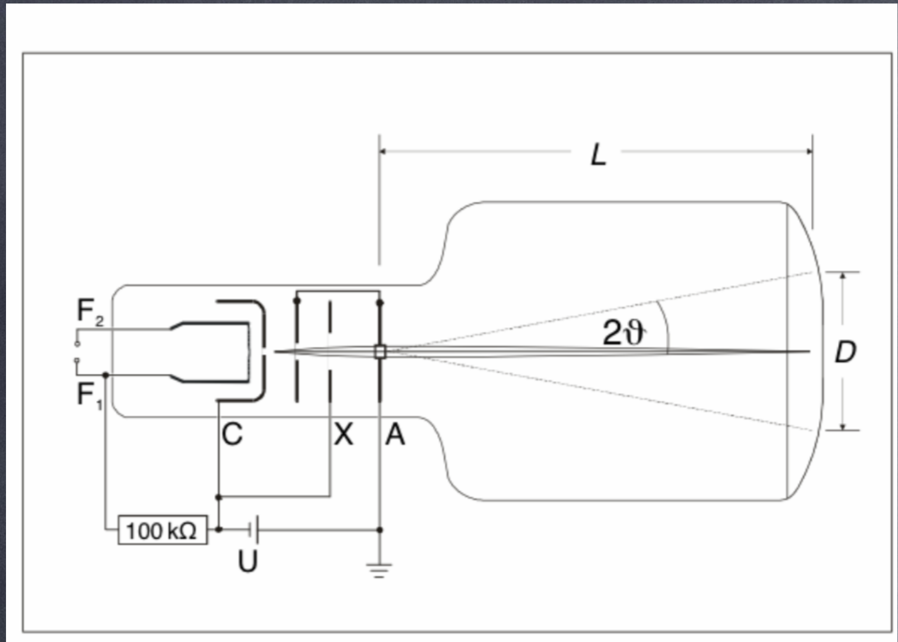
The wavelength of the electrons is

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

$$eU = \frac{1}{2} m v^2$$

$$v^2 = \frac{2eU}{m} \qquad v = \sqrt{\frac{2eU}{m}} \qquad p = mv = m\sqrt{\frac{2eU}{\cancel{m}}} = \sqrt{\frac{2eU m^{\cancel{2}}}{\cancel{m}}}$$

graphite target



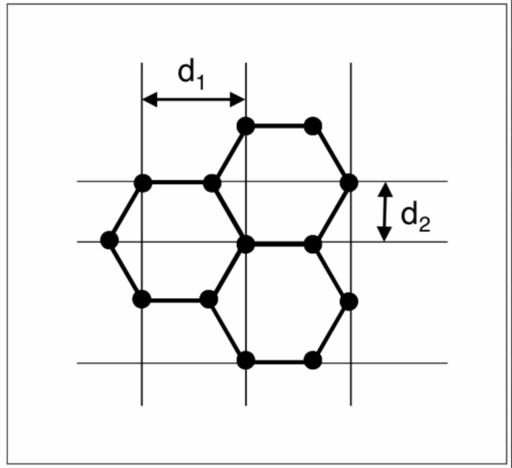
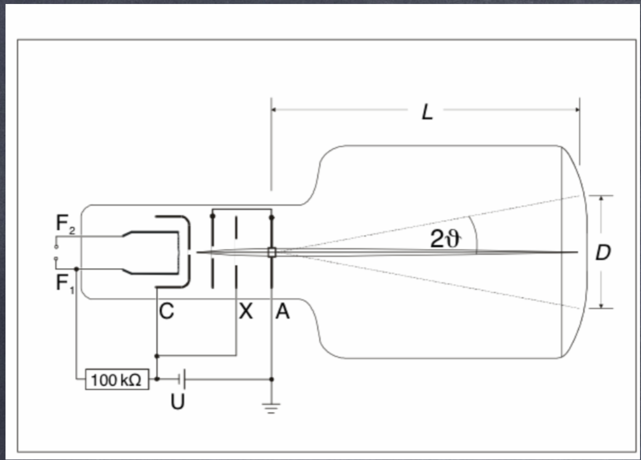




