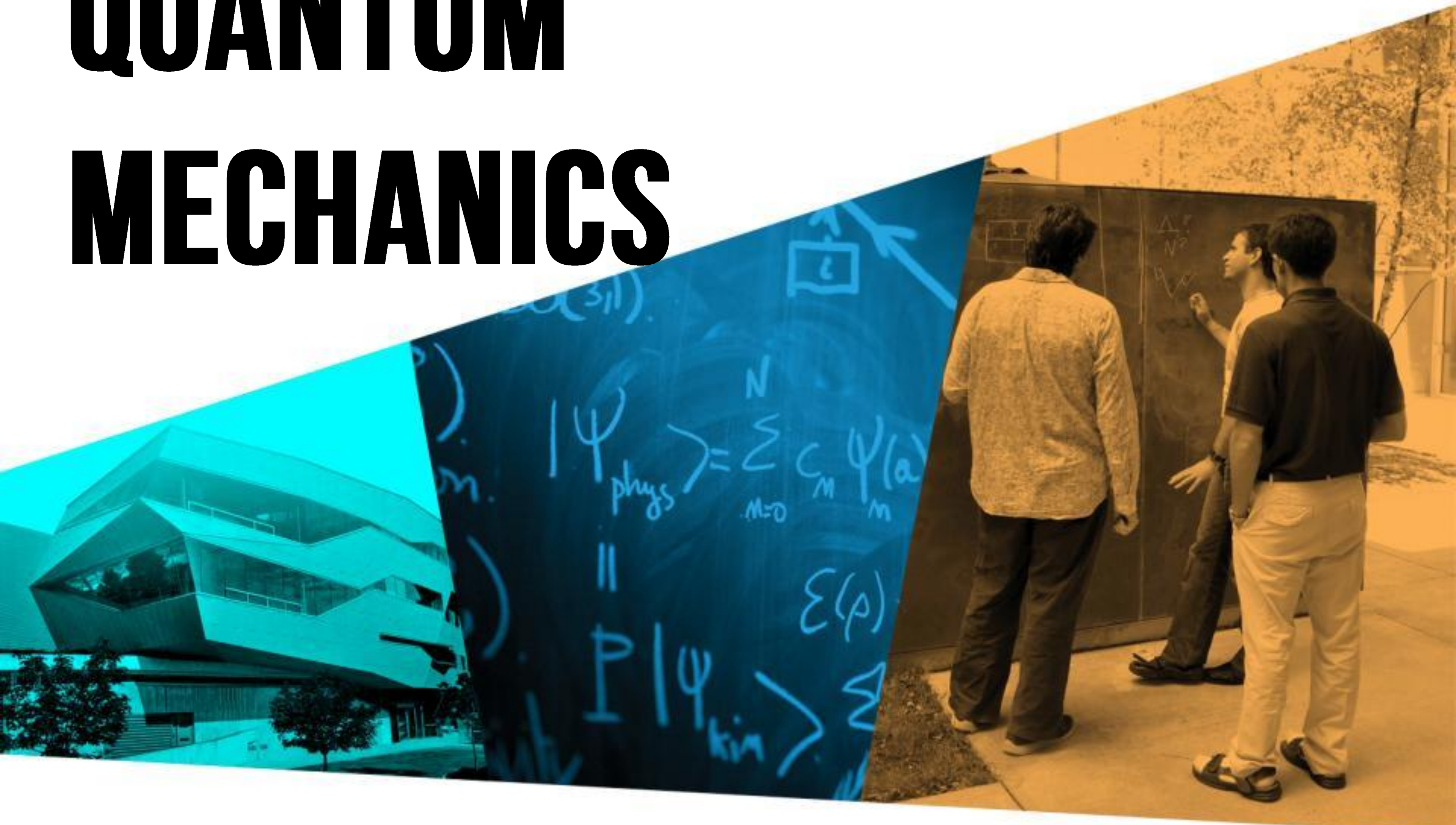
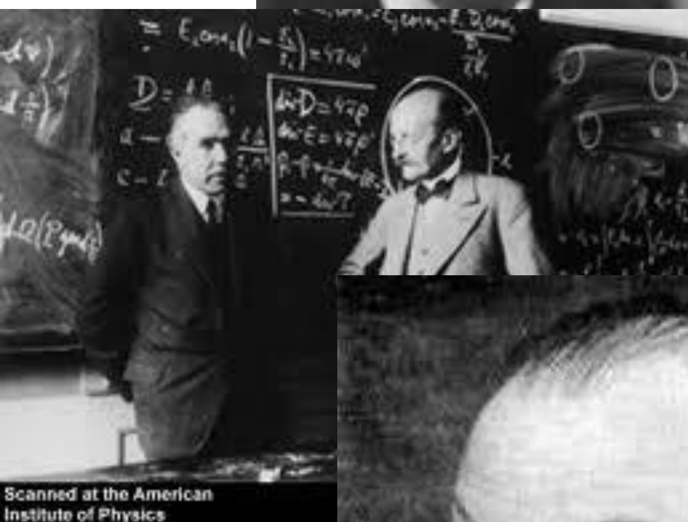
QUANTUM MECHANICS



PERIMETER INSTITUTE FOR THEORETICAL PHYSICS





Scanned at the American
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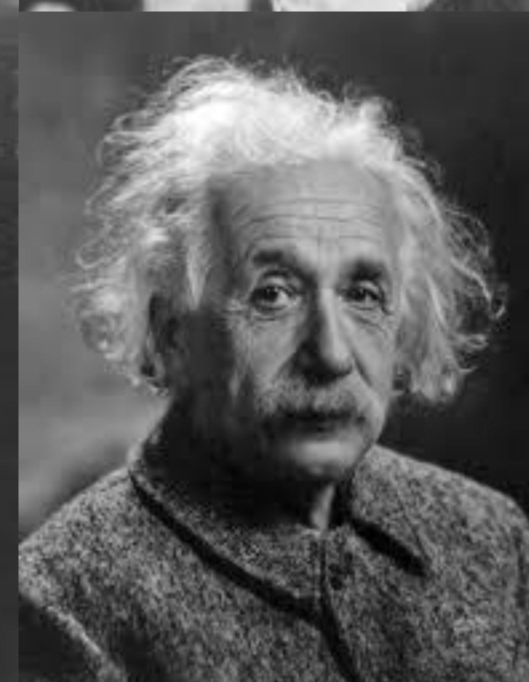
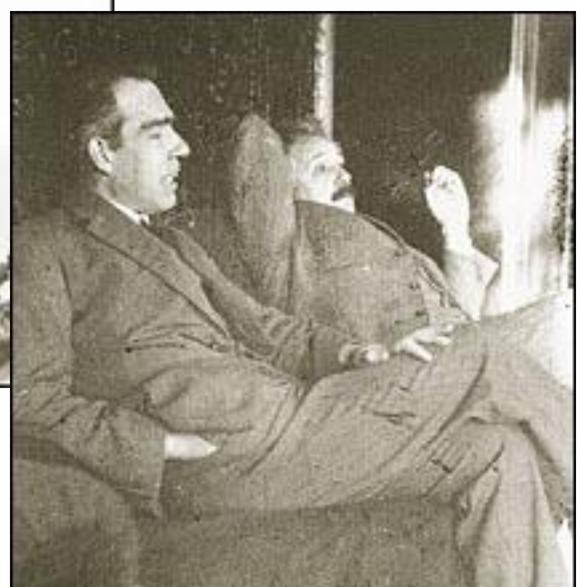
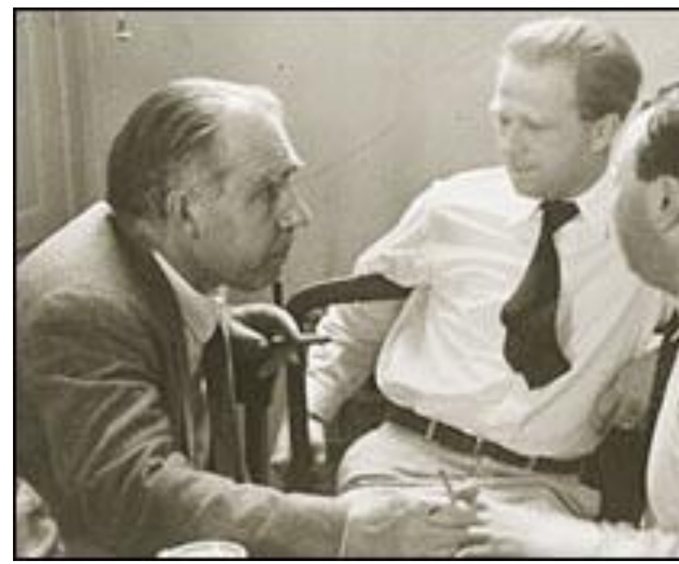


Since my talks with Bohr often continued till long after midnight and did not produce a satisfactory conclusion, ...both of us became utterly exhausted and rather tense.

--Heisenberg, recollection





Double Slit with Classical Particles (POE)

PREDICT

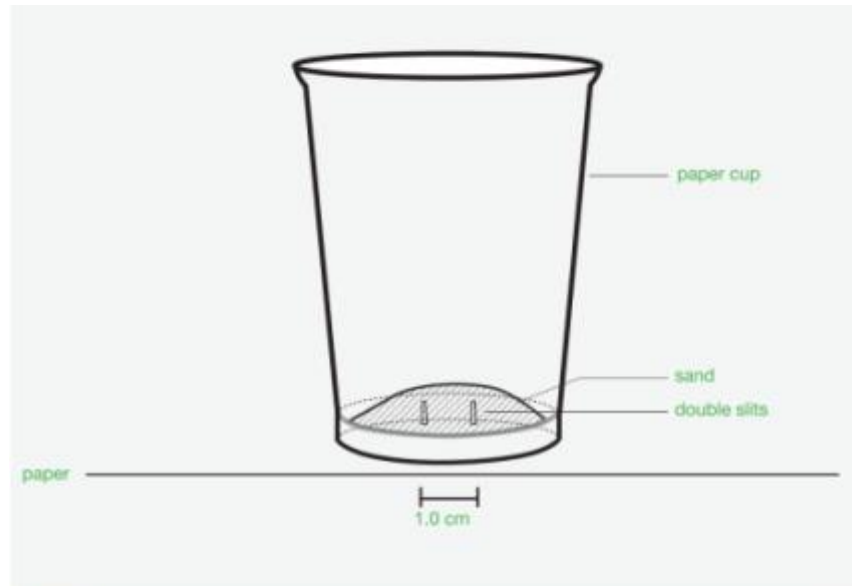


Figure 1 Be sure to keep the cup still and on the tabletop when pouring the sand through the slits.

Double Slit with Classical Particles (POE)

Using your white boards, please sketch and provide **three (3) describing words** of what you think will happen.

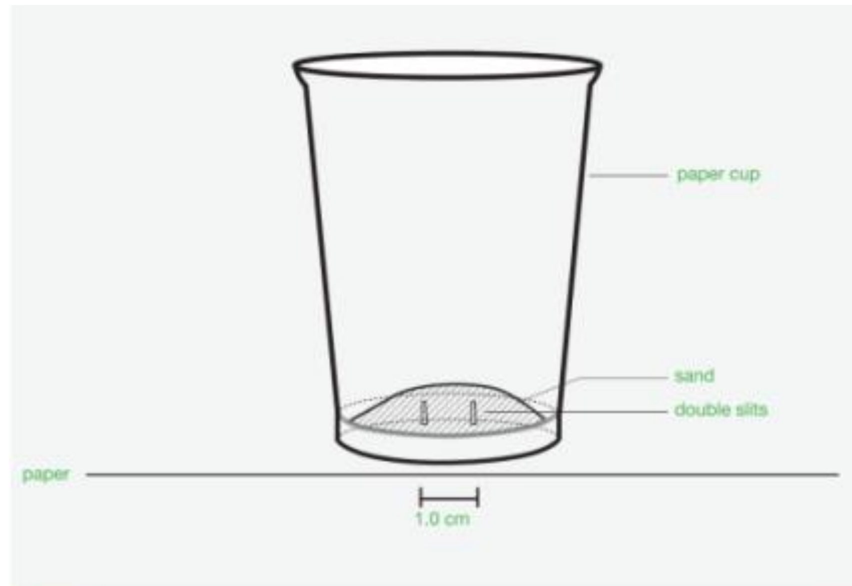


Figure 1 Be sure to keep the cup still and on the tabletop when pouring the sand through the slits.

Double Slit with Classical Particles (POE)

Classical particles…
collide
localized

Particle Model of Nature

What is a particle?

- Localized object
- Only in one place at a time
- Can bounce off other particles

Double Slit with Classical Waves (POE)

Predict what happens when waves travel through the two slits. Write down **three (3) describing words** about the properties of waves.

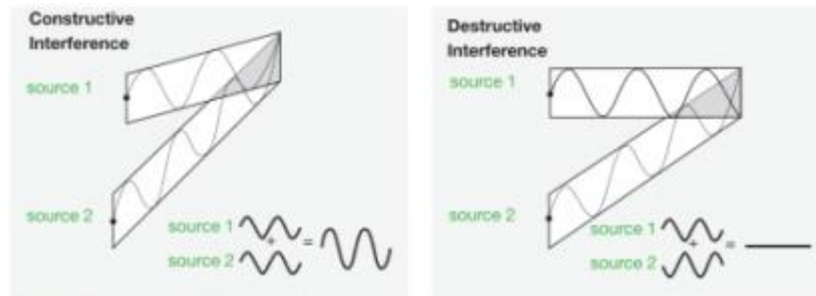


Figure 2 Recall the constructive interference and destructive interference of classical waves.

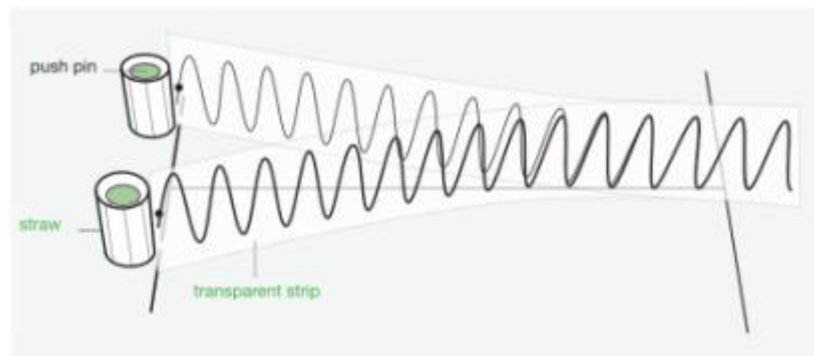
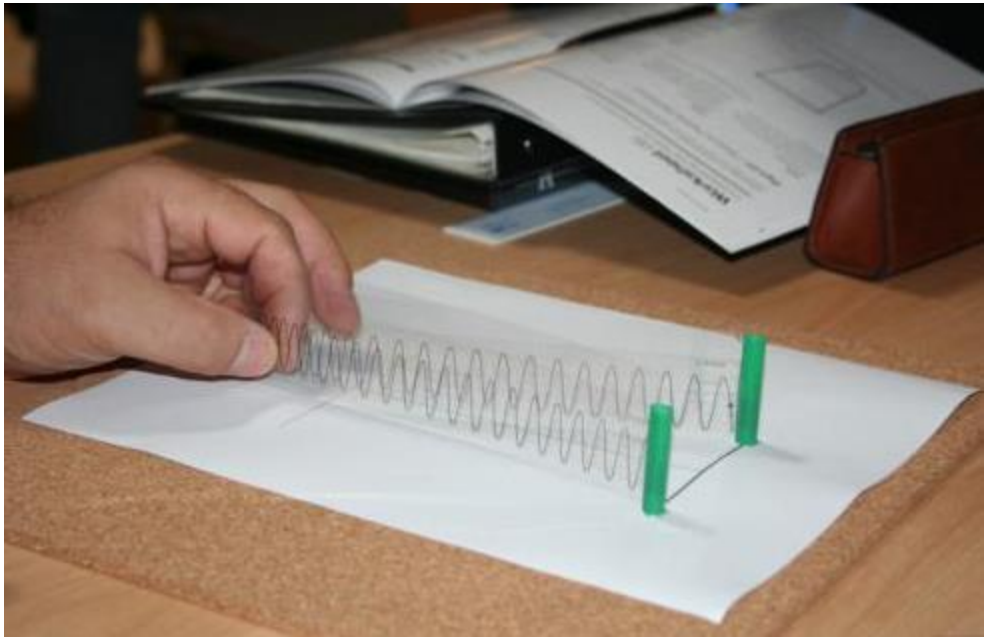


Figure 3 Use waves drawn on transparencies to observe interference.

Double Slit with Classical Waves (POE)

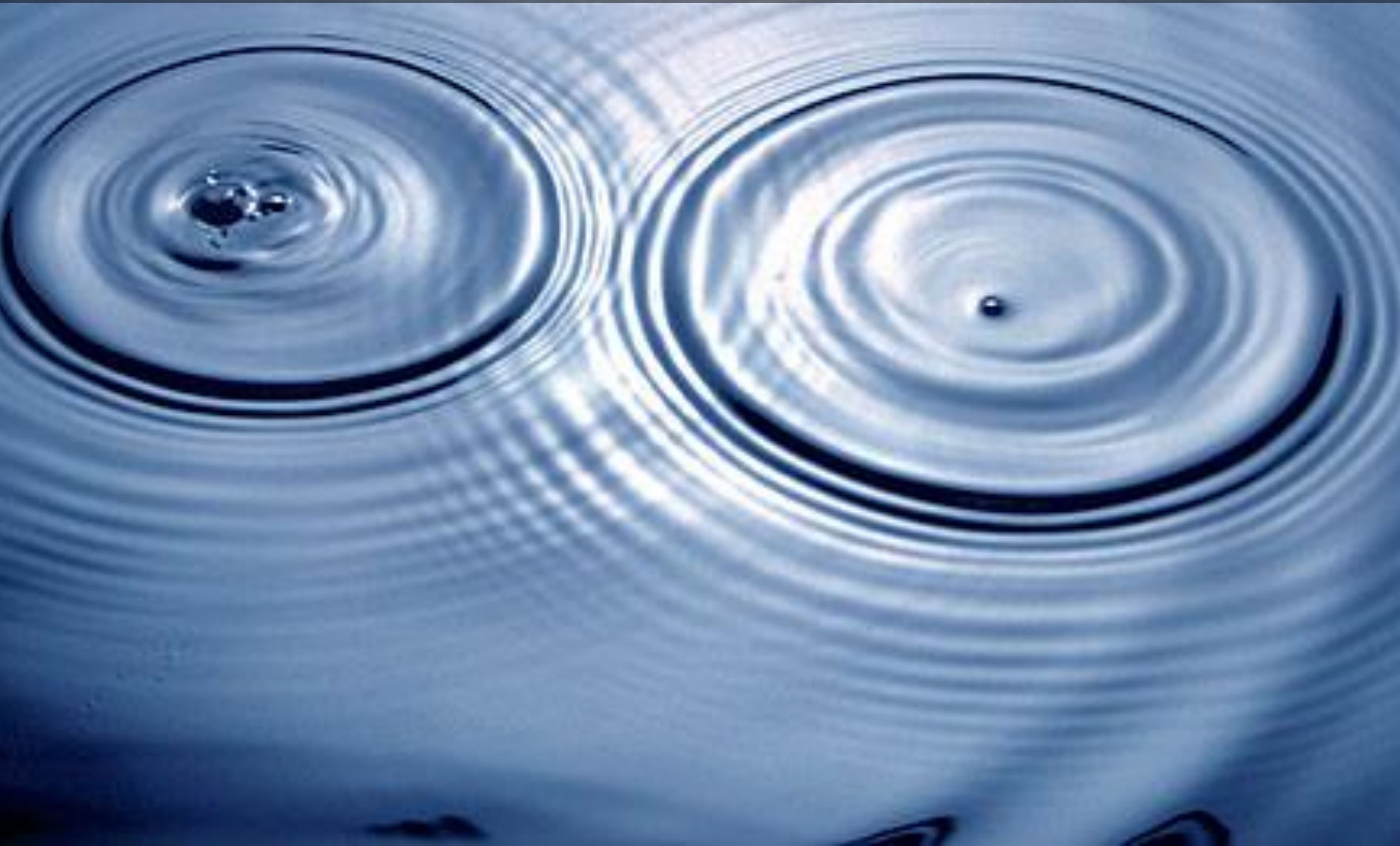


Classical waves…

interfere

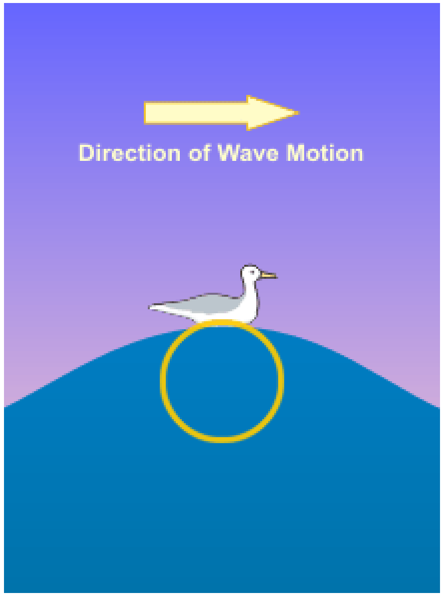
non-localized

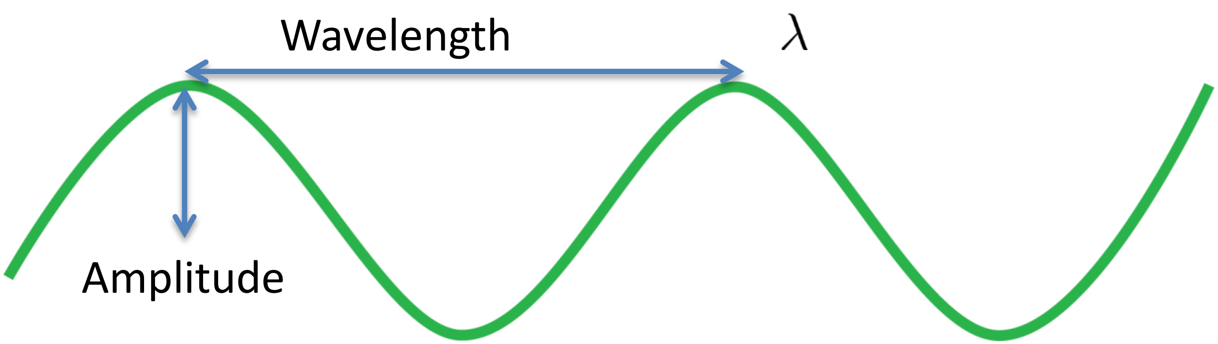
WAVES



Waves 101

Waves Transport Energy



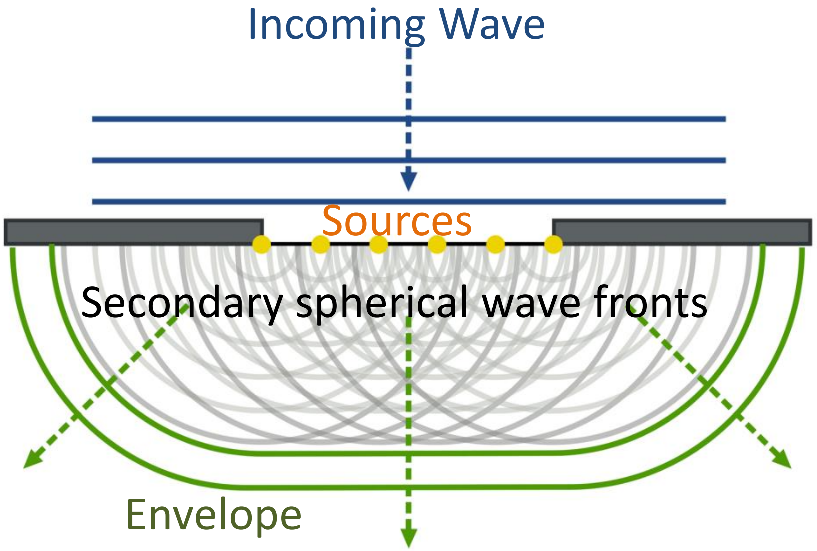


$$v = f \times \lambda$$

The speed of the wave is determined by the medium.