Fig. 3 Lattice plane spacings in graphite:
$d_1 = 2.13 \cdot 10^{-10}$ m
$d_2 = 1.23 \cdot 10^{-10}$ m

lattice spacings $d_1, d_2$



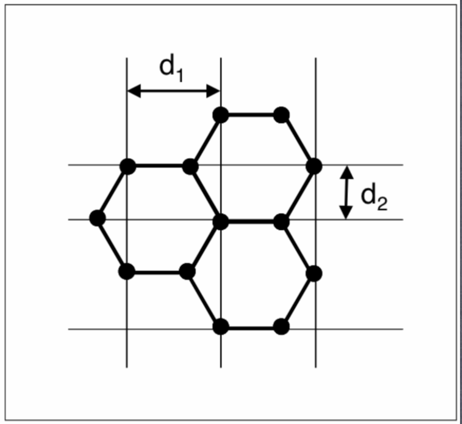




Fig. 3 Lattice plane spacings in graphite:
$d_1 = 2.13 \cdot 10^{-10}$ m
$d_2 = 1.23 \cdot 10^{-10}$ m

condition for diffraction:

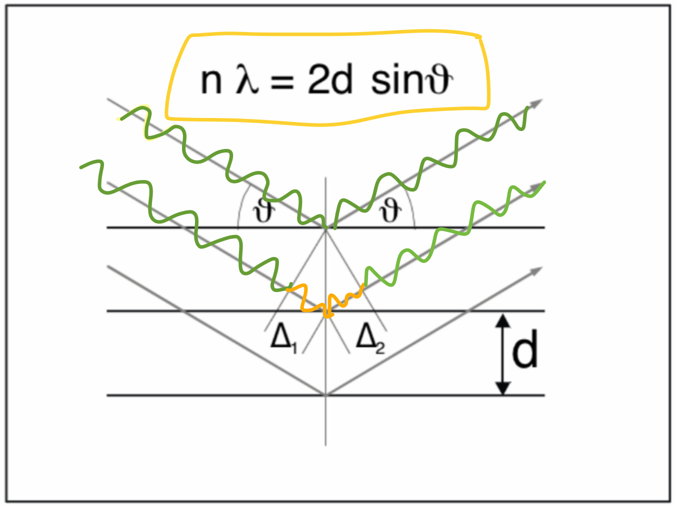
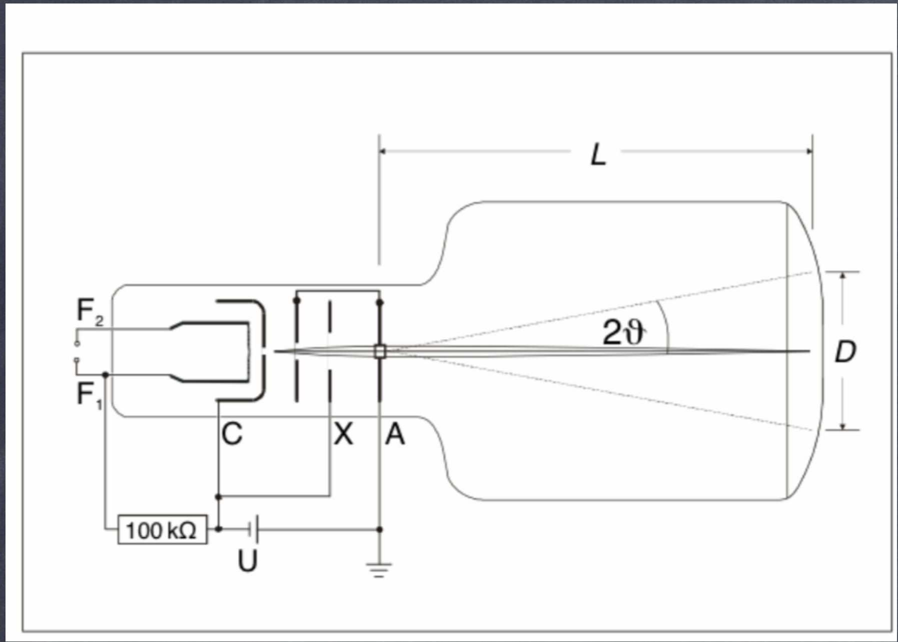



Fig. 2: Schematic representation of the Bragg condition.

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




by geometry :

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

small-angle approximations

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

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

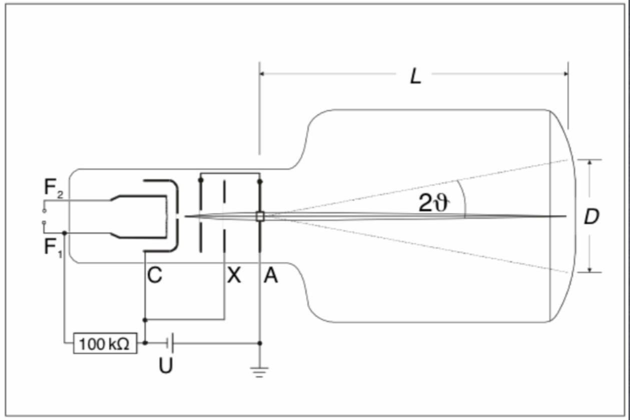
we have $n\lambda = 2d\sin\theta$

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

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

$$D = \frac{n\lambda 2L}{d} \qquad n = 1, 2, 3, \ldots$$

This tells us where we will see the bright rings



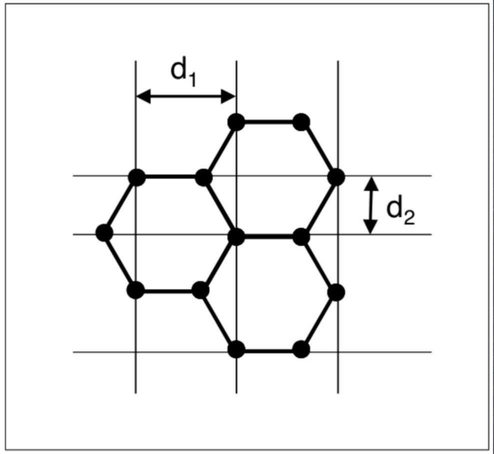




Fig. 3 Lattice plane spacings in graphite:
$d_1 = 2.13 \cdot 10^{-10}$ m
$d_2 = 1.23 \cdot 10^{-10}$ m

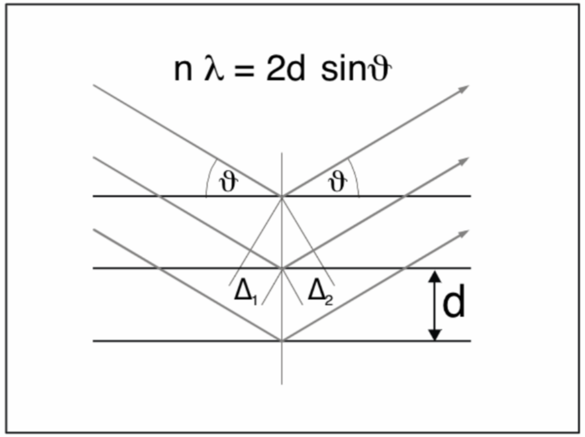



Fig. 2: Schematic representation of the Bragg condition.

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

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

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

For $n=1$

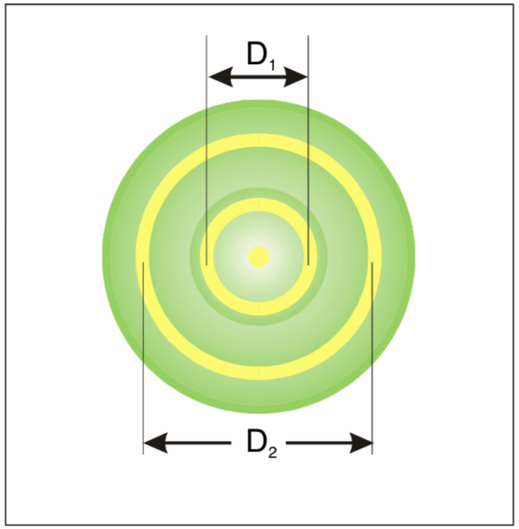



Fig. 1: Schematic representation of the observed ring pattern due to the diffraction of electrons on graphite. Two rings with diameters $D_1$ and $D_2$ are observed corresponding to the lattice plane spacings $d_1$ and $d_2$ (Fig. 3).