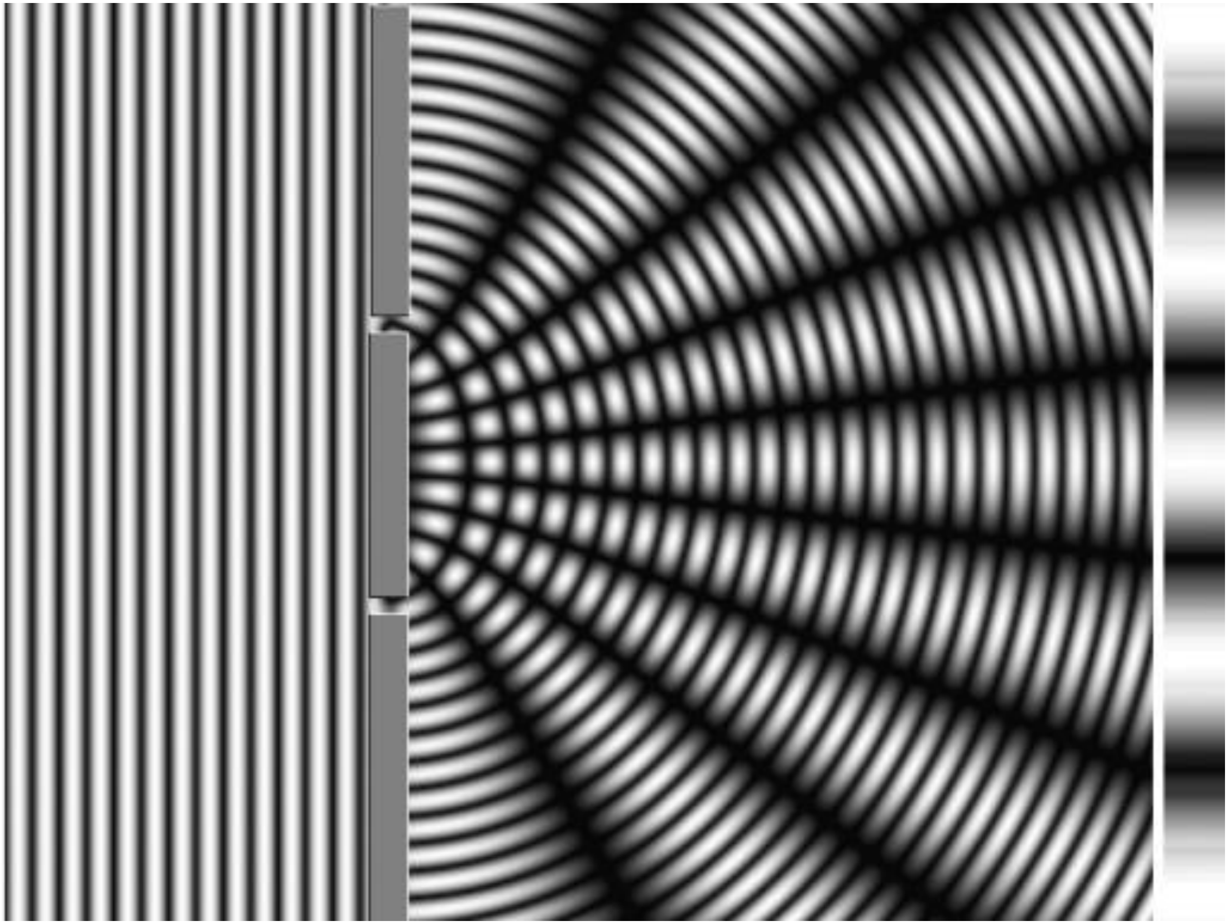
Waves Spread Out (Diffract)

Huygens' Principle

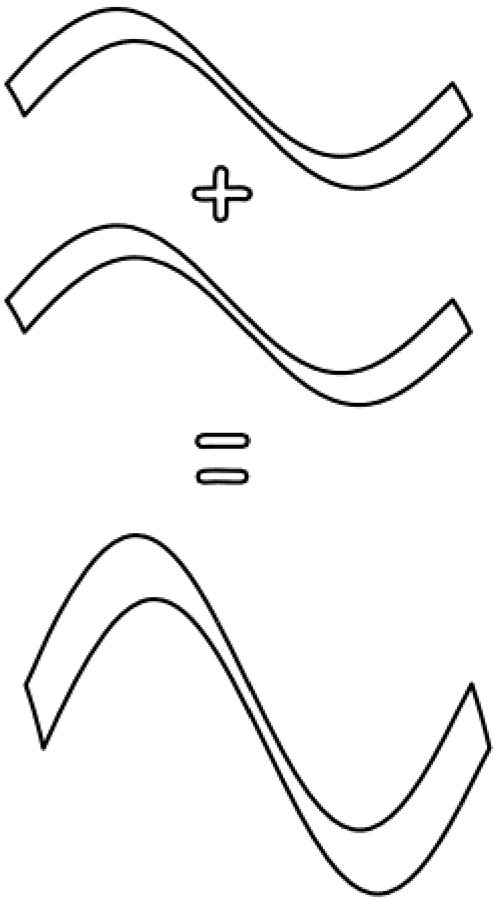


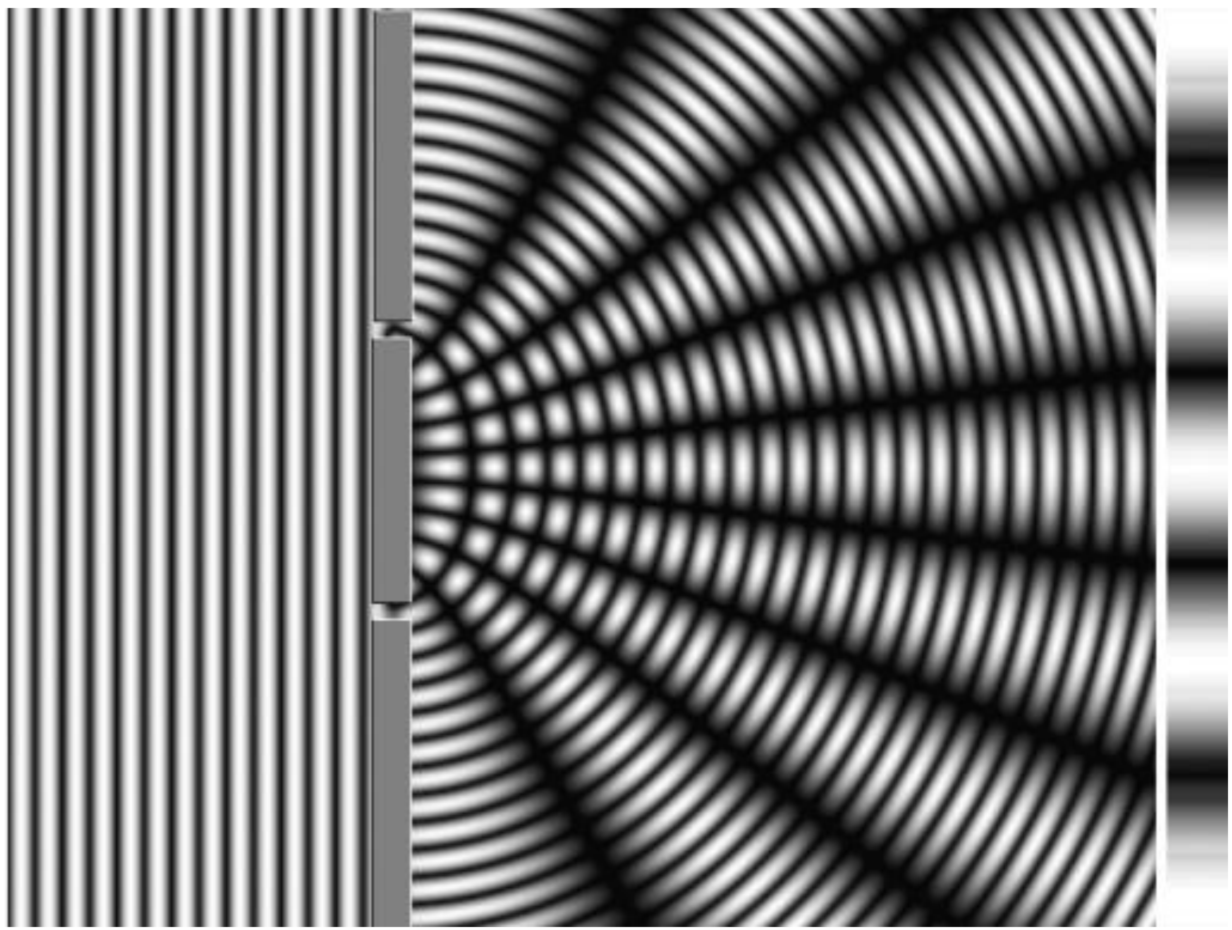
Each point disturbed by the advancing wave front can be viewed as a source of spherical waves. The new front is the envelope of these secondary spherical wave fronts.

WAVES Interfere



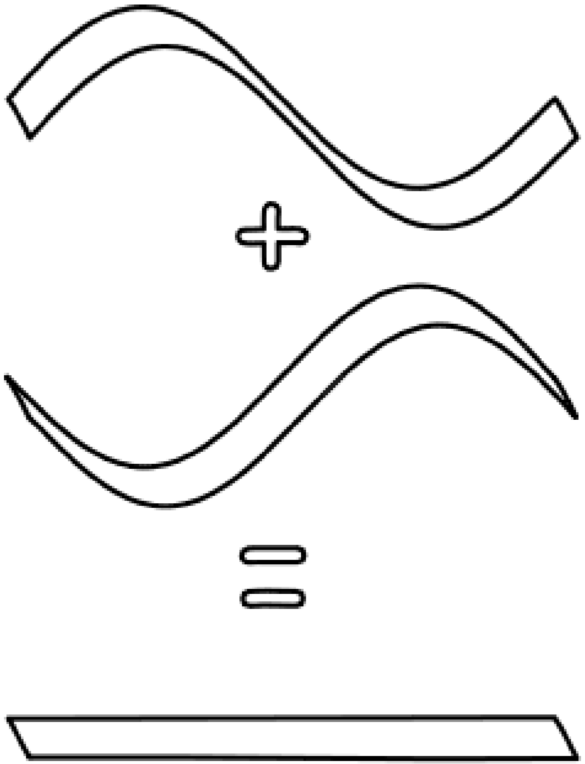
WAVES Interfere



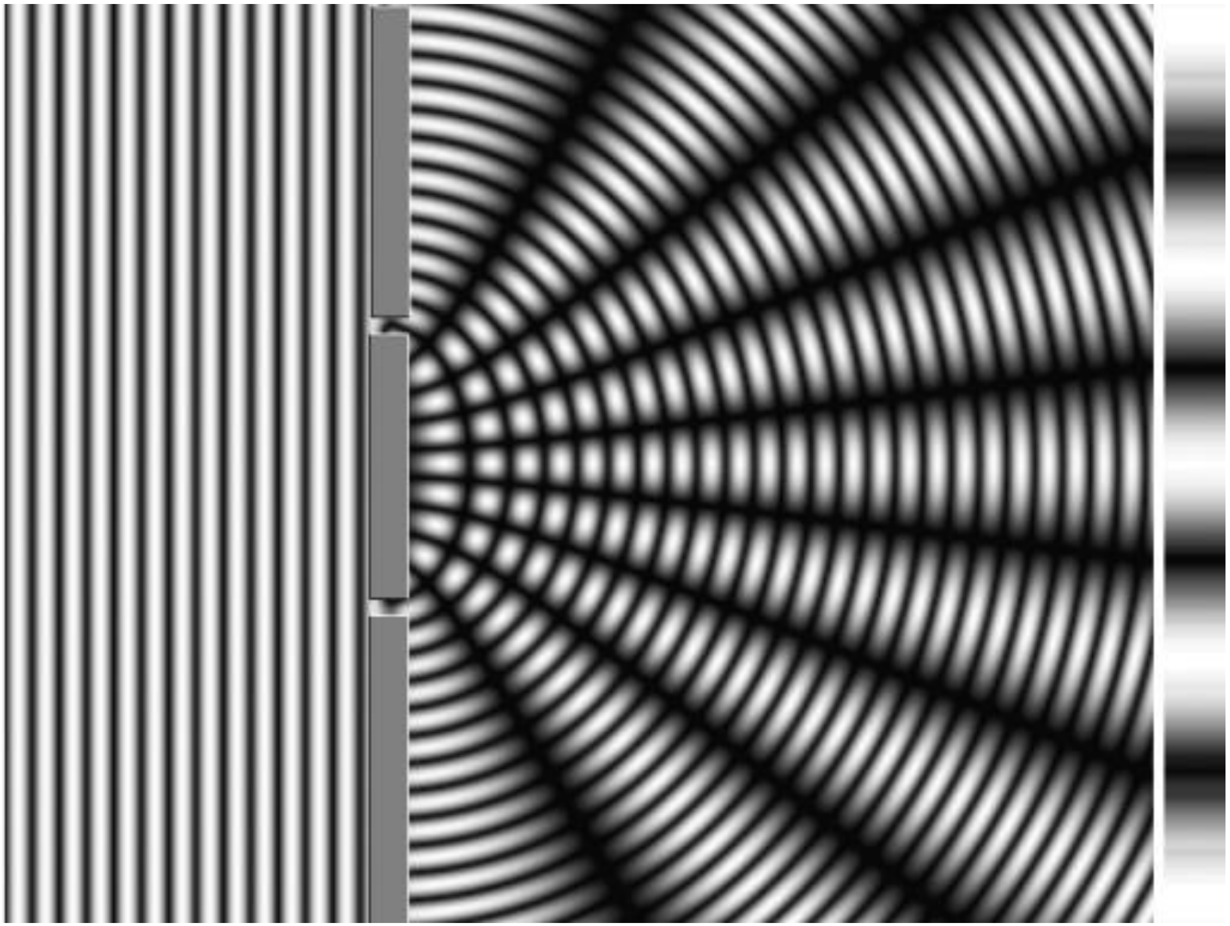


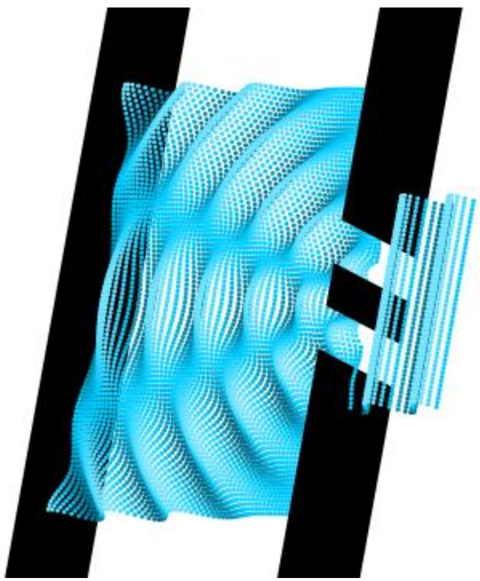
CONSTRUCTIVE

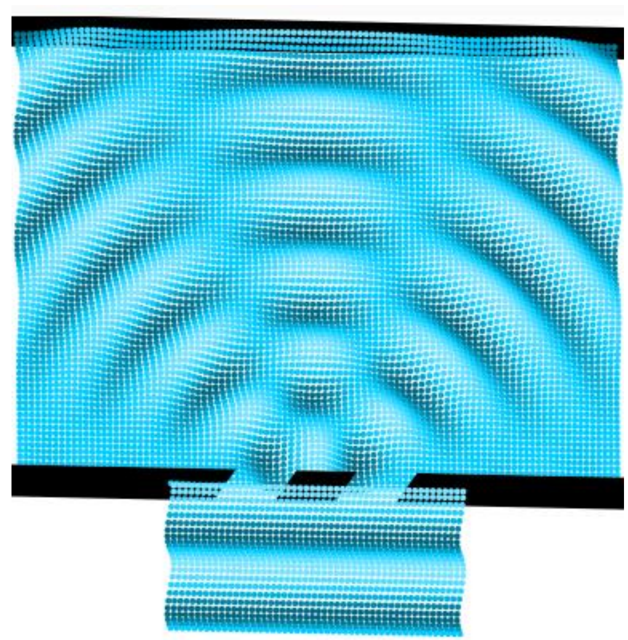
WAVES Interfere

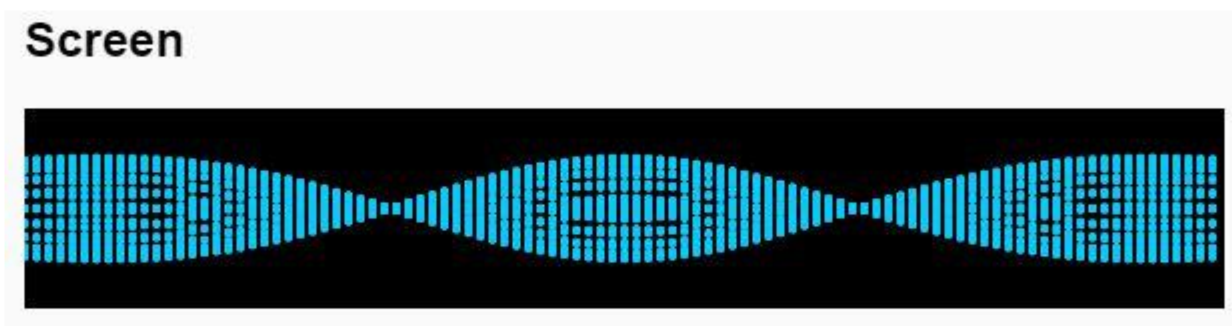


DESTRUCTIVE

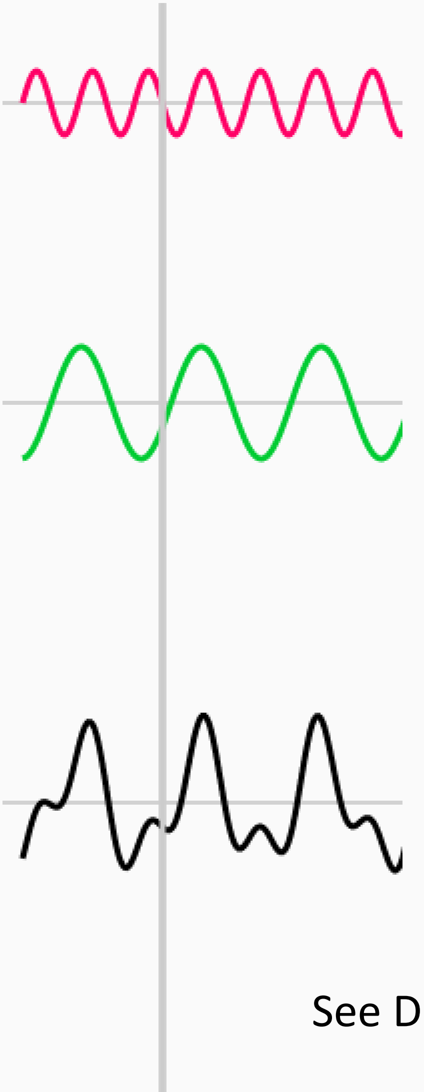







Screen

Make your own waves and interference patterns!



Wave 1

Amplitude = 16 Wavelength = 28 Phase = 0°

Amplitude

Wavelength

Phase

Wave 2

Amplitude = 28 Wavelength = 60 Phase = 86°

Amplitude

Wavelength

Phase

Resultant Wave

Measure amplitude by sliding slider

Wave 1 Amplitude = 0
Wave 2 Amplitude = -12.3
Resultant Amplitude =-12.3

See Demo folder in D2L!