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:

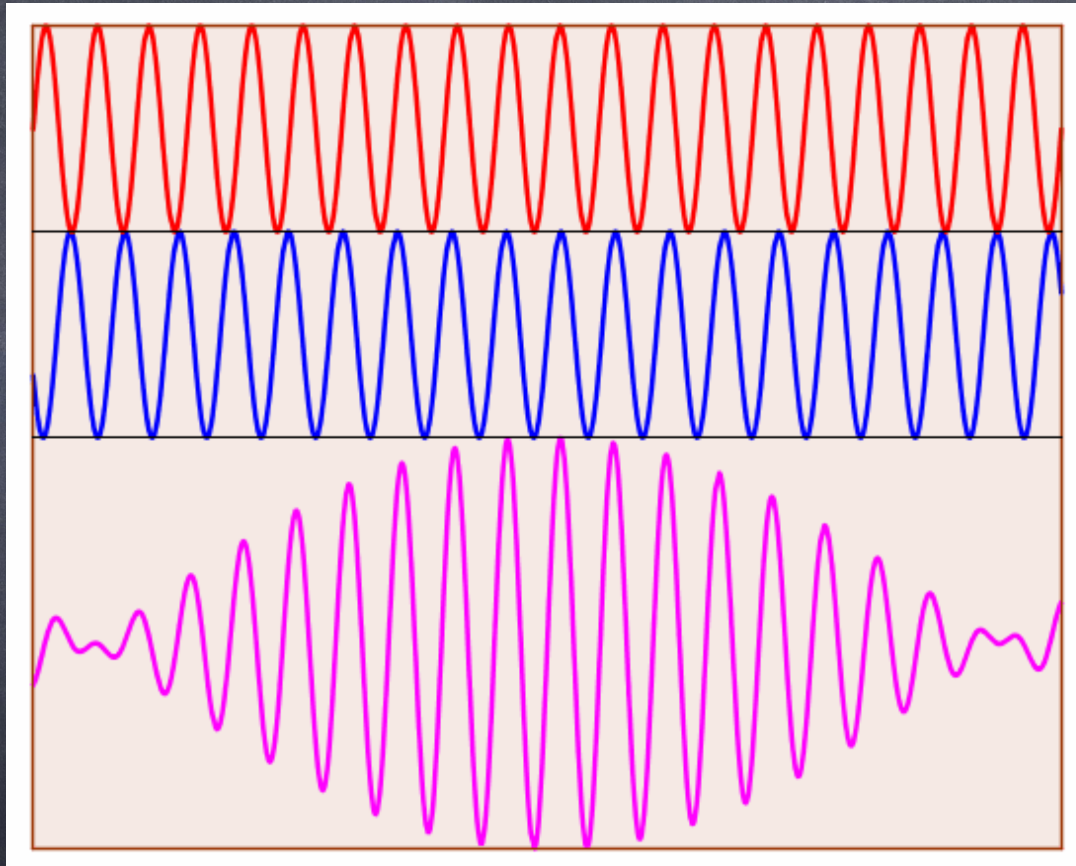
perfect sine wave with an exact $\omega$ + $k$