Wave Model of Nature

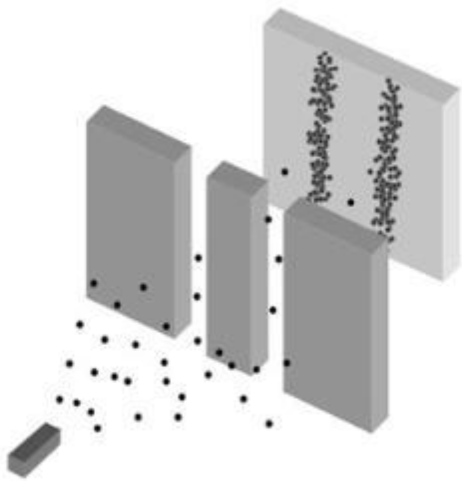
What is a wave?

- Non-localized
- Spread out
- Able to interfere and pass through other waves

Summary

Particles

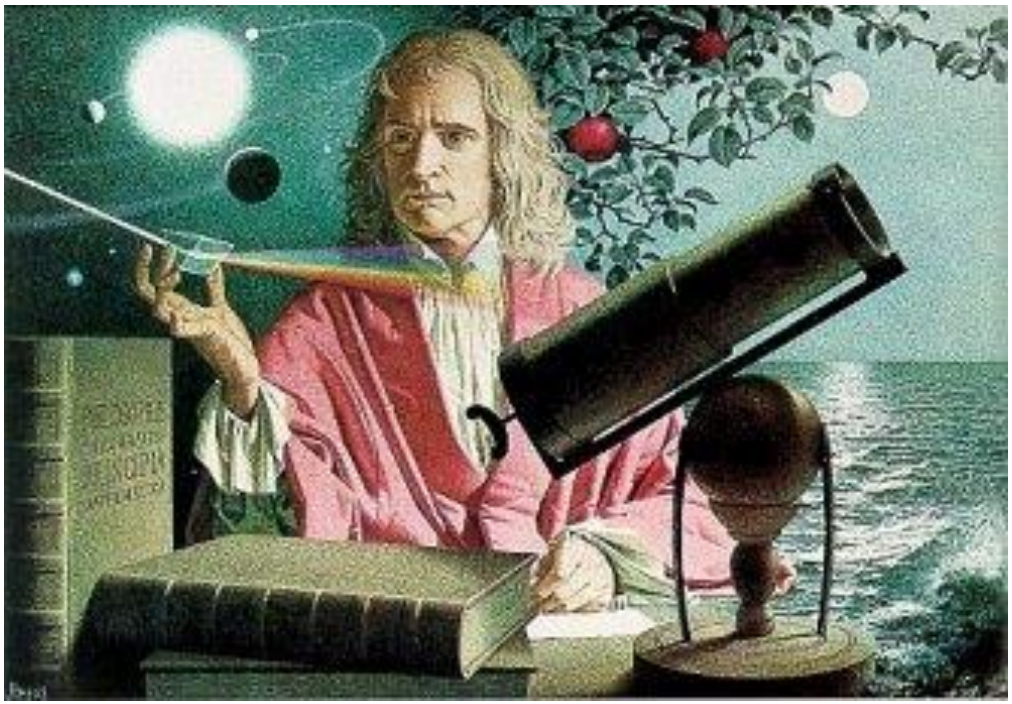
- Localized
- One place at a time
- Can bounce off other particles



Waves

- Non-Localized
- Spread out
- Can pass through other waves

NEWTON'S MODEL - *Light is a Particle*

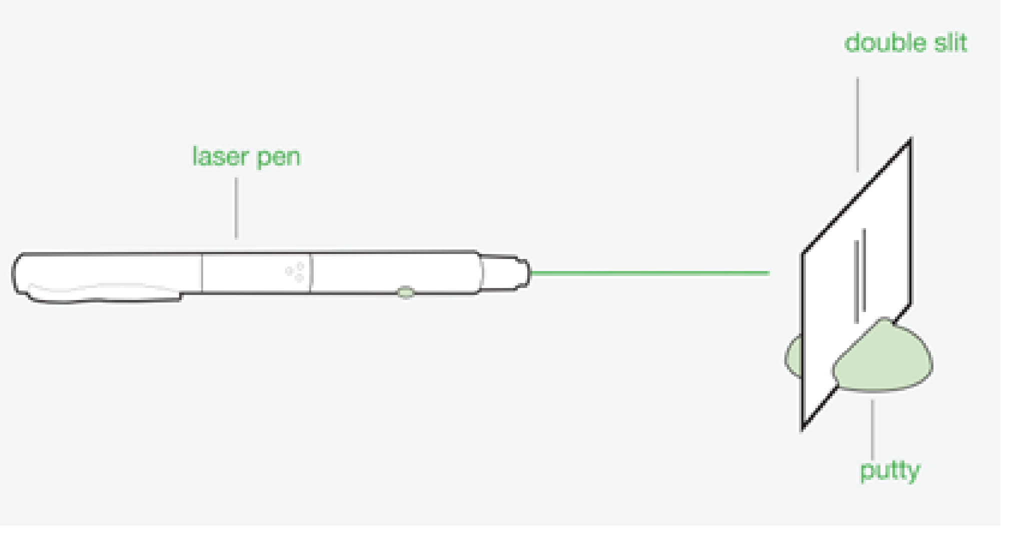



Google earth

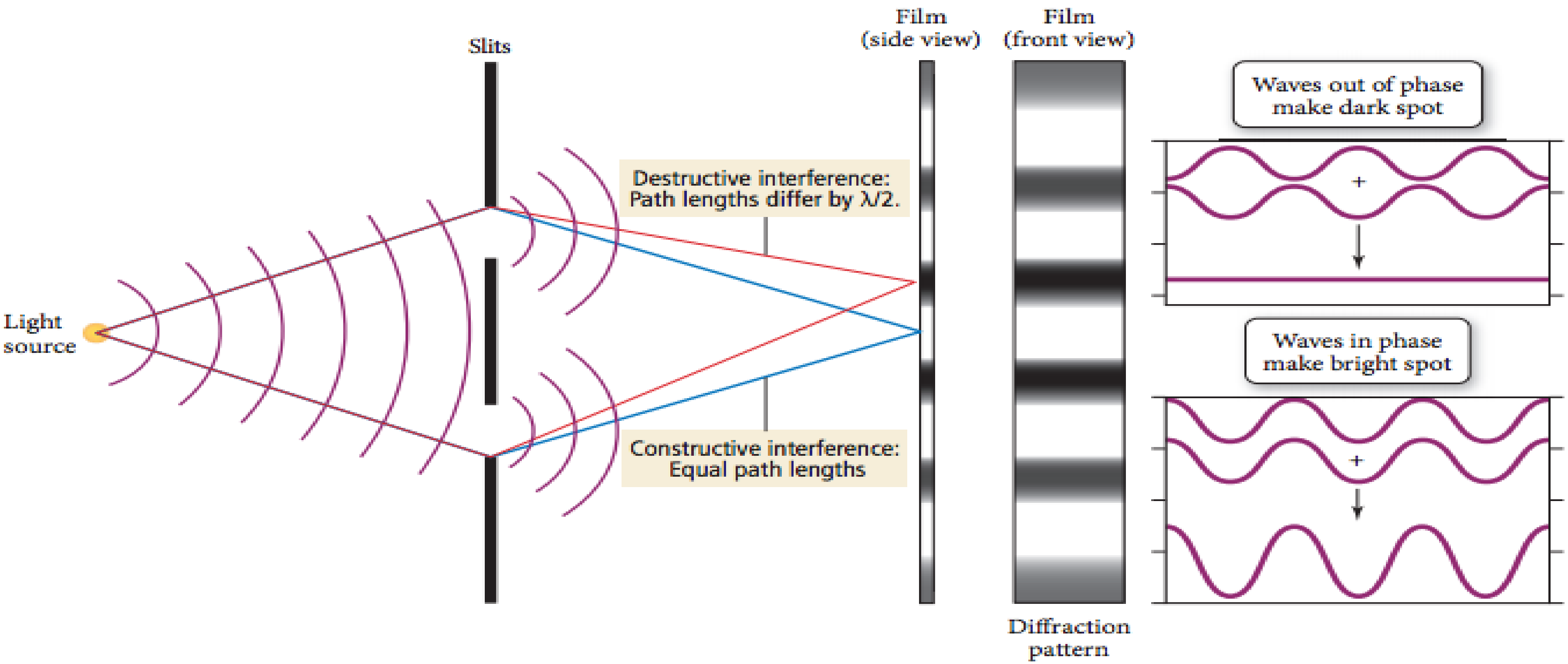
HUYGEN'S MODEL - Light is a Wave

What is light? A particle or a wave?

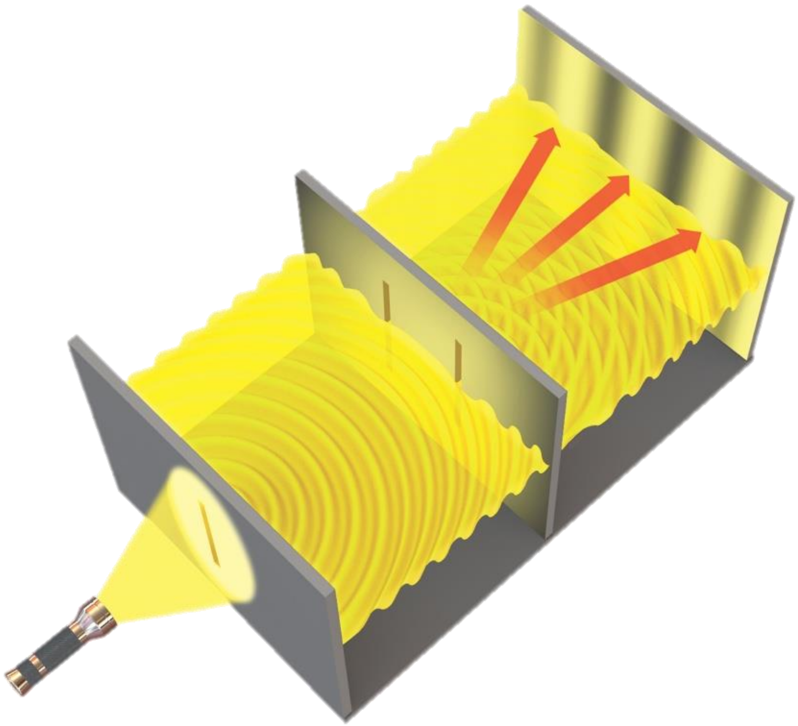
Sketch your Prediction



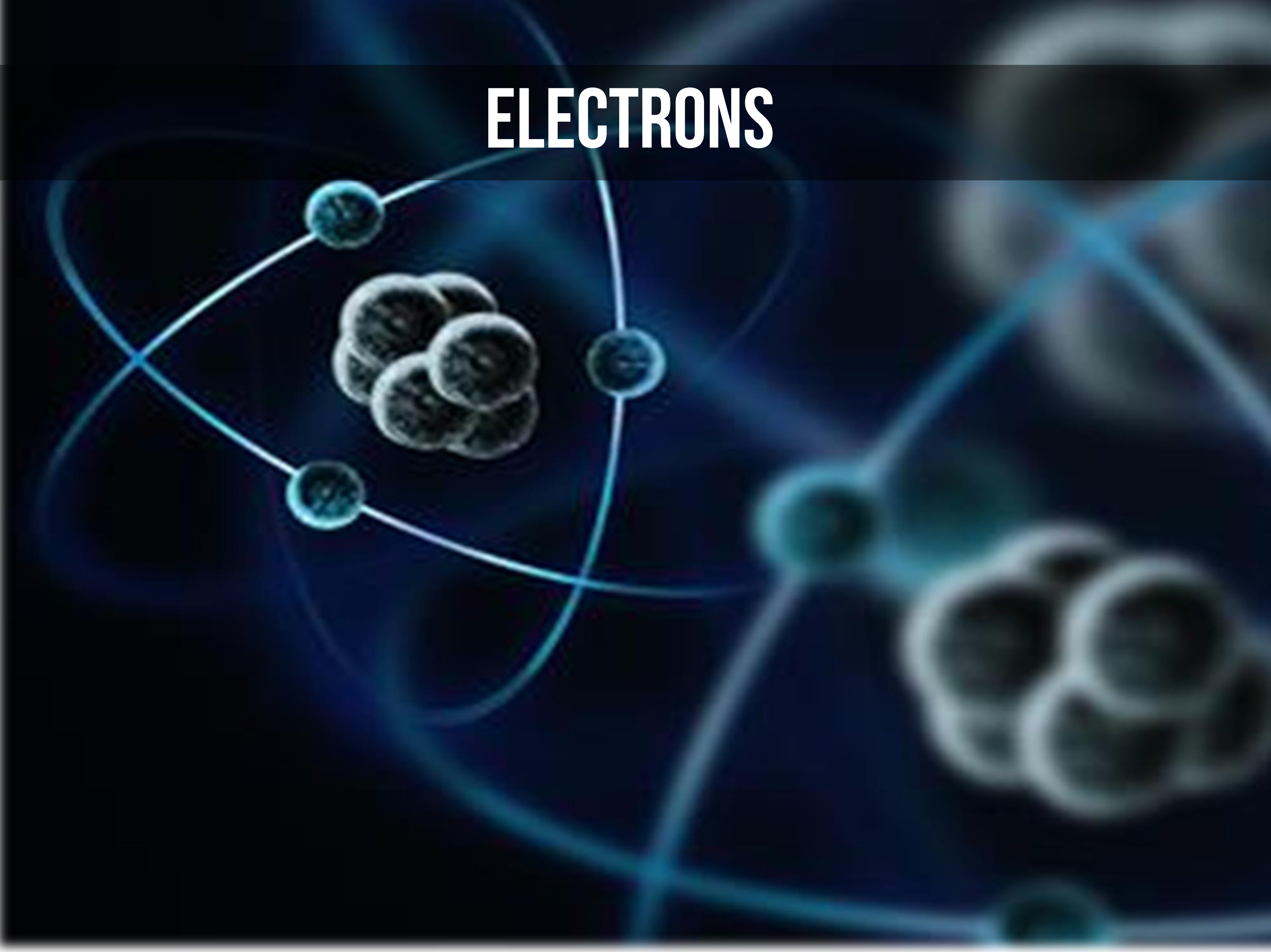
Light Seems like a Wave



YOUNG'S EXPERIMENT- Light is a Wave



ELECTRONS



Electrons

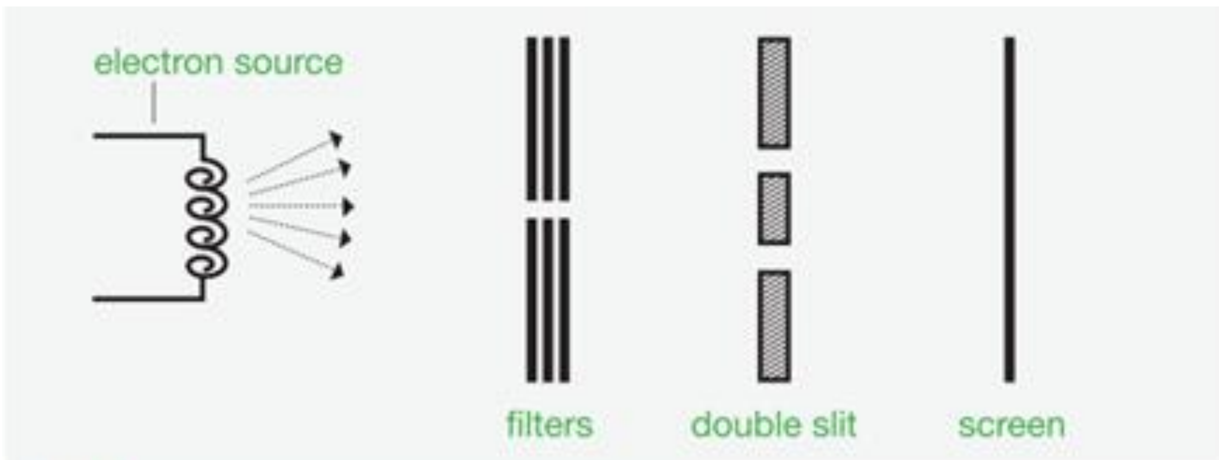
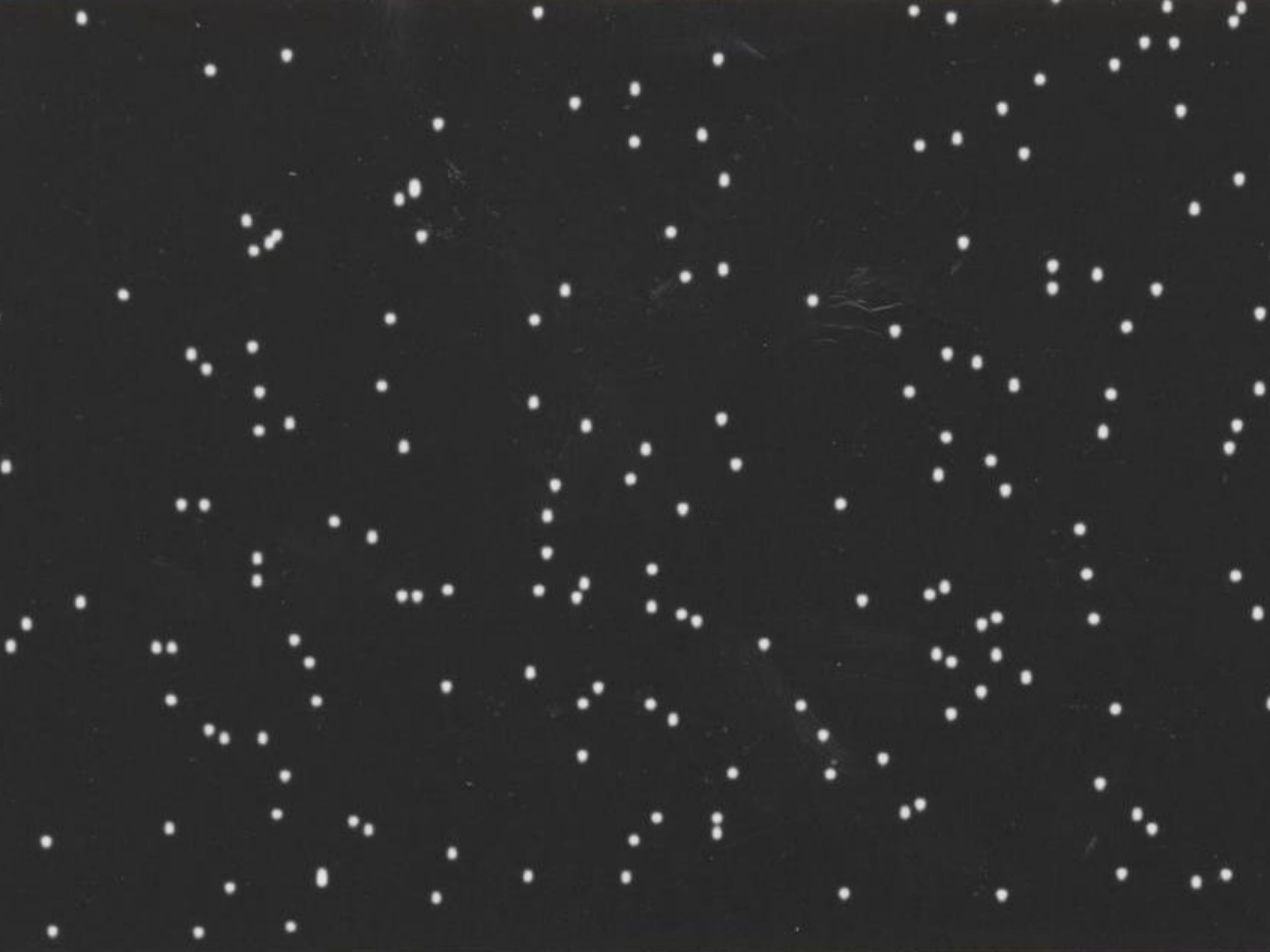
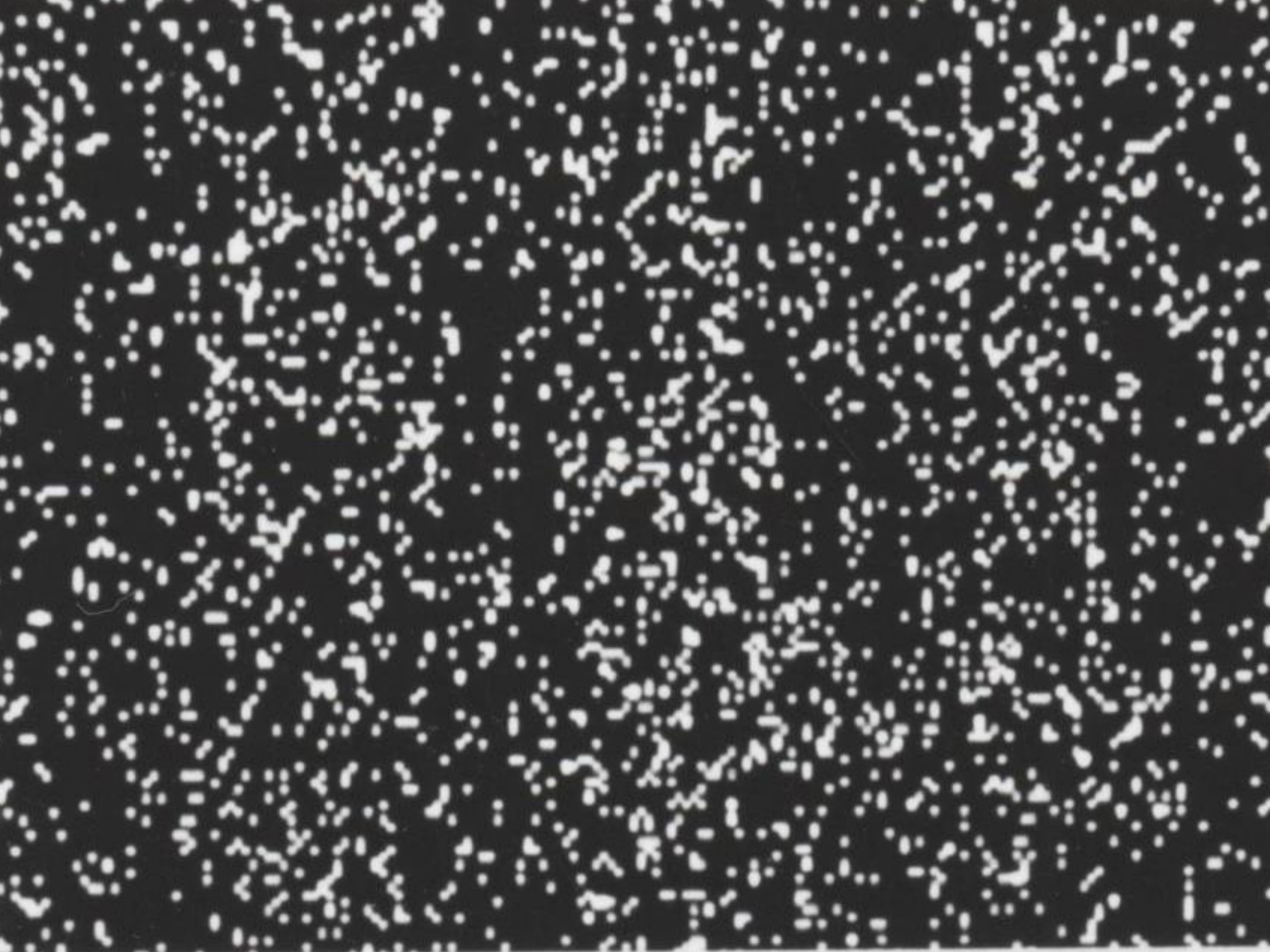