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 $\omega$ + $K$

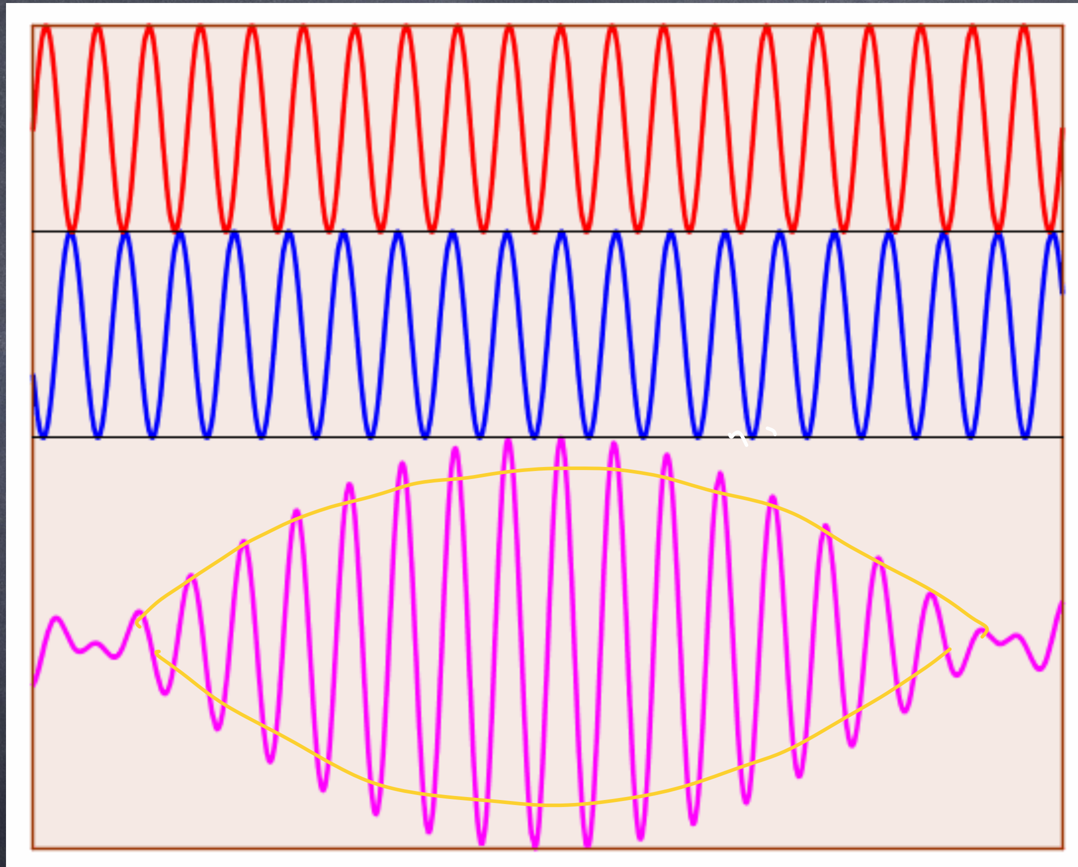


combination

(video on lecture notes web page)

Two waves of slightly different $\omega$ + $K$

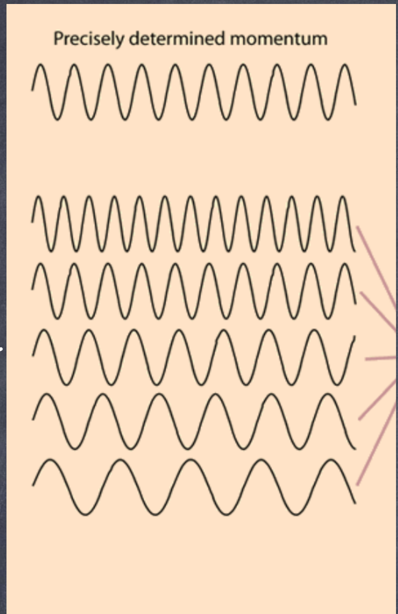
combination



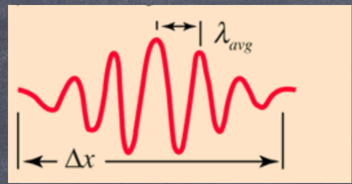
wave packet is the envelope of the added waves.

range of $\lambda$, $\Delta\lambda$

$\lambda_1$ ⋮ $\lambda_i$ ⋮ $\lambda_n$




wave packet represents the location of a particle




$\Delta x$ : location range of ptcl.

Each individual wave has its own $\lambda_i \rightarrow$ own $w_i, k_i$

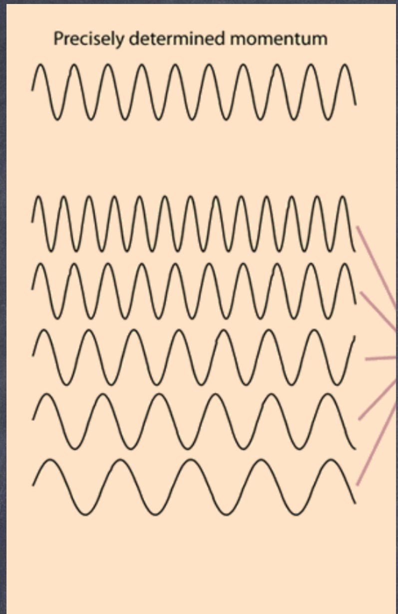
$$V_i = \frac{w_i}{k_i}$$

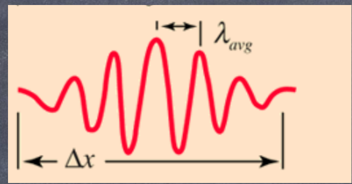
$$\Delta\lambda = \lambda_n - \lambda_1 \Rightarrow \Delta K = \frac{2\pi}{\Delta\lambda}$$