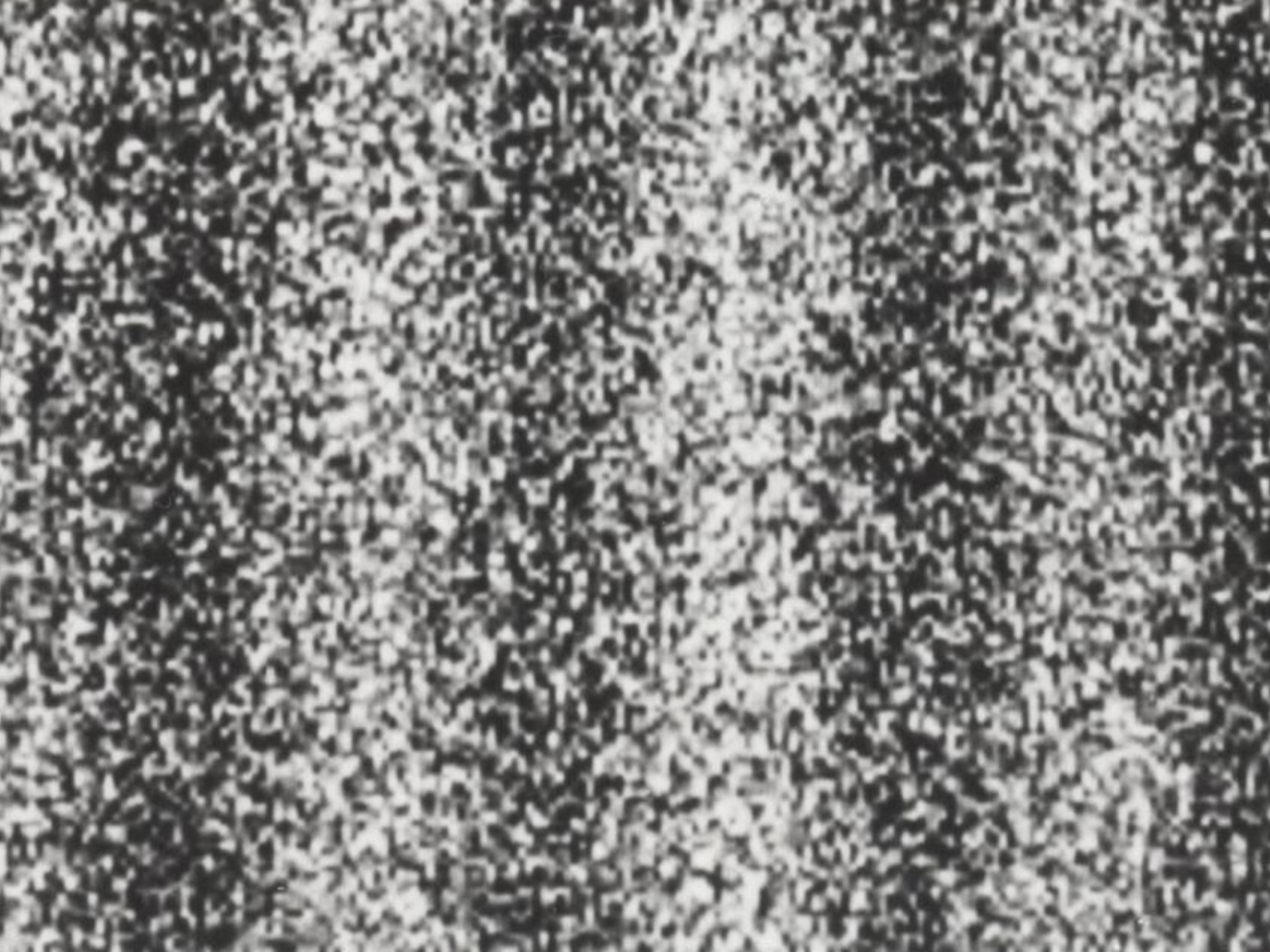
Figure 3 Experiment set-up (not to scale)

Electron 2-slit experiment:

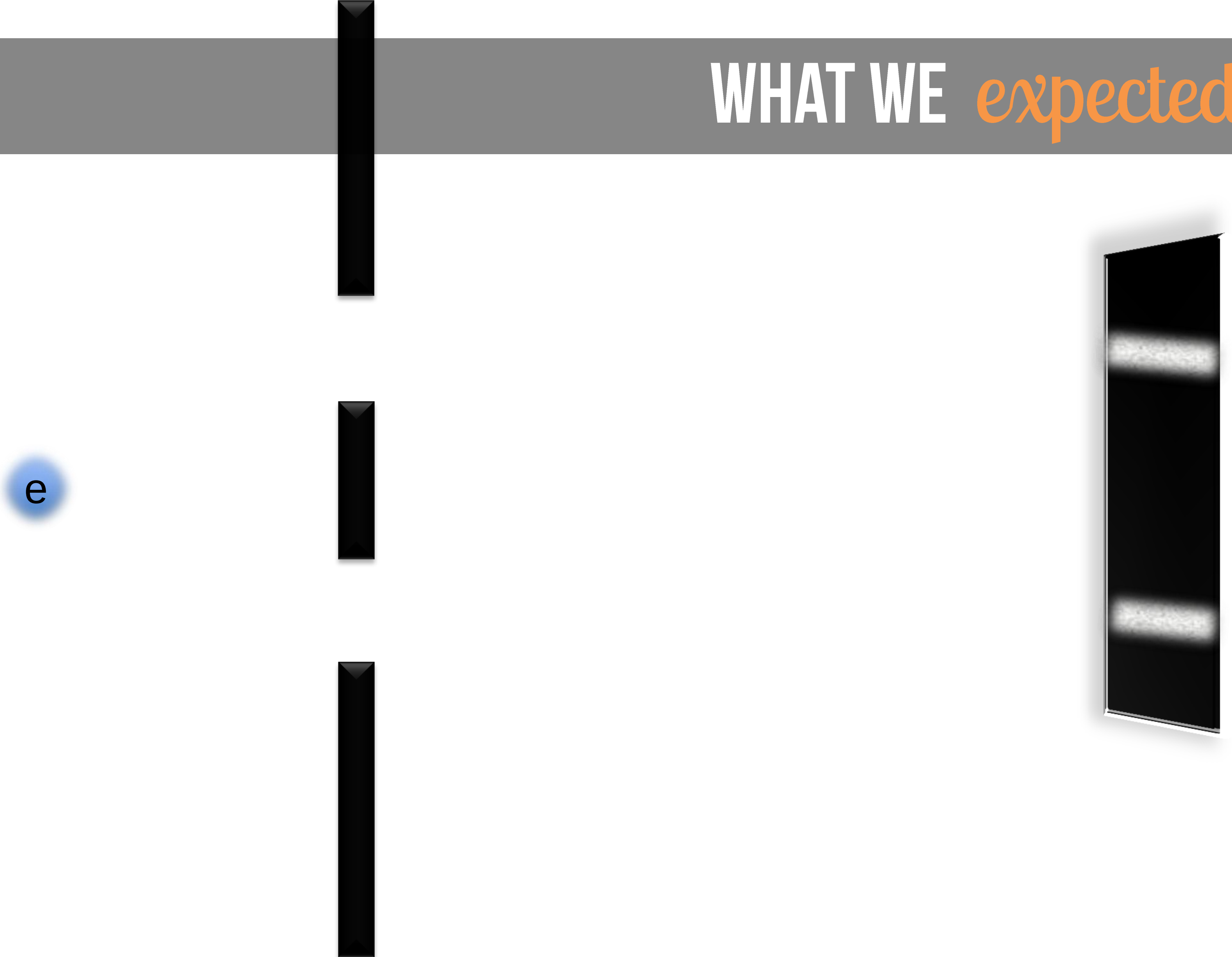
From: Dr. B. King



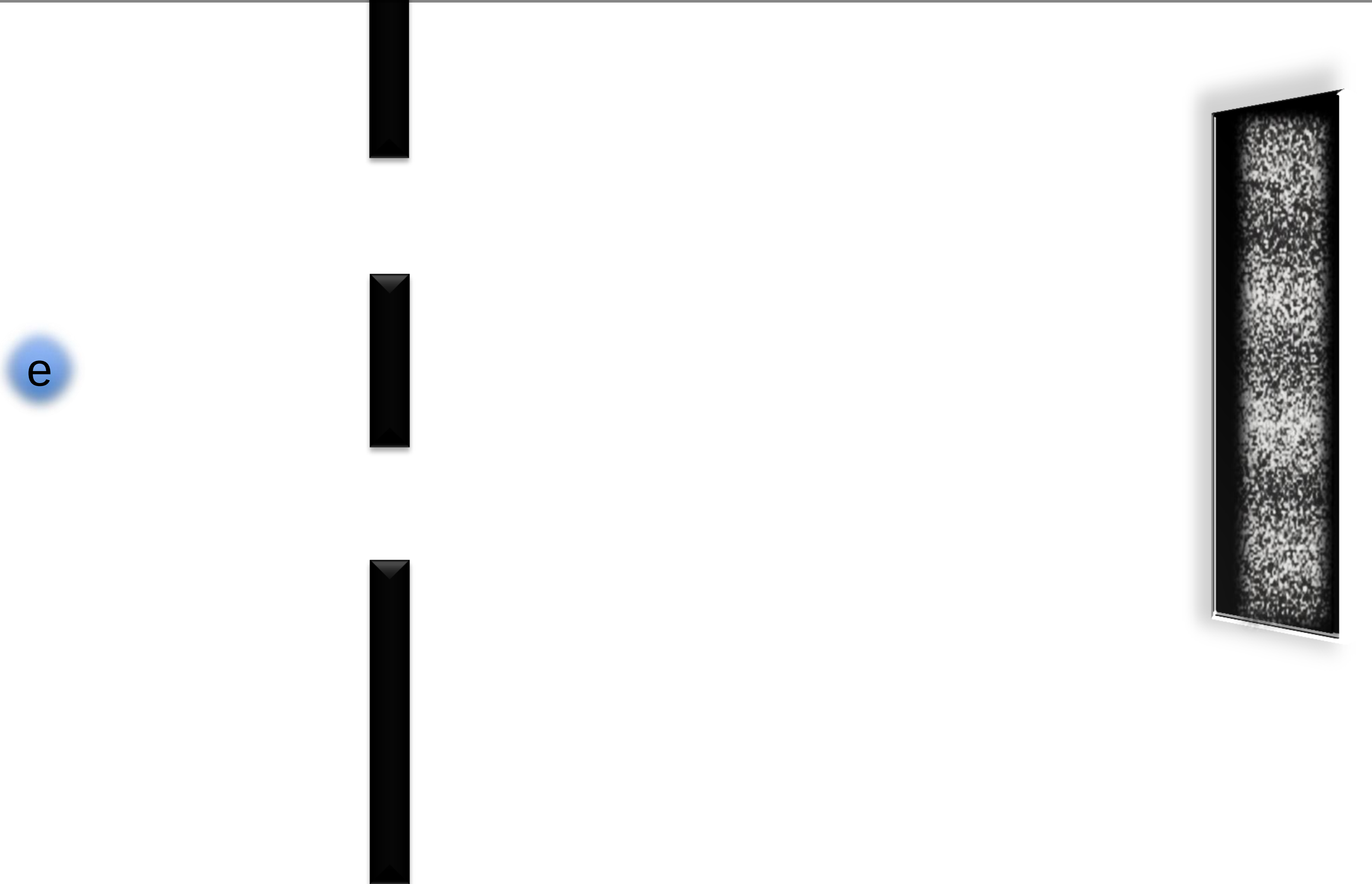




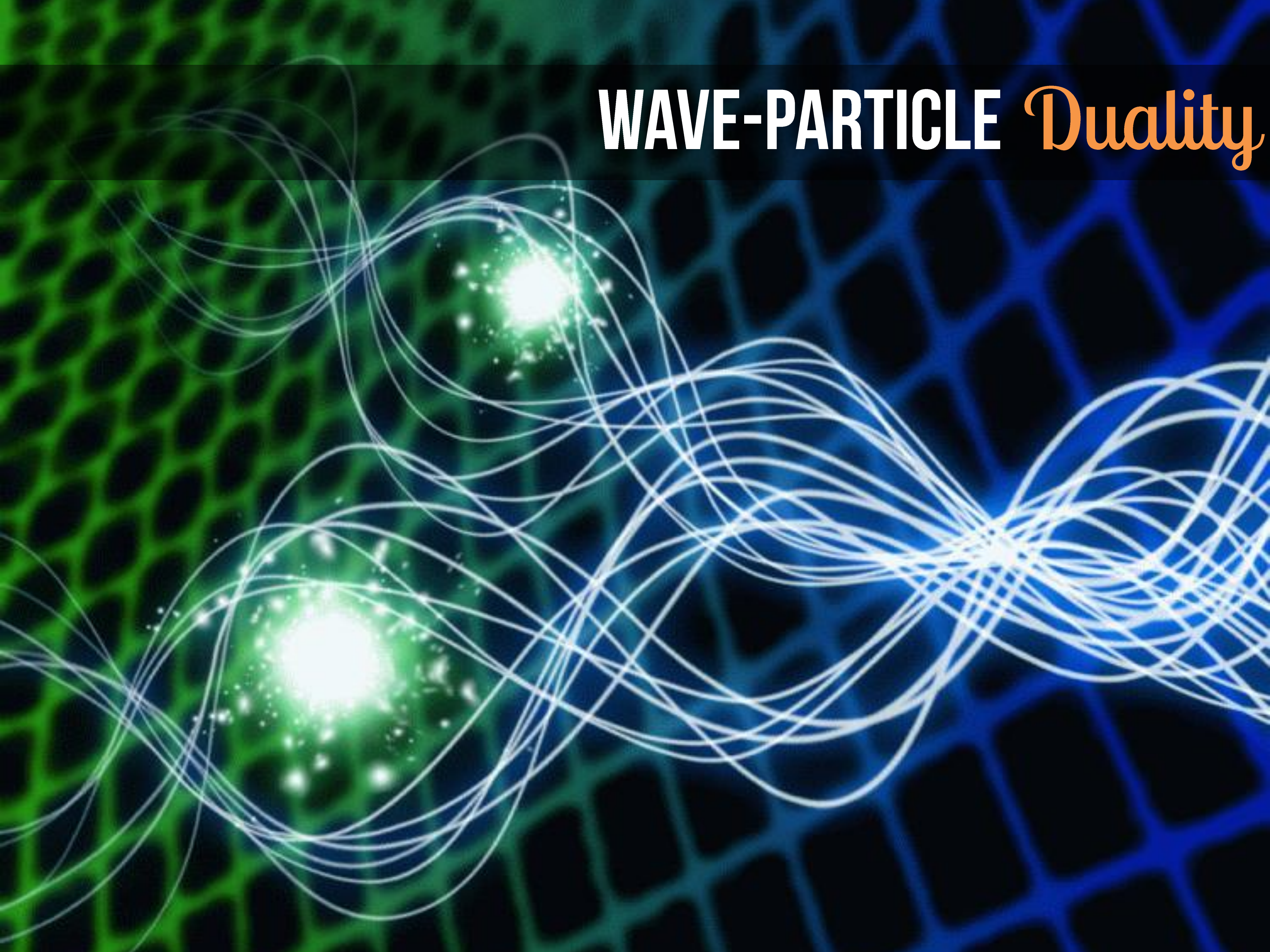
WHAT WE *expected*



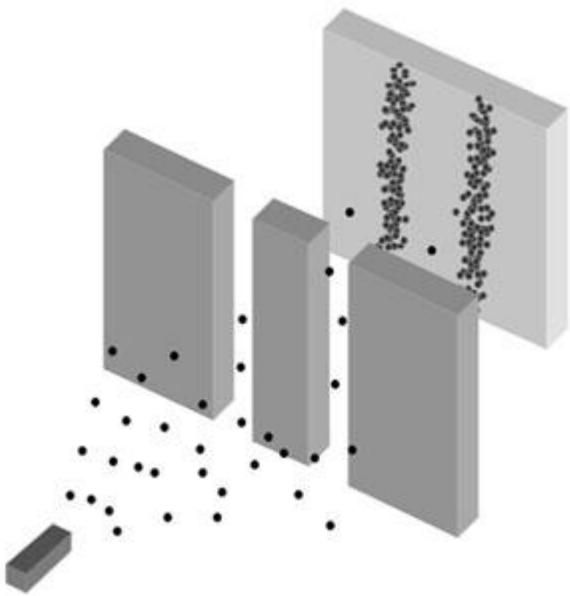
WHAT WE *actually see*



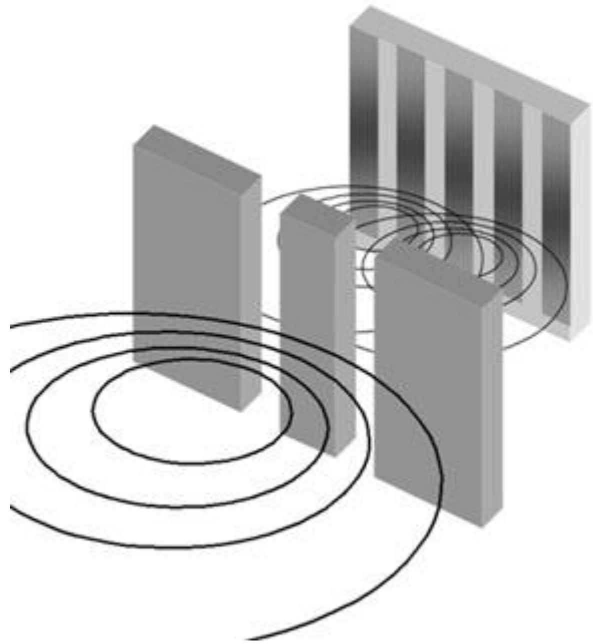
WAVE-PARTICLE Duality



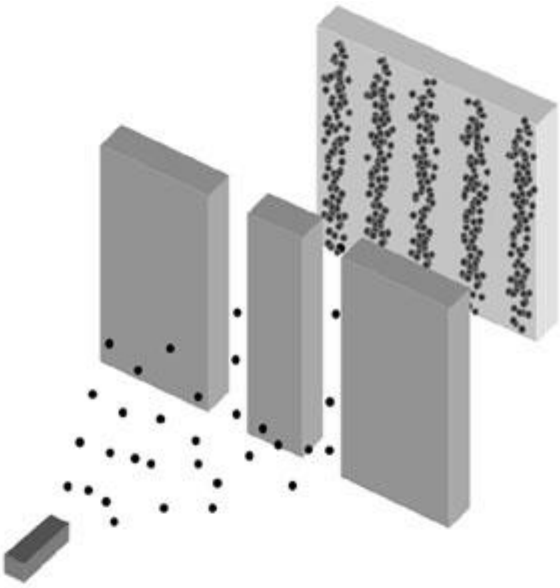
Particles



Waves



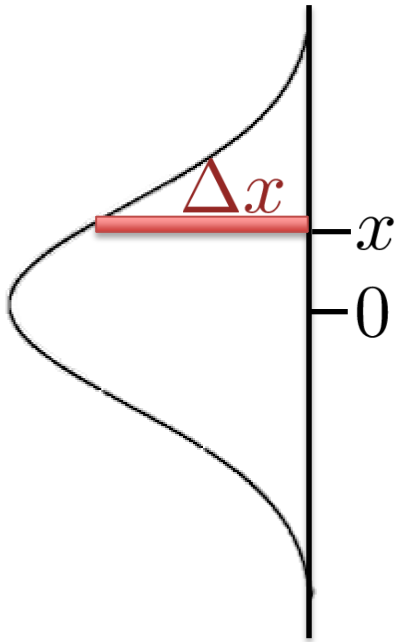
Electrons



The Beginning of the End

- Prior to the late 19th century, we viewed the universe as:
  - divisible into particles (matter) and waves (light)
  - smooth on small scales (no structure on scales smaller than atoms)
  - deterministic, so that if you know the state of a system *now*, you can know its state at any time by using the laws of kinematics and dynamics

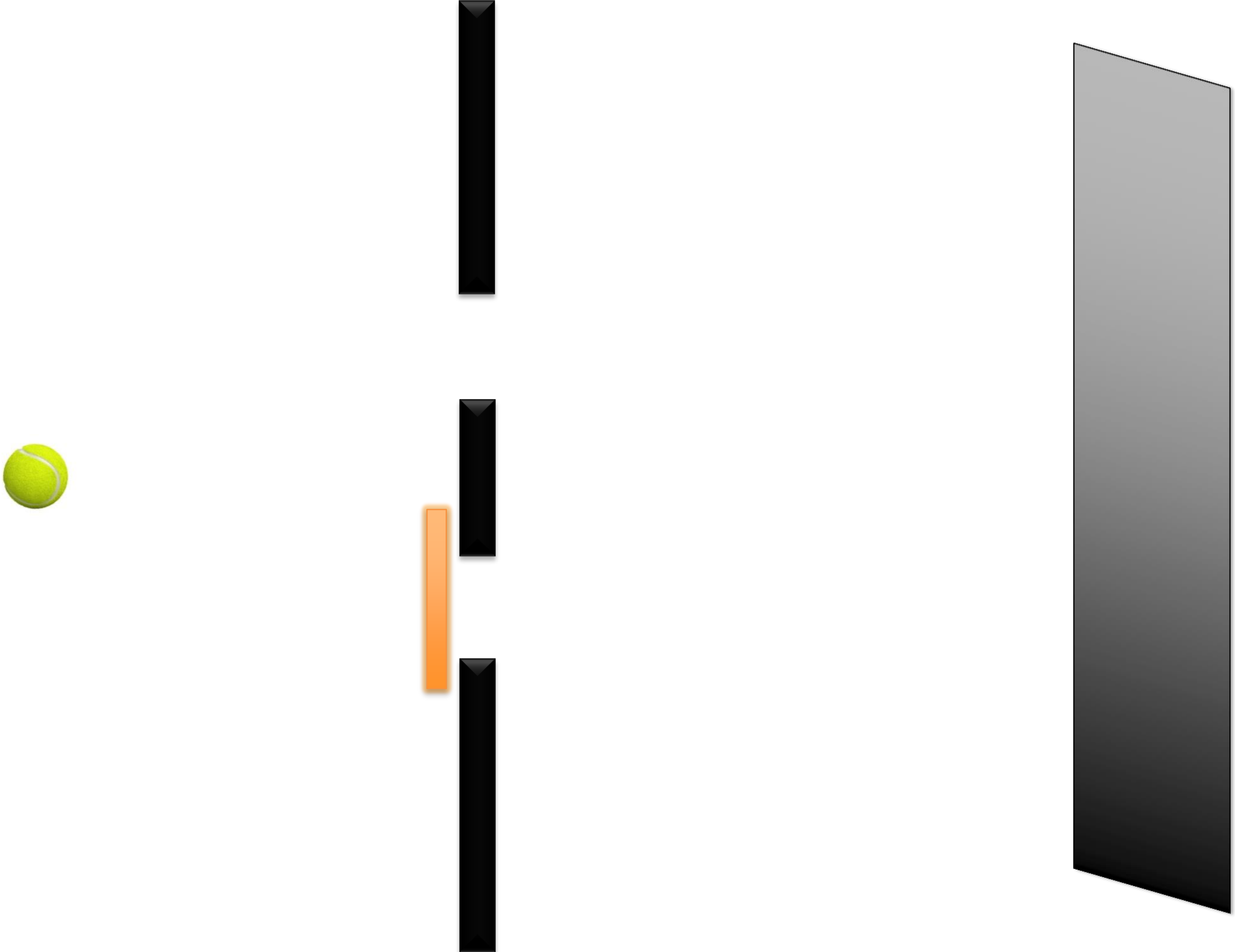
Probability

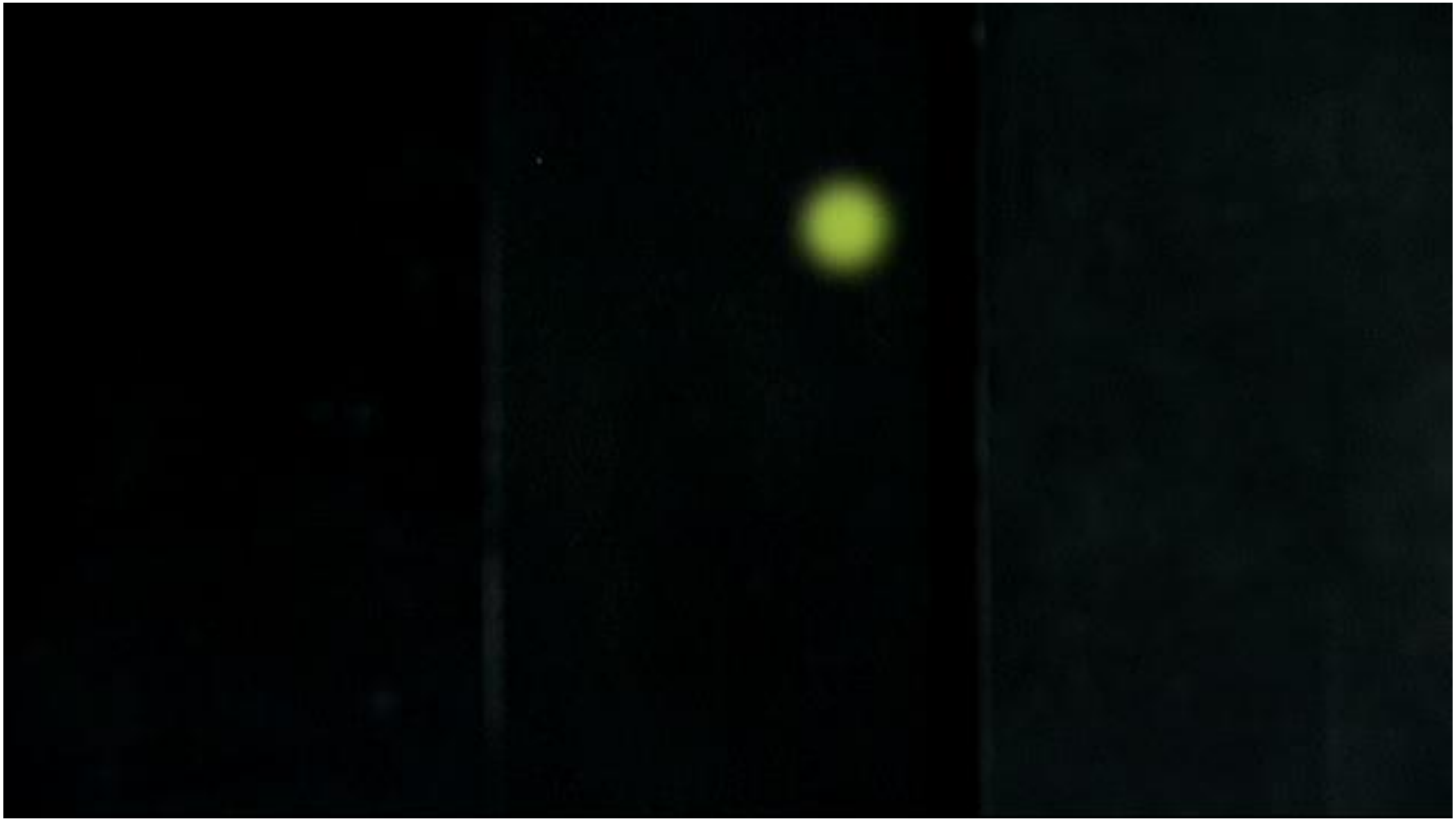


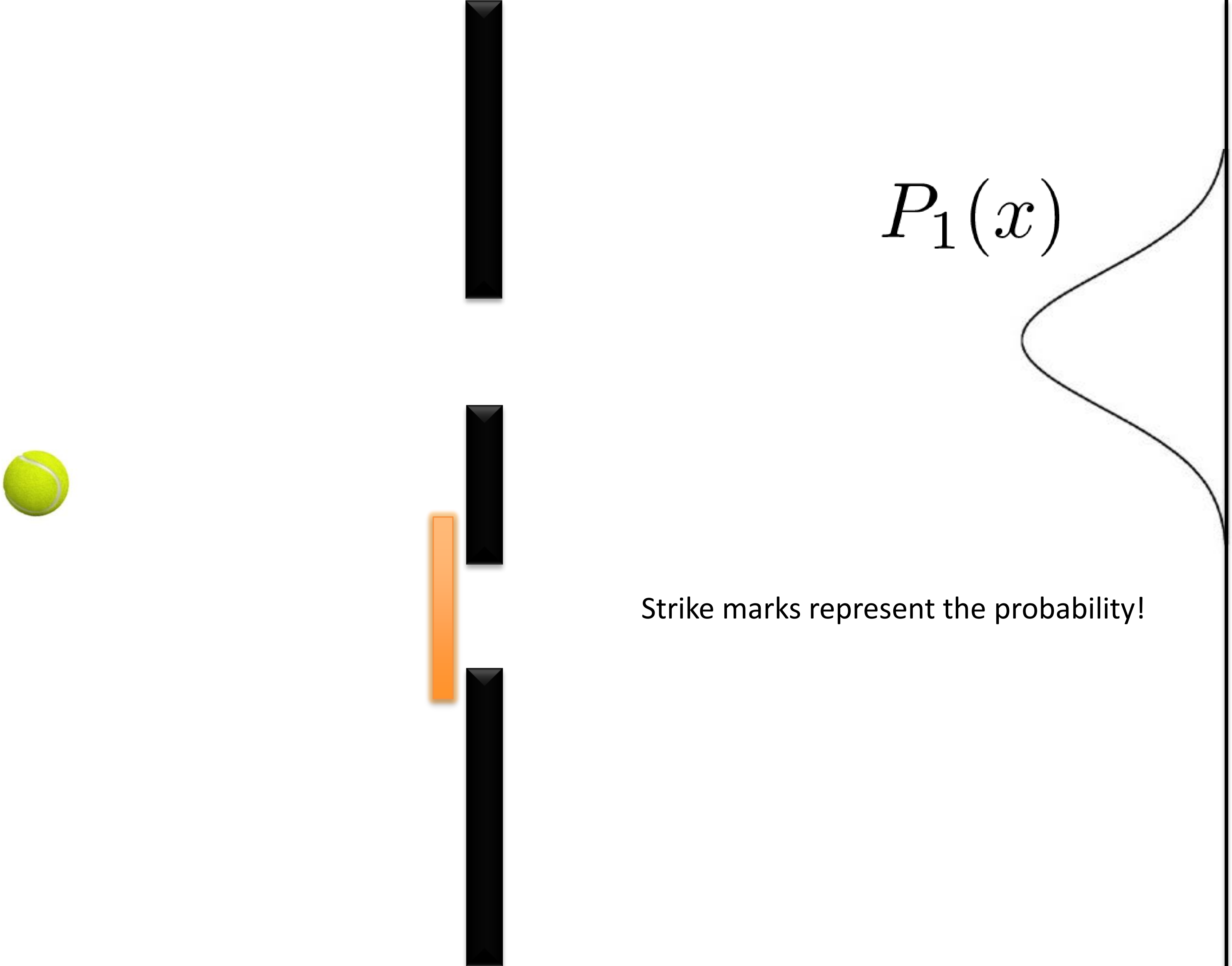
$$P(x)\Delta x$$

Probability a particle will hit a region with width Δx centered at pt. x

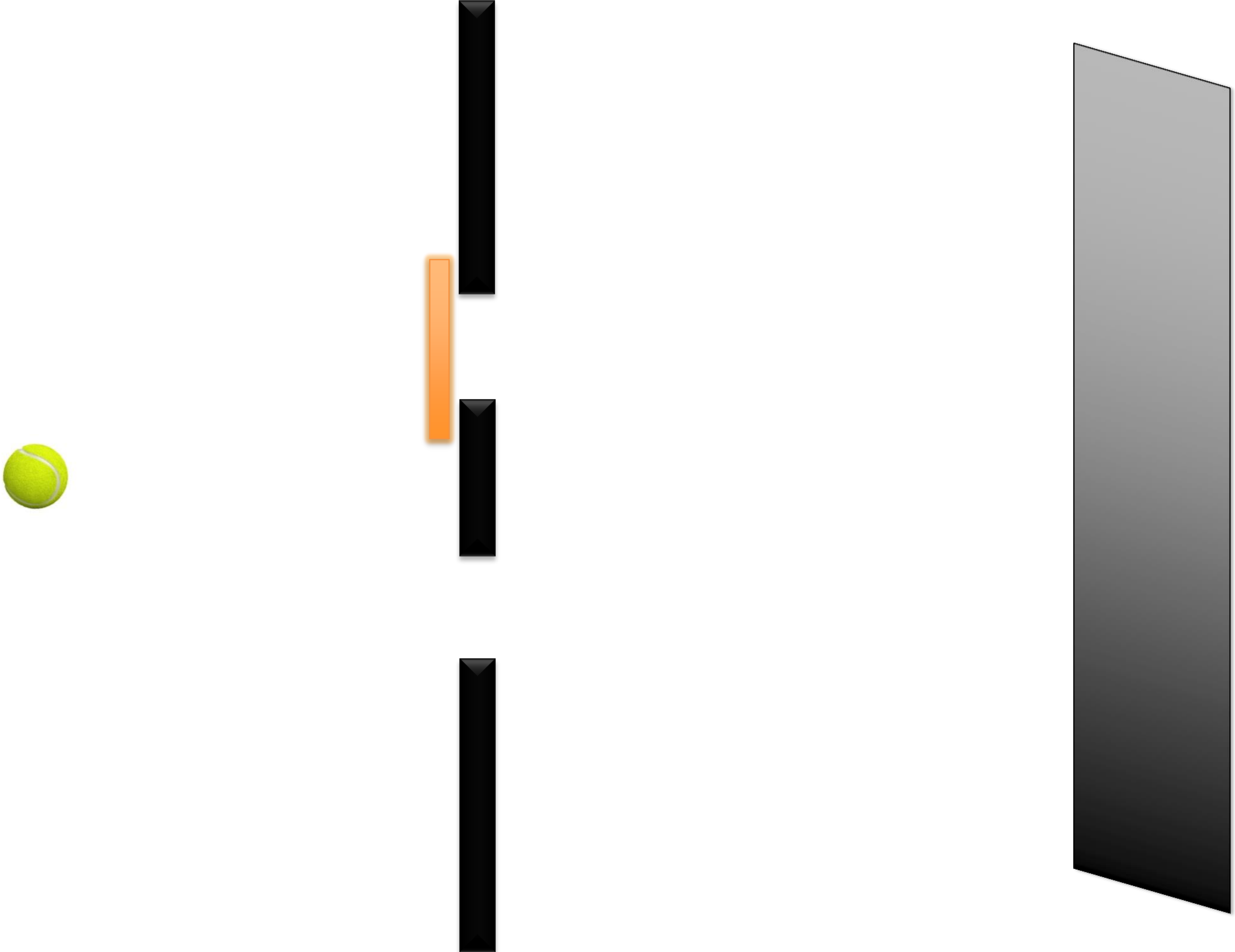
The sum of all such rectangles is the total area under the curve P(x). It represents the total probability that any given particle will hit somewhere on the screen, which must be 1 (100%).