The wave packet has a range of $\Delta K$ & $\Delta W$

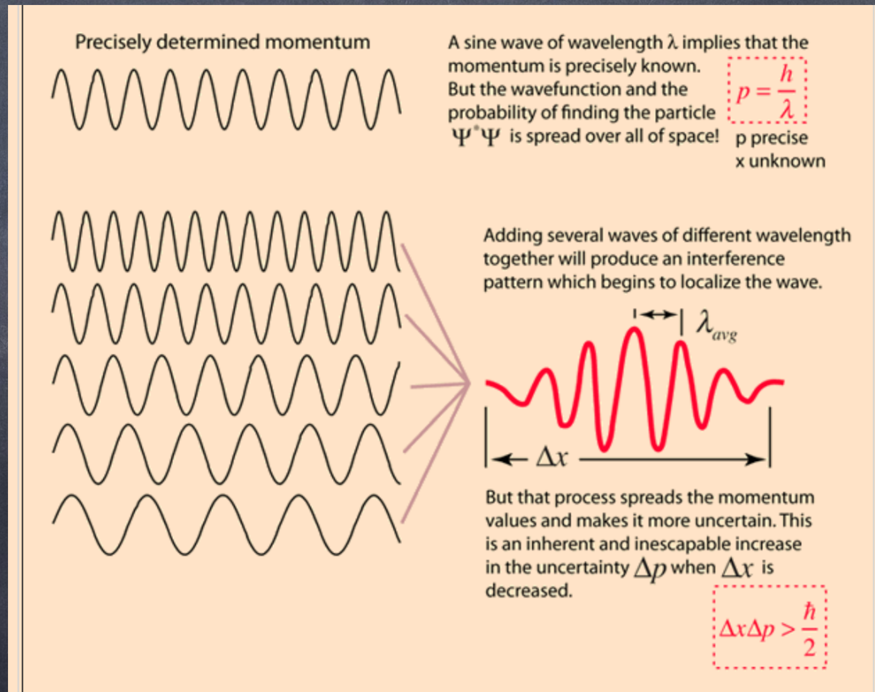
The wave packet has its own velocity, $\underbrace{V_g}_{\text{group velocity}} = \dfrac{\Delta W}{\Delta K}$

The average of the individual waves has a velocity $V_p$ = phase velocity $= \dfrac{W_{avg}}{K_{avg}}$