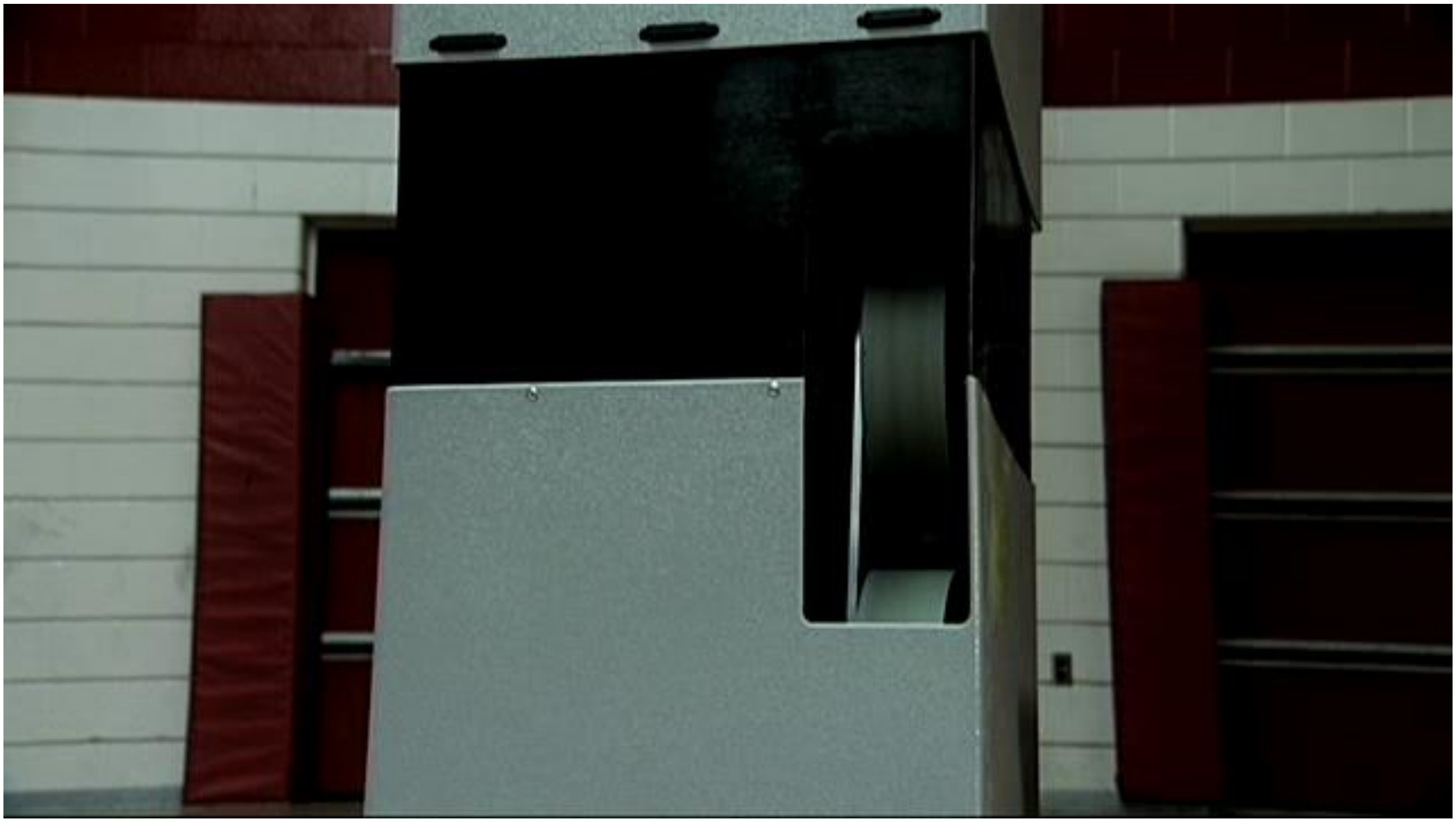


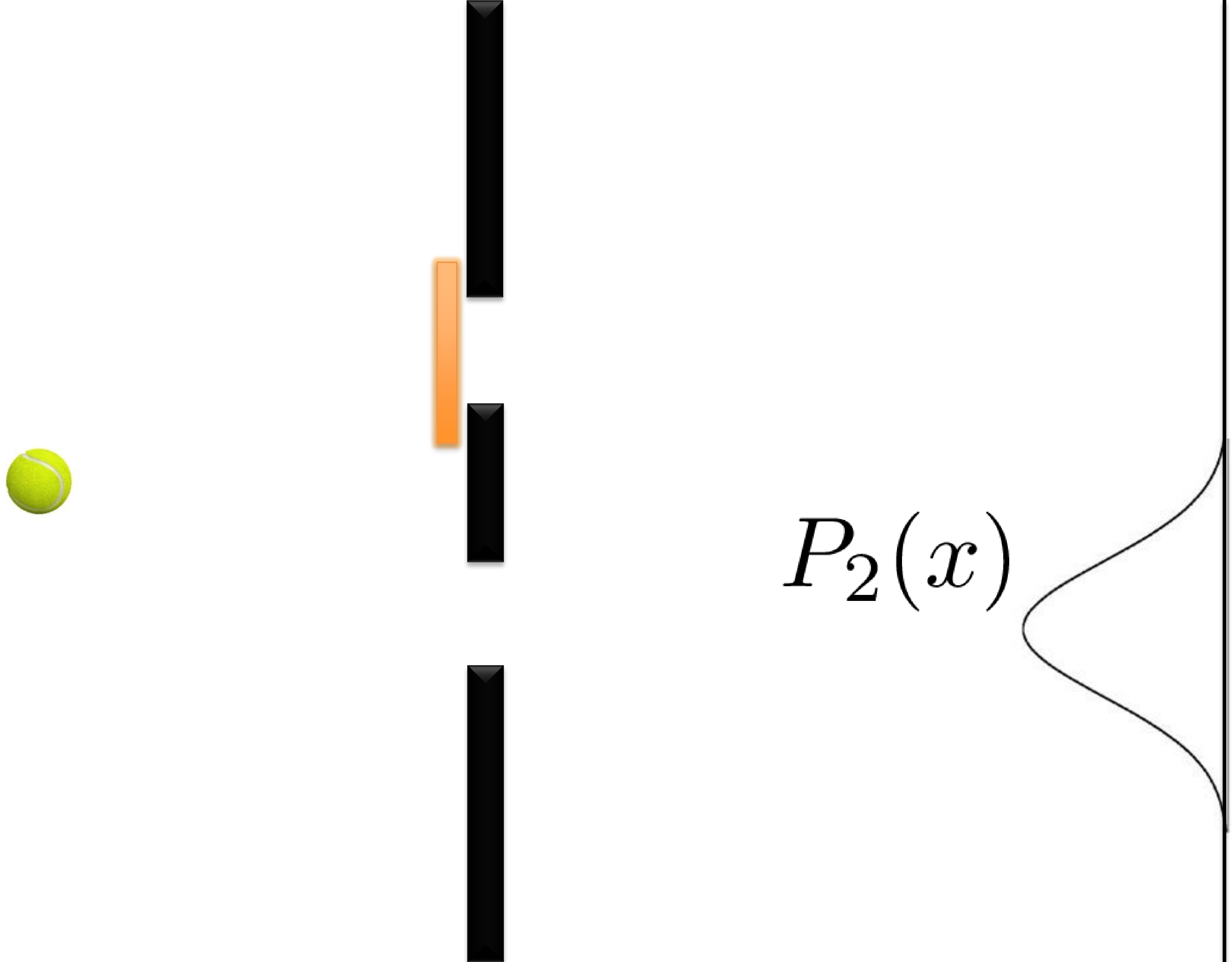




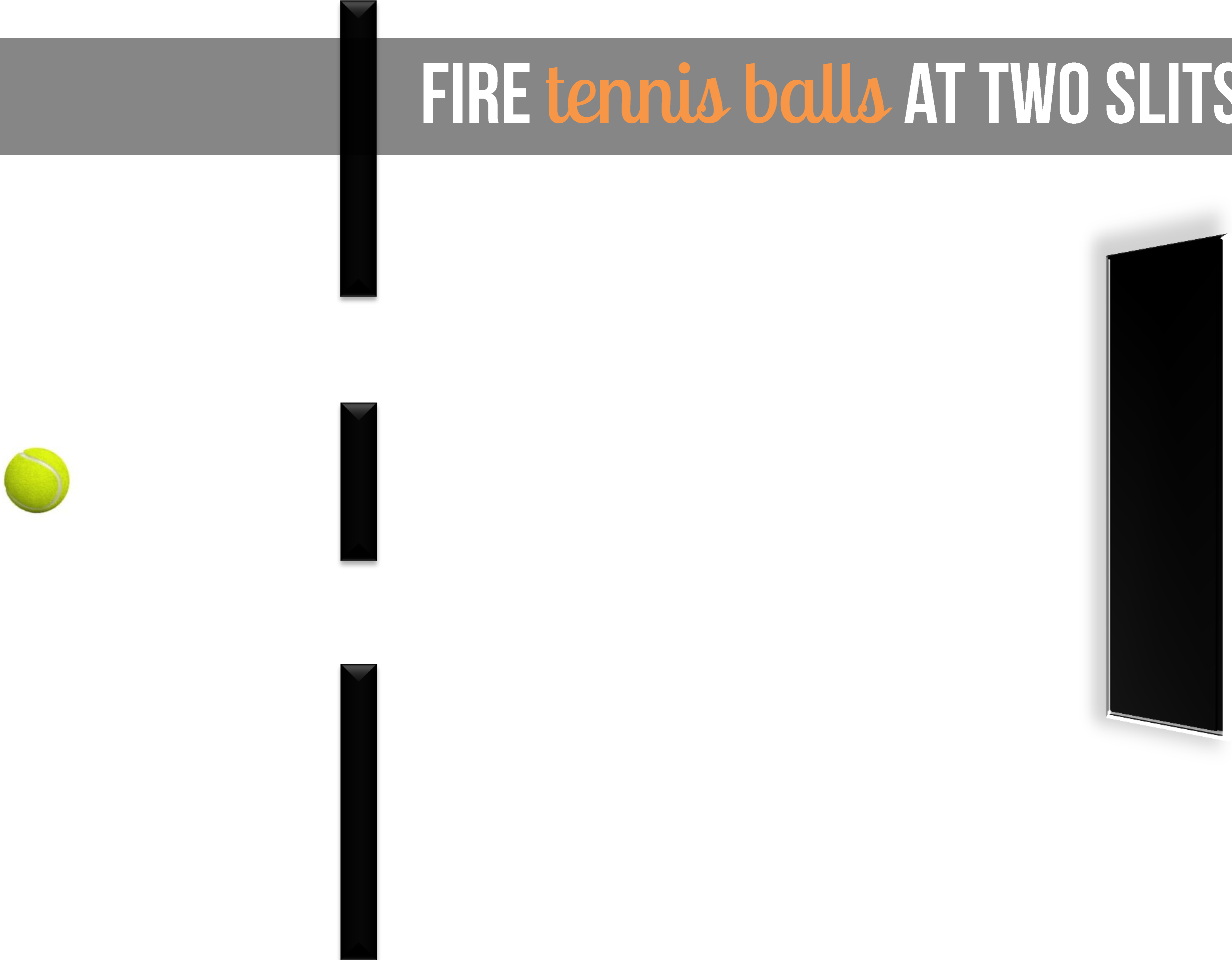
$P_1(x)$
Strike marks represent the probability!



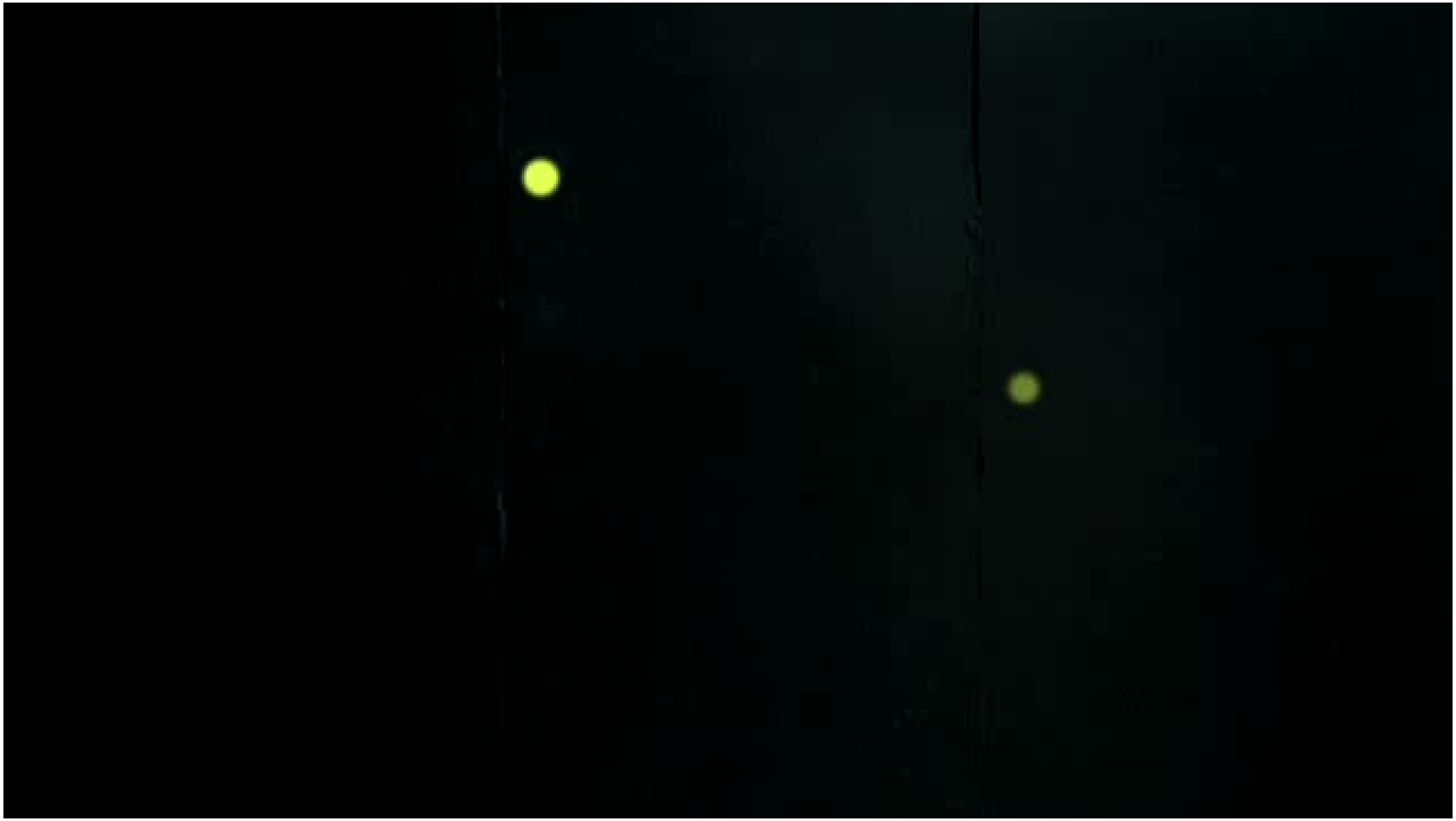


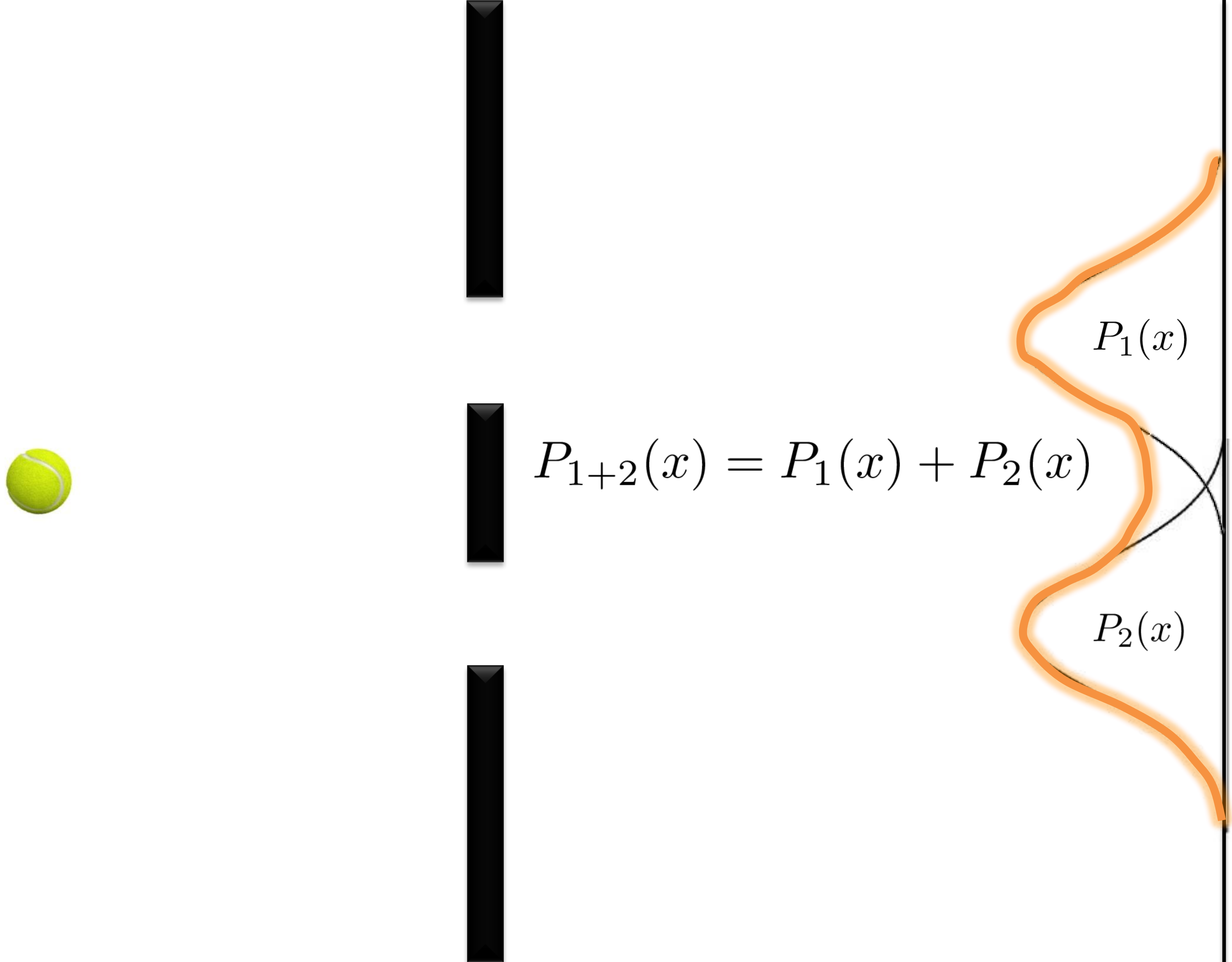

$P_2(x)$

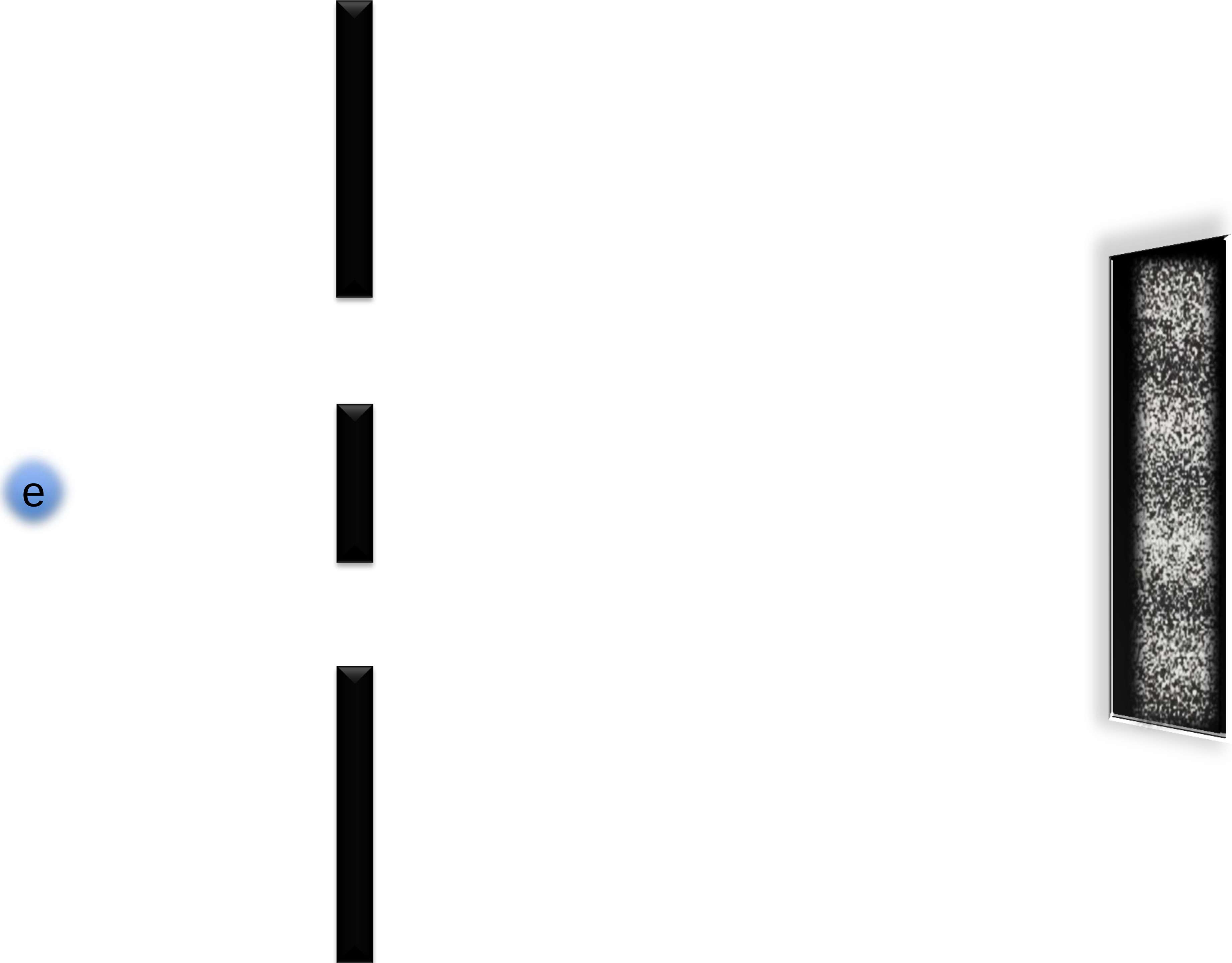
FIRE *tennis balls* AT TWO SLITS



TENNIS BALLS ARE localized




$P_1(x)$
$P_{1+2}(x) = P_1(x) + P_2(x)$
$P_2(x)$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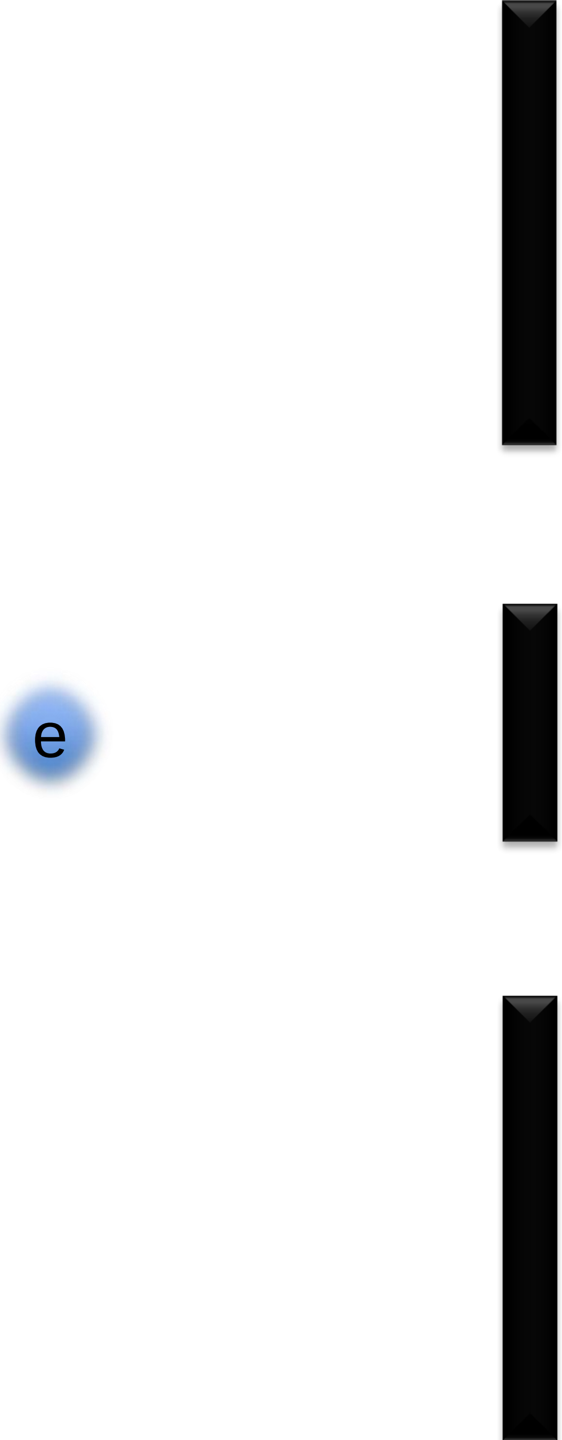
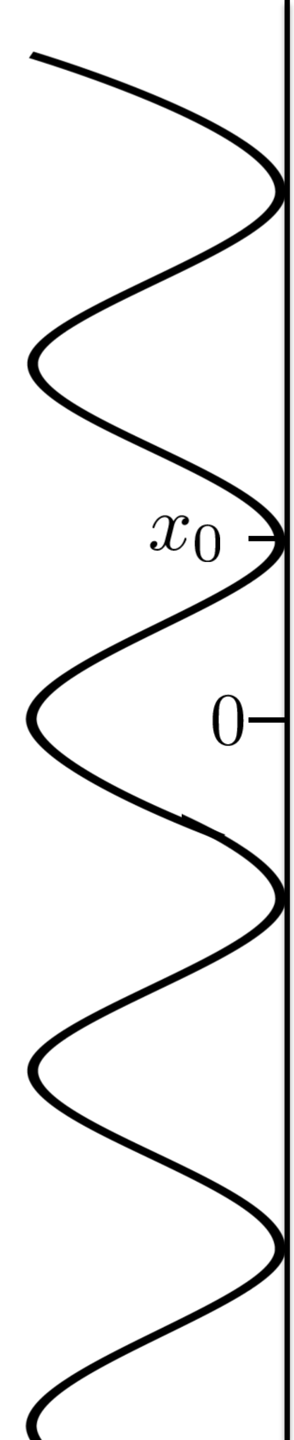


$$P_{1+2}(x) \neq P_1(x) + P_2(x)$$

There are places like x_0! When only 1 slit is open electrons hit there, but when both slits are open no electrons hit there!!!

How can this be???

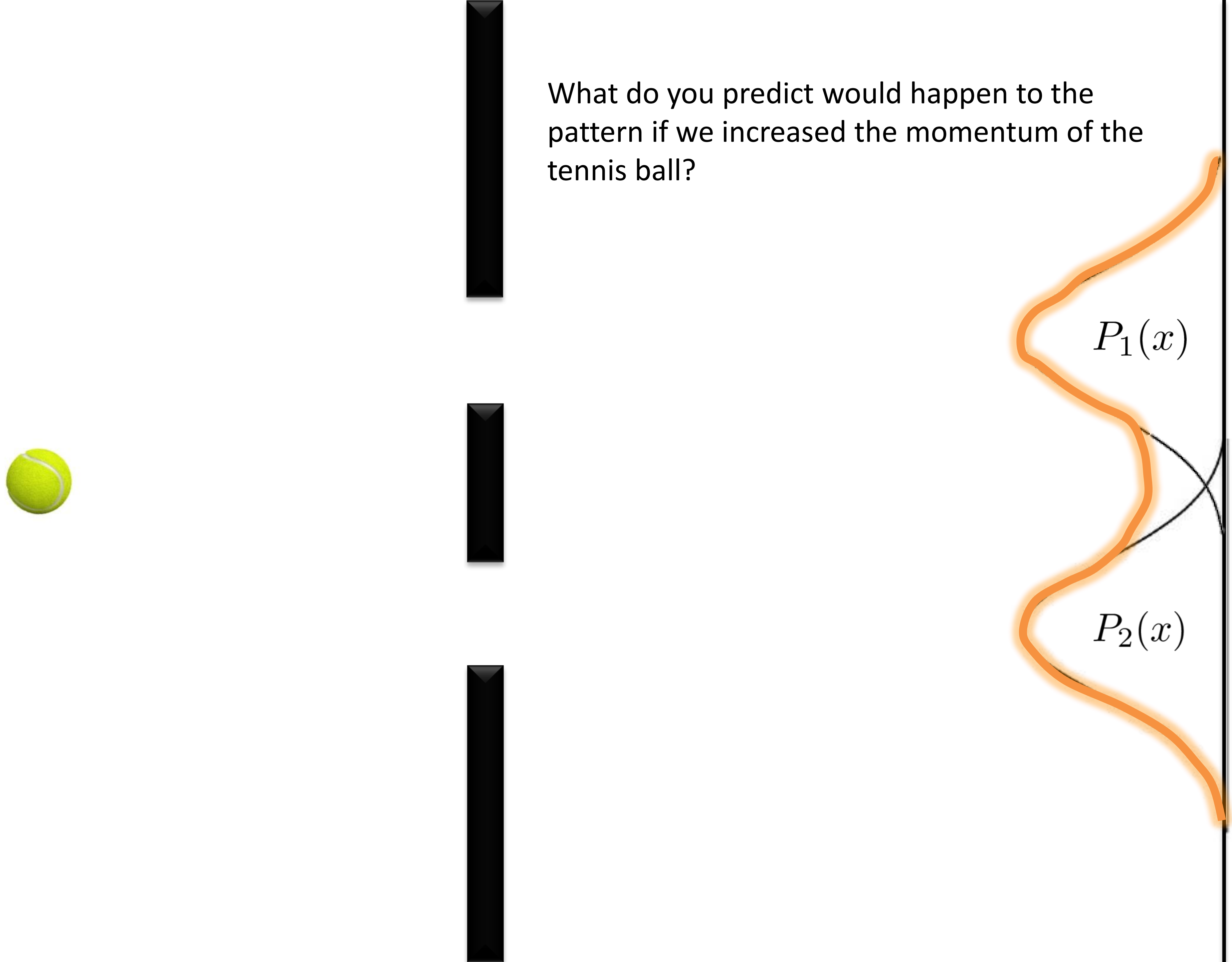


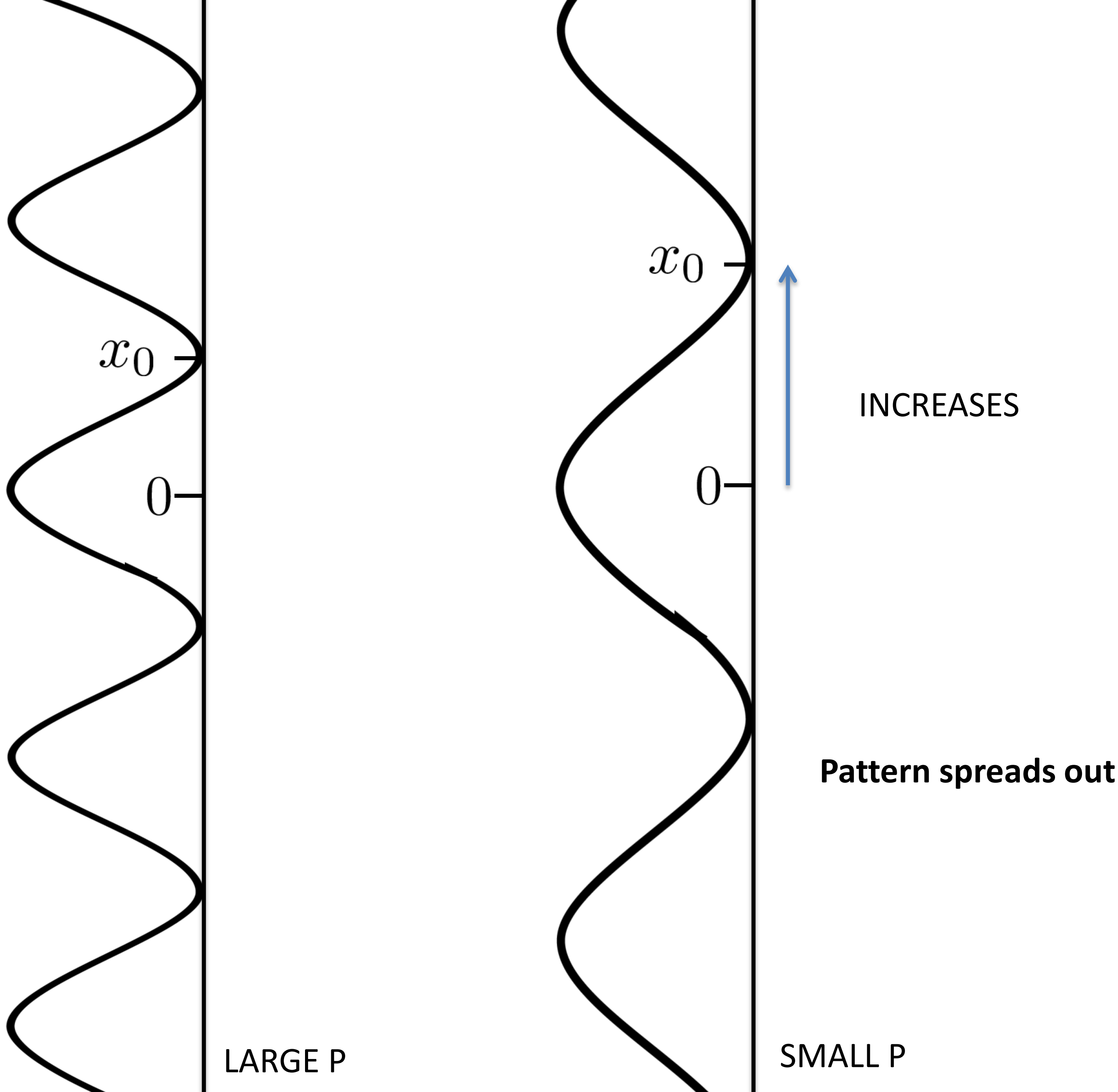
Can we explain electron behaviour with classical physics?

- Ricochet
- Non-contact force at slit edges
- Collisions

- Experiments show same results even when electrons are much smaller than slit, neutrons are employed and electrons are fired one at a time!

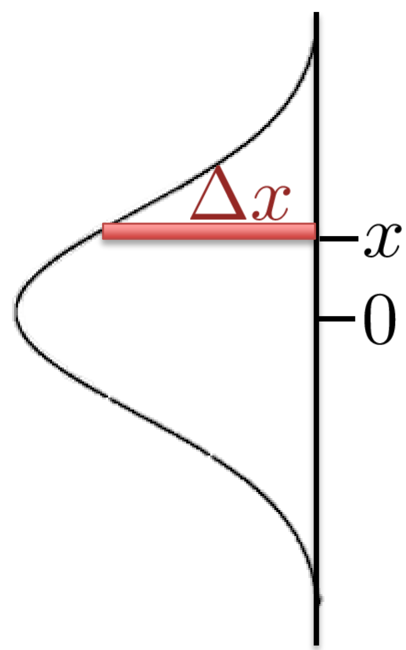
What do you predict would happen to the pattern if we increased the momentum of the tennis ball?




x_0
0
LARGE P
x_0
0
INCREASES
Pattern spreads out!
SMALL P

Probability Pattern

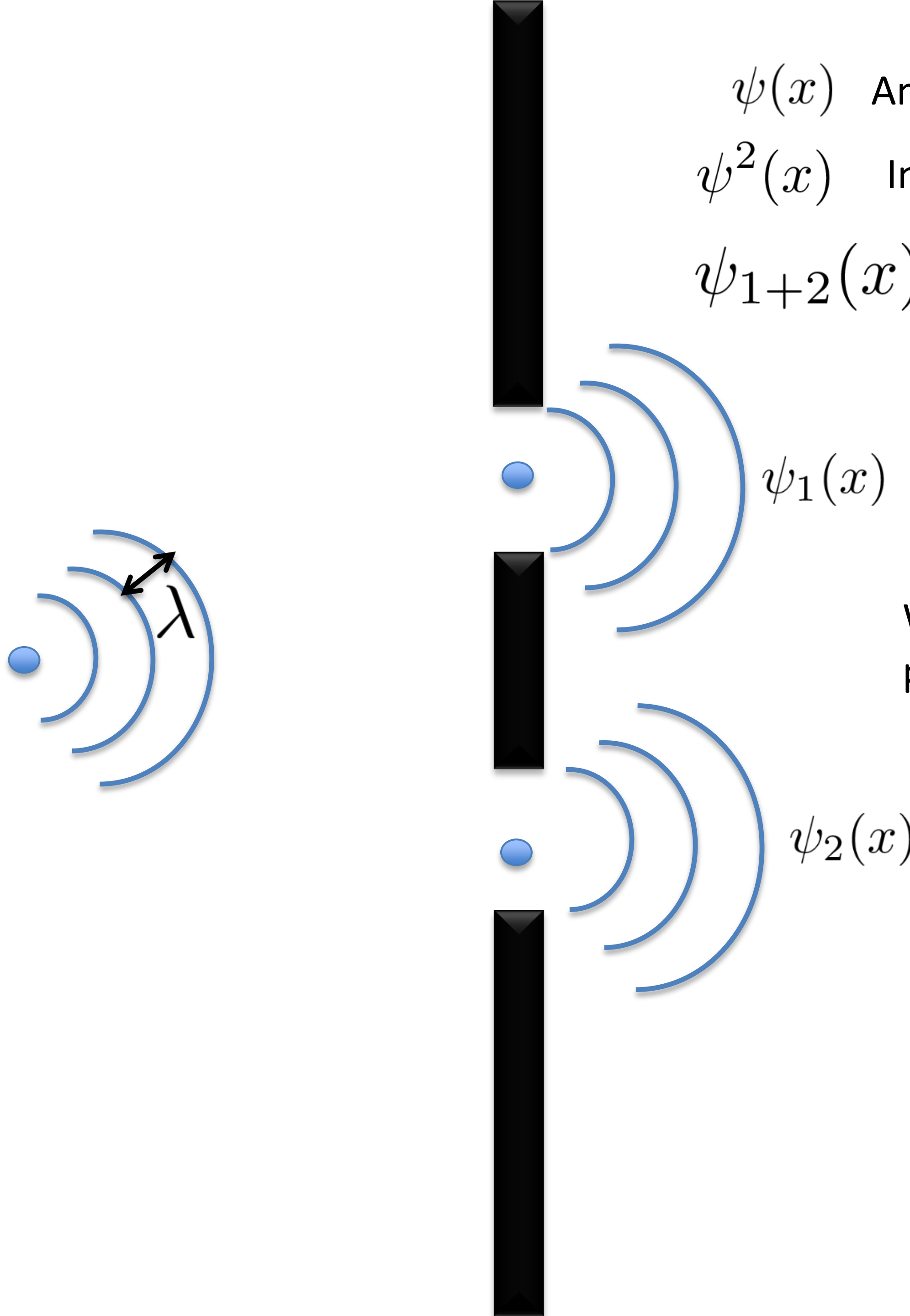
- As the momentum of the electrons is reduced, the probability pattern P(x) spreads out, but it must spread out in such a way the the total area under it remains equal to one.



$\psi(x)$ Amplitude of oscillation at x

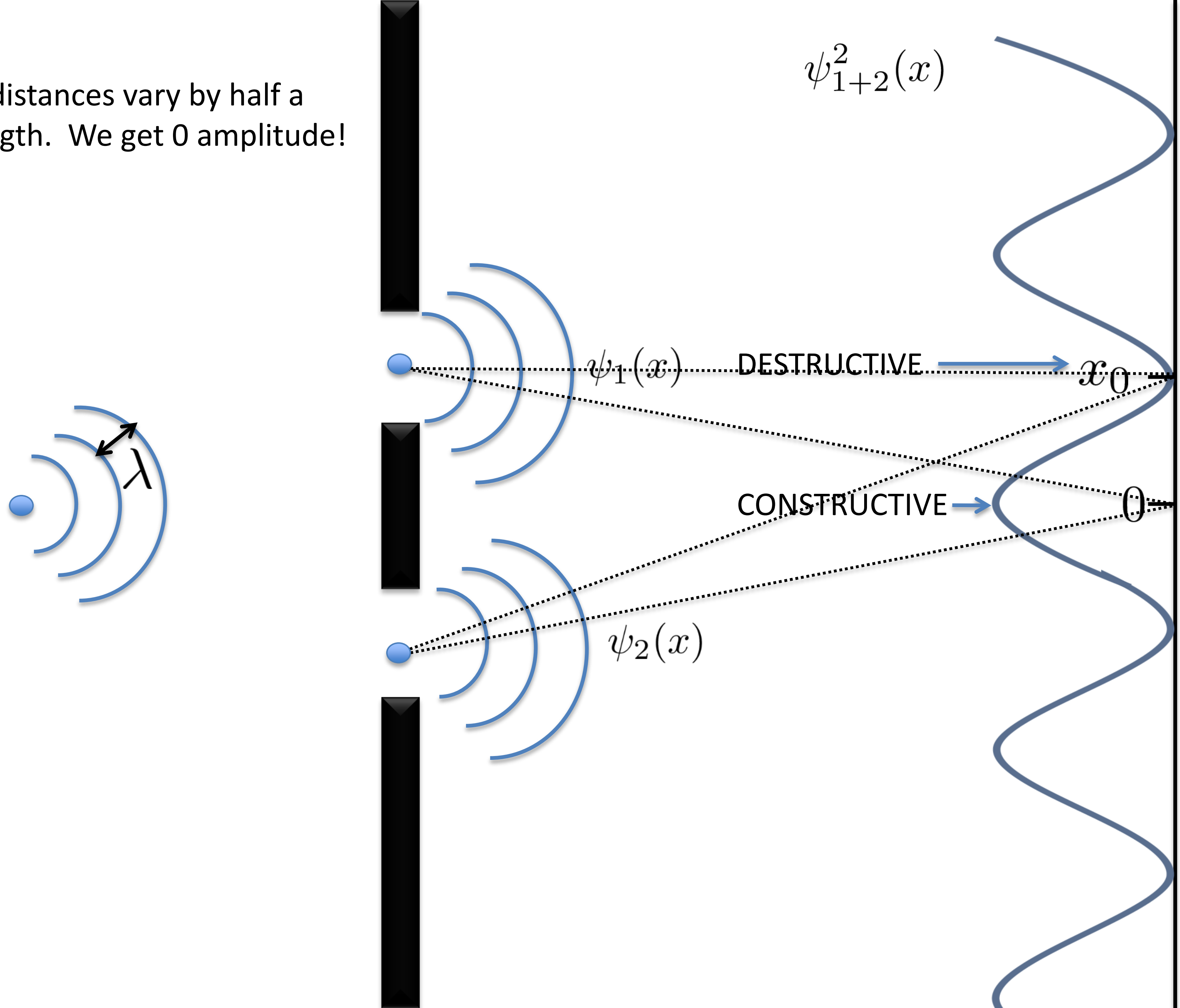
$\psi^2(x)$ Intensity of wave at x

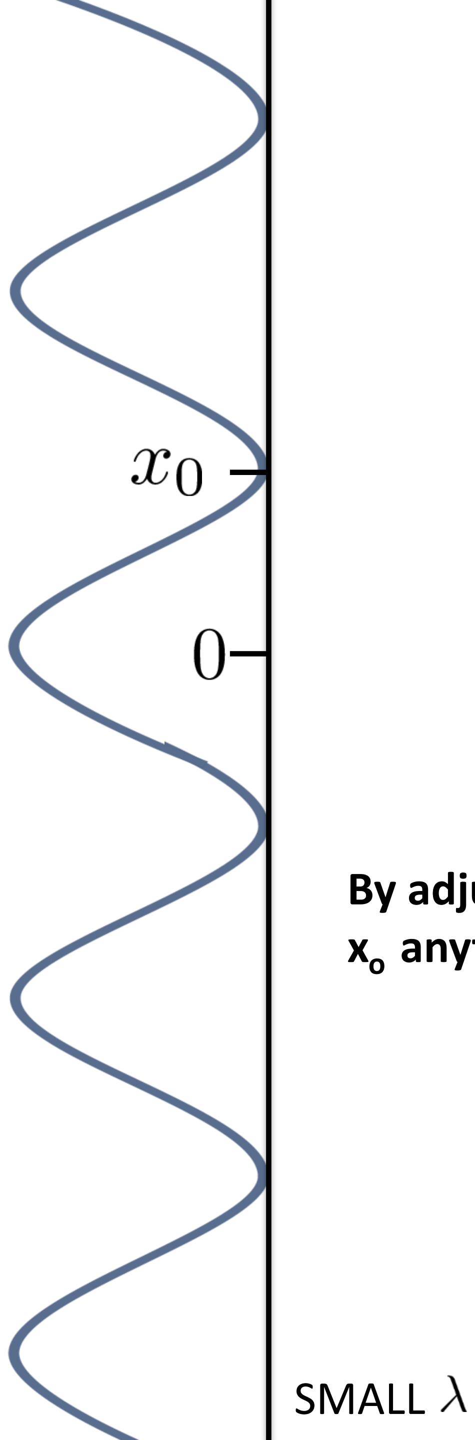
$$\psi_{1+2}(x) = \psi_1(x) + \psi_2(x)$$



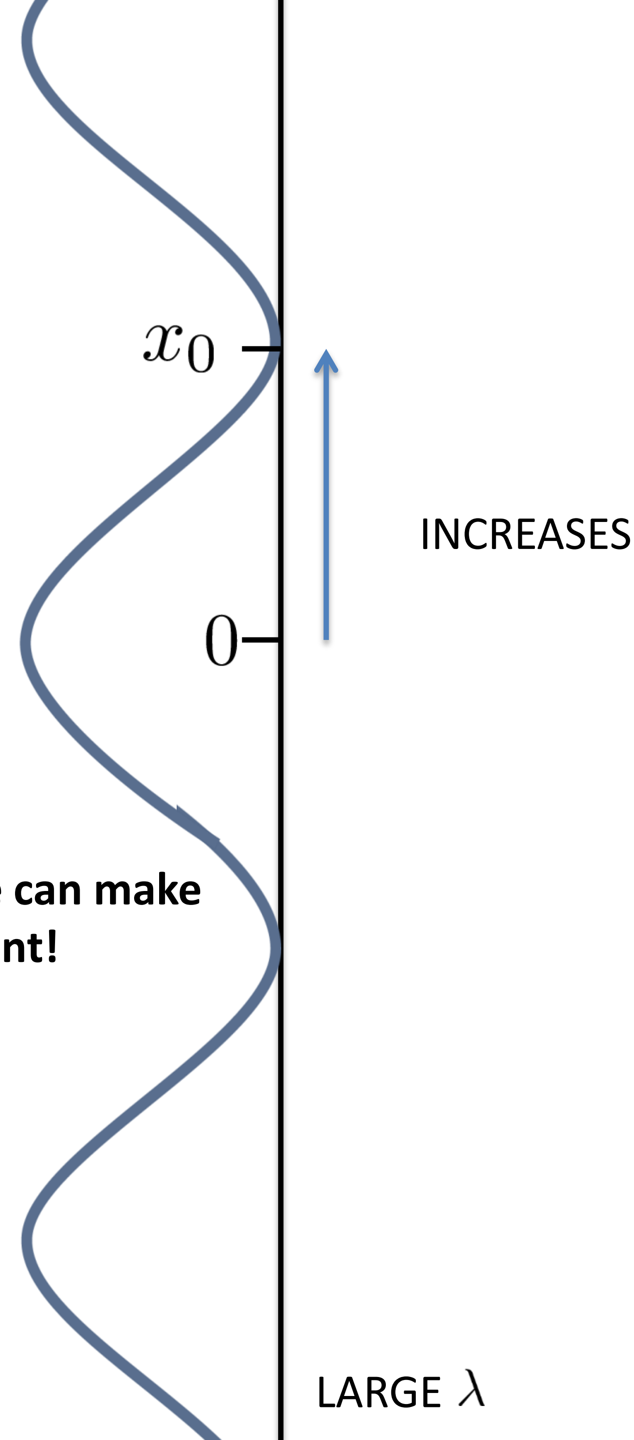
What will the wave intensity pattern $\psi^2_{1+2}(x)$ look like?

At $x=x_o$ distances vary by half a wavelength. We get 0 amplitude!





By adjusting λ we can make x_o anything we want!



- Detailed measurements show that given any double slit experiment with electrons of momentum p, a double slit experiment with waves can be set up such that $\psi^2(x)$ **exactly matches** the probability pattern $P(x)$!

Electrons are similar to Waves!

- Wave intensity is similar to electron probability $\psi^2(x) = P(x)$

- There seems to an inverse relationship between wavelength and momentum!

- We find $\lambda = \dfrac{h}{p}$

h is a proportionality constant!

How could you determine h?

- Experiment
  - Electrons with momentum p produce a pattern
  - Repeat with waves and find λ such that
    $$\psi^2(x) = P(x)$$
  - Given these values find $h = \lambda p$
- h is the same regardless of particle (electron, photons, neutrons) and no matter the momentum!

Planck's Constant

- We have a new fundamental constant!

$$h = 6.626068 \times 10^{-34} m^2 kg/s$$

Adding Wave Amplitudes

We saw that for e- $P_{1+2}(x) \neq P_1(x) + P_2(x)$

Let's see why!

We know from waves that wave amplitudes **add**!

$$\psi_{1+2}(x) = \psi_1(x) + \psi_2(x)$$

But *Particle Probabilities = Wave Intensity* (**square** of the amplitude)

$$P_{1+2}(x) = \psi_{1+2}^2(x)$$

$$\begin{aligned} P_{1+2}(x) &= [\psi_1(x) + \psi_2(x)]^2 \\ &= \psi_1^2(x) + \psi_2^2(x) + 2\psi_1(x)\psi_2(x) \\ &= P_1(x) + P_2(x) + 2\psi_1(x)\psi_2(x) \end{aligned}$$

CROSS TERM!

The cross term accounts for the difference!

Replacing F=ma

The double slit experiment shows us that particles like electrons do not obey F=ma from Newtonian mechanics.

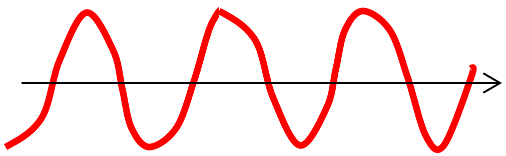
Instead they obey wave mechanics and the de Broglie relationship

$$F = ma \longrightarrow \lambda = \frac{h}{p}$$

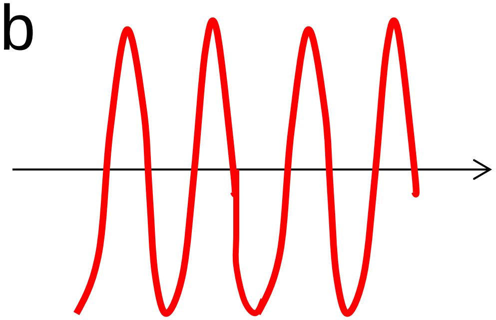
"What path does the particle follow?" → *"What is the probability the particle will hit here or there on the screen?"*

Three particles with equal mass are associated with the following matter waves. Rank, from largest to smallest, the speed of these particles.

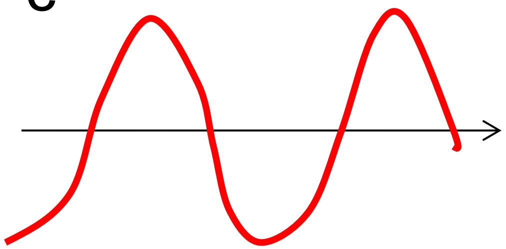
a



b



c



A. $v_a > v_b > v_c$

B. $v_b > v_c > v_a$

C. $v_a > v_c > v_b$

D. $v_b > v_a > v_c$

E. $v_c > v_a > v_b$

A bullet is fired from a rifle. The end of the rifle is a circular aperture. Is diffraction a measurable effect?

A. No, because only charged particles have a de Broglie wavelength.
B. No, because a circular aperture never causes diffraction.
C. No, because the de Broglie wavelength of the bullet is too large.
D. No, because the de Broglie wavelength of the bullet is too short.
E. Yes

Photons

We see waves behaving like particles!

De Broglie Relation For Photons

- Einstein's famous equation $E = mc^2$ expresses the equivalence of mass and energy for particles at *rest*.

- For particles with motion (momentum, p), the full equation reads:

$$E = \sqrt{m^2c^4 + p^2c^2}$$

- Photons are moving but have zero rest mass, so the equation reduces to $E = cp$

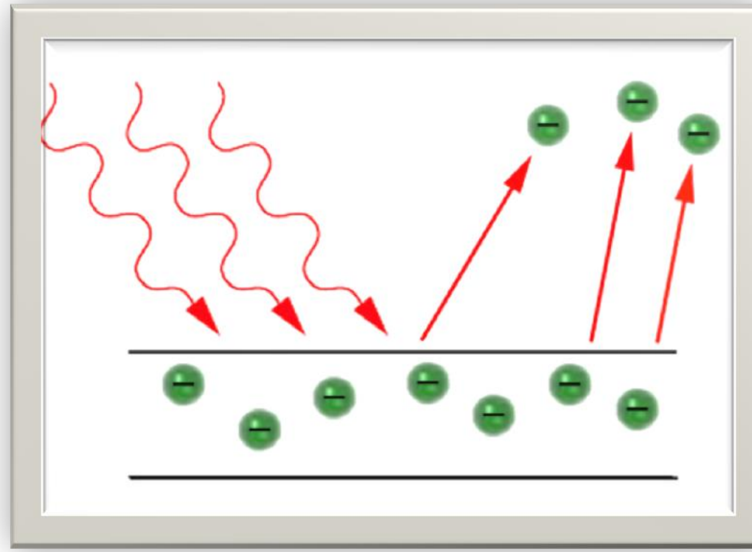
- **Photons have momentum!**

De Broglie Relation For Photons

- Combine $E = cp$ with the de Broglie relation and simplify using the universal wave equation $c = f \times \lambda$ to find the relation between the **energy** of a photon and its **frequency**.

- Which colour of photon requires more energy to produce: red (low-frequency) or blue (high-frequency)? Why?

EINSTEIN'S IDEA - Photons



SUMMARY

Sand and tennis balls are *classical* particles that obey Newton's law: $F = ma$. A force is needed to deflect their trajectory.

Electrons are *quantum* particles that obey the de Broglie relation: $\lambda = h/p$. As happens in *wave diffraction*, just passing through a hole can deflect their trajectory!

Electrons also exhibit *wave interference*. A single electron passing through two or more holes interferes *with itself*!

Photons are also quantum particles that obey the de Broglie relation: $\lambda = h/p$. This relation can be rewritten as $E = hf$.

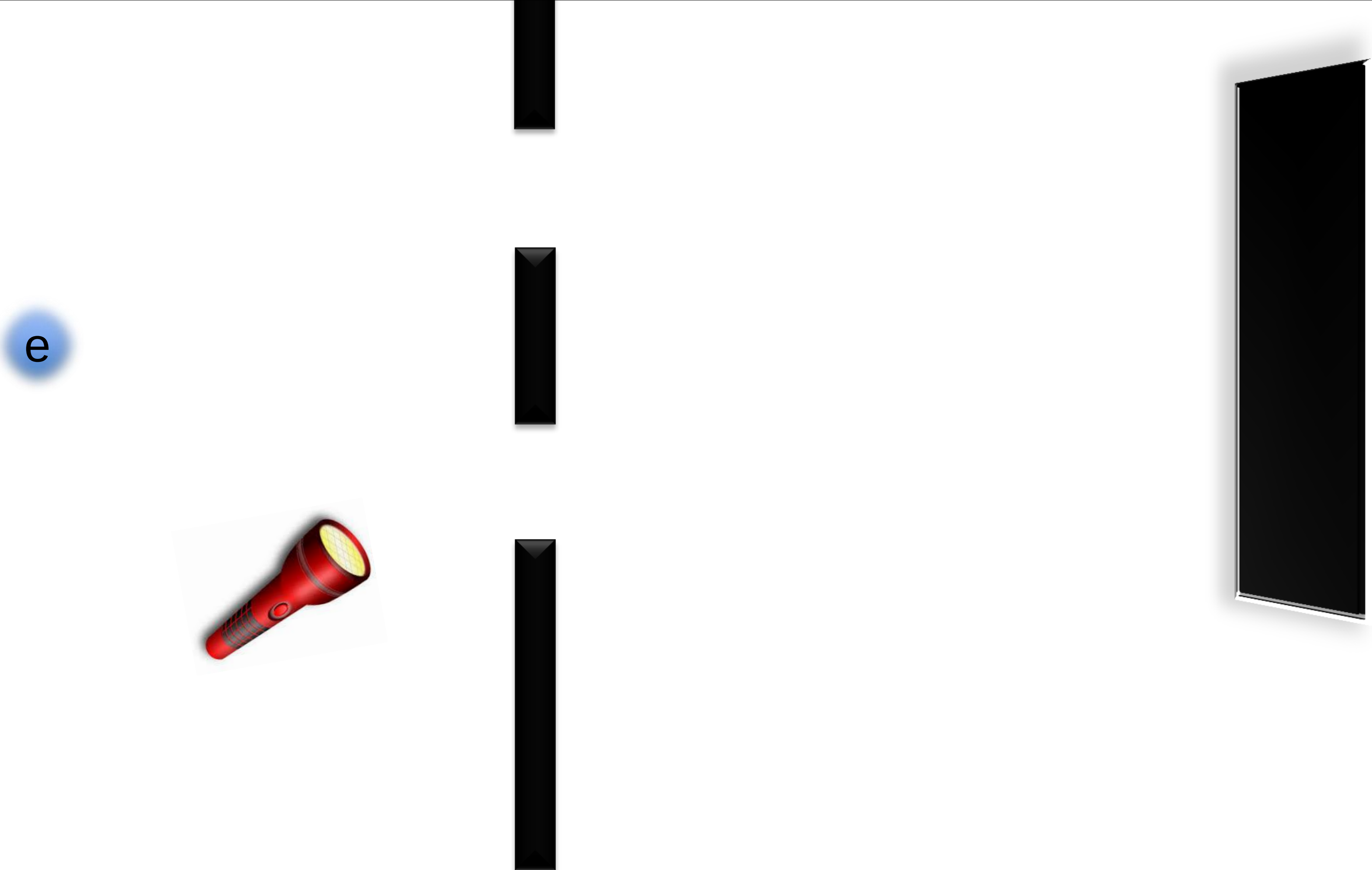
All matter and radiation is made of quantum particles that obey the *same* universal law: $\lambda = h/p$.

We can think of quantum particles as **particles behaving like waves** (e.g., electrons diffracting and interfering), or as **waves behaving like particles** (e.g., light hitting the screen as individual particles).

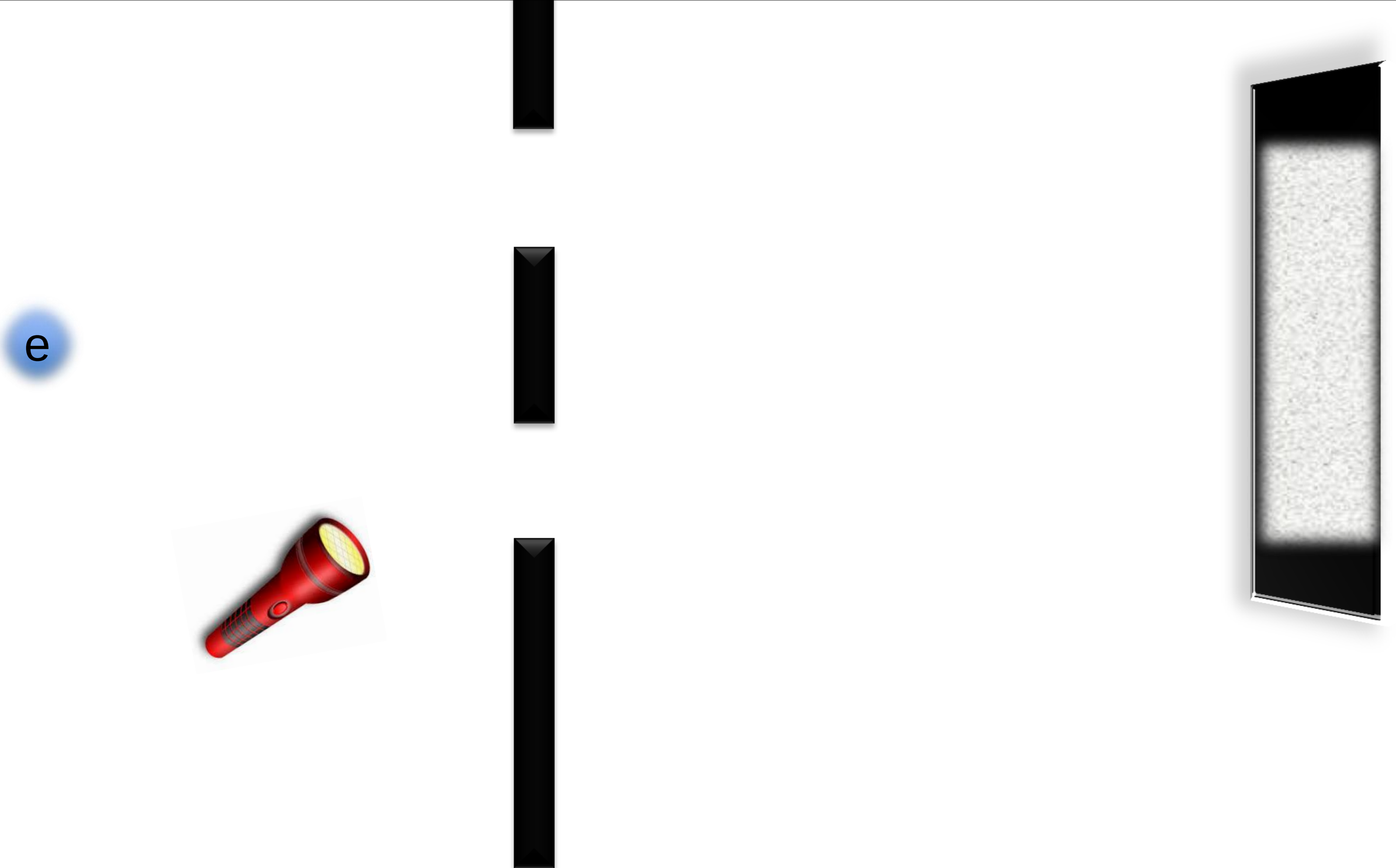
This *wave-particle duality* represents one of the most important discoveries (and mysteries!) in all of science.

WHAT IS THE ELECTRON doing?

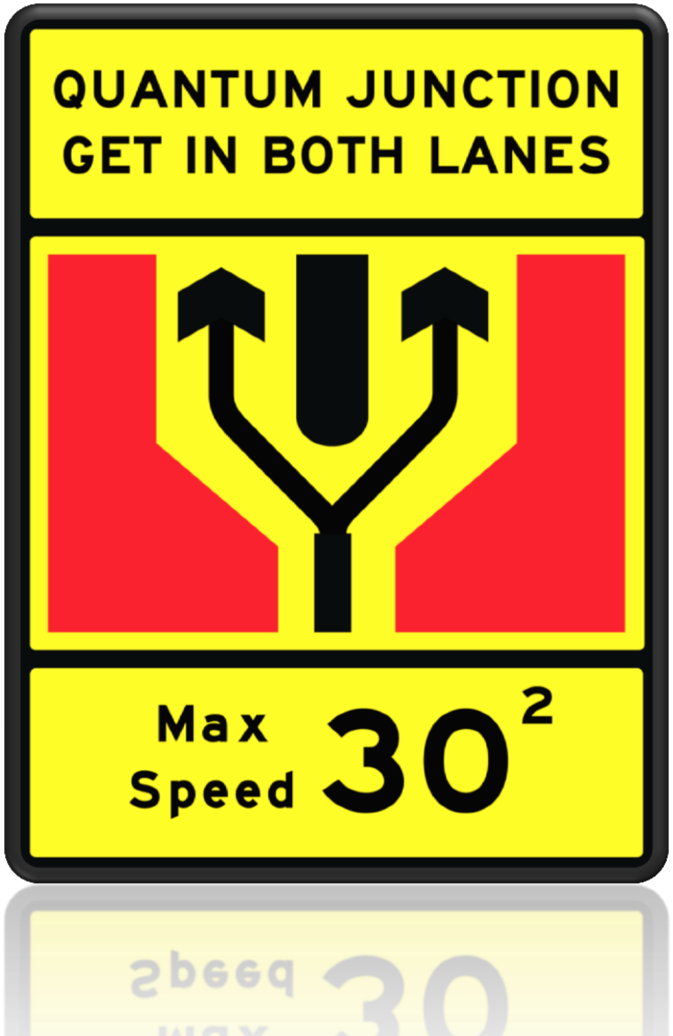
LET'S HAVE A look!



Interference pattern disappears!



QUANTUM Superposition



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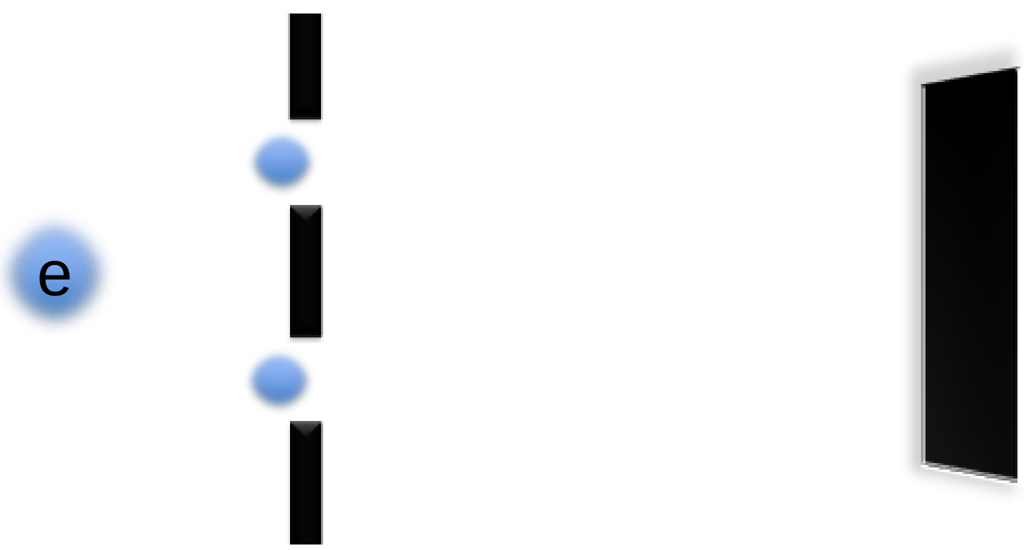
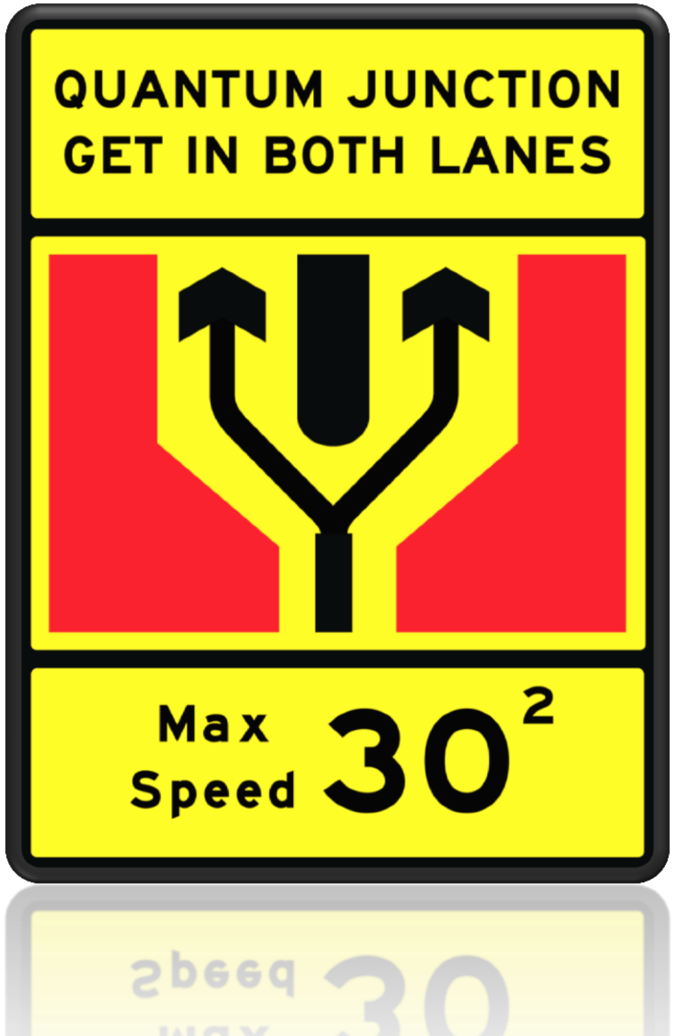
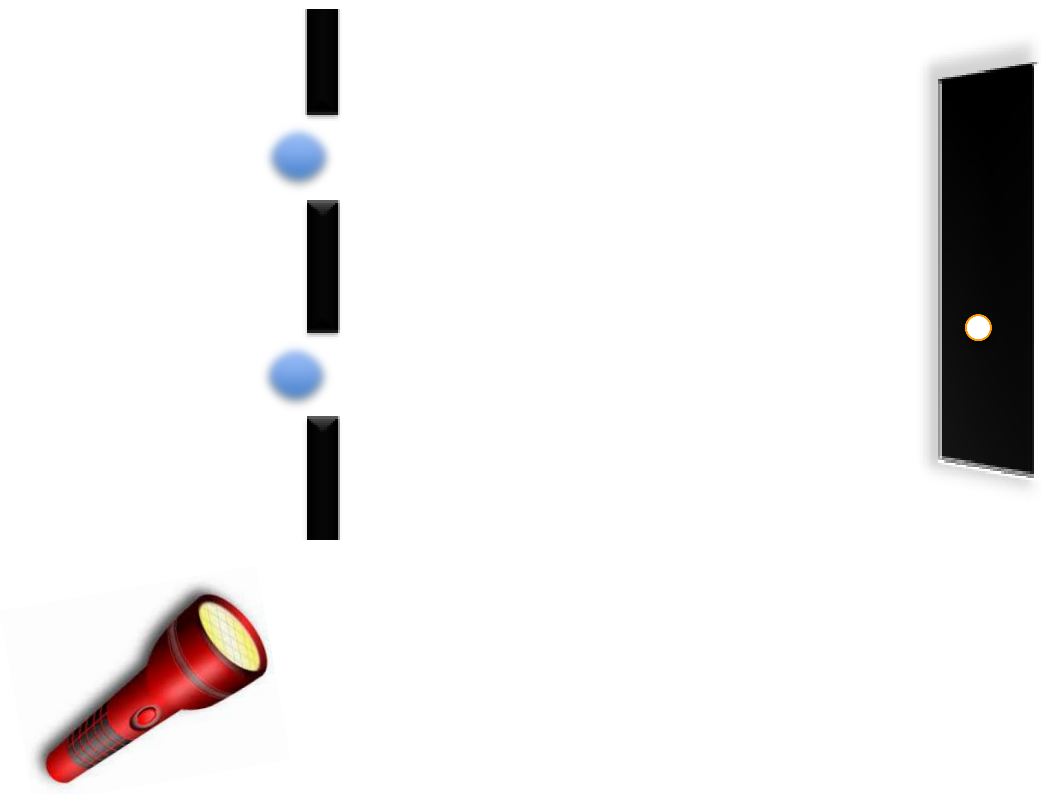