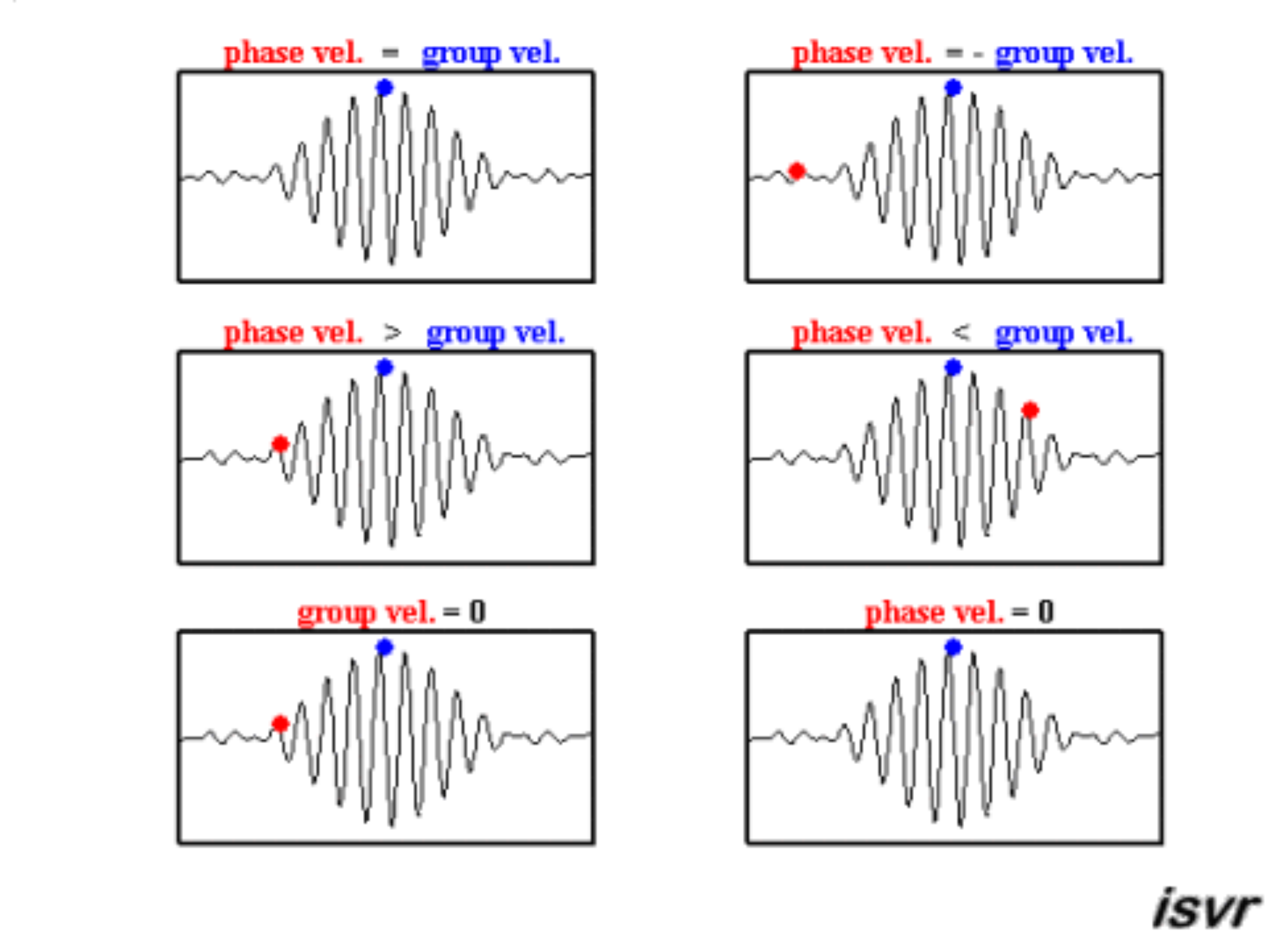

Precisely determined momentum


$\lambda_{avg}$
$\Delta x$

$p = h/\lambda$


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.
$\lambda_{avg}$
$\Delta x$
But that process spreads the momentum values and makes it more uncertain. This is an inherent and inescapable increase in the uncertainty $\Delta p$ when $\Delta x$ is decreased.
$\Delta x \Delta p > \frac{\hbar}{2}$

(video on lecture notes web page)



A general property of waves is that

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

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

$\Delta k$ : range of wave numbers

$\Delta x$ : location, or size of wave packet.

we can multiply these equations by

$\hbar$ : Planck constant, $\frac{h}{2\pi} = \hbar$

$$p = \frac{h}{\lambda} = \hbar k \qquad \epsilon = h\nu = \hbar \omega$$

$$\boxed{\begin{array}{l} \Delta p \, \Delta x \sim \hbar \\ \Delta \epsilon \, \Delta t \sim \hbar \end{array}}$$

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 $\epsilon$ & $t$ simultaneously.

This is expressed as:

$$\boxed{\begin{array}{c}\Delta p\,\Delta x \geq \frac{\hbar}{2} \\ \Delta E\,\Delta t \geq \frac{\hbar}{2}\end{array}}$$

Heisenberg's uncertainty principle (s).

$\Delta t$: time available for measurement

$\Delta E$: uncertainy in measured energy

$\Delta p$: uncertainty in measured momentum

$\Delta x$: uncertainty in position.

If you know $\lambda$ 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?


← infinitely tall box: $U(x)$ potential barrier goes to $\infty$

→ outside box, particle is not here

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: $P(x=0) = 0 \quad P(x=L) = 0$

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

The energy of the particle is $\epsilon = \underset{\text{(kinetic)}}{K} + \underset{\text{(potential)}}{U}$

The wave equation for quantum mechanics is:

Schroedinger wave equation: (time-independent)

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

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

we can simplify the above to:

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

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

Now, let's call $k^2 = \frac{2mE}{\hbar^2}$ $\longrightarrow$ then $\boxed{E = \frac{k^2\hbar^2}{2m}}$ (1)

this is a constant not Kinetic energy $K$,

and write (a) as $\boxed{\frac{\partial^2\Psi(x)}{\partial x^2} = -k^2\Psi(x)}$ (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, $\psi(x) = A\sin kx + B\cos kx$

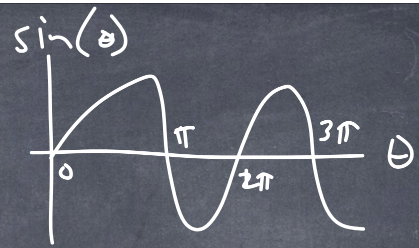
we know that $\psi(x=0) = 0 \quad \psi(x=L) = 0$

$$\psi(x=0) = 0 = \underbrace{A\sin k(0)}_{0} + B\underbrace{\cos k(0)}_{1} = B$$

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 $n$ = integer

$n = 0, 1, 2, 3, \dots$

we get that $k = \frac{n\pi}{L}$ for $n = 0, 1, 2, 3, \dots$

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

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

$$\boxed{E_n = \frac{n^2h^2}{8mL^2}, \quad n = 1, 2, 3, \dots}$$

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

for $n=1$, $\epsilon_1 = \frac{h^2}{8mL^2}$ and $\epsilon_n = n^2 \epsilon_1$

for $n = 1, 2, \ldots$

The energy is quantized.

$\psi(x) = A \sin kx = A_n \sin\left(\frac{n\pi x}{L}\right)$ for $n=1,2,\ldots$

what is $A_n$?

$A_n$ : constant for each $n$

we use $\int_0^L \psi^2(x)\,dx = 1$ must be true.

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

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

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

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

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

For this integral: $\displaystyle\int_a^b \sin^2 x \, dx = \frac{1}{2}\left(x - \frac{1}{2}\sin 2x\right)\Big]_a^b$

For our case: $\displaystyle A_n^2 \frac{L}{n\pi}\left[\frac{\theta}{2} - \frac{\sin 2\theta}{4}\right]_0^{n\pi} = A_n^2 \frac{L}{\cancel{n\pi}} \cdot \cancel{n\pi} = 1$

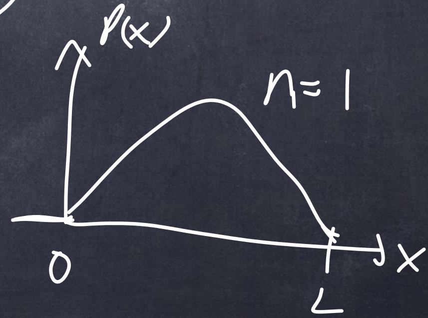
we find that $A_n = \sqrt{\frac{2}{L}}$ (independent of $n$)

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

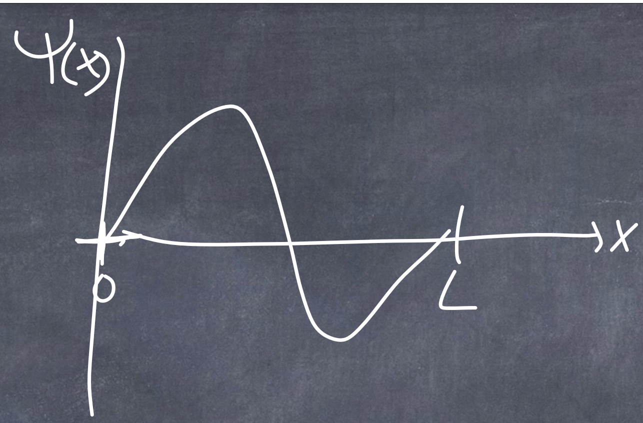
$n$: are the quantum numbers

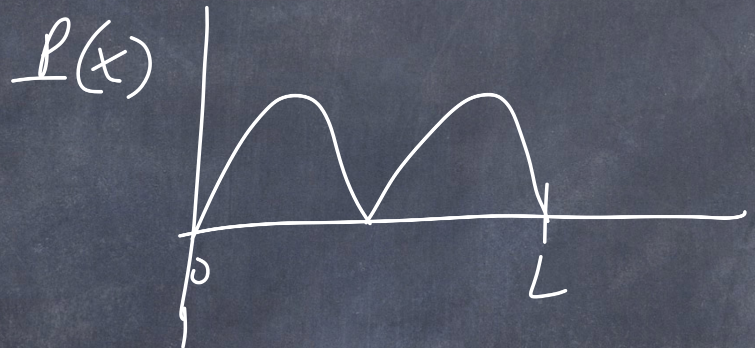
If $n = 1$, then $\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$


$\rho(x) = \psi^2(x)$



For $n=2$




The classical limit $n \to$ large number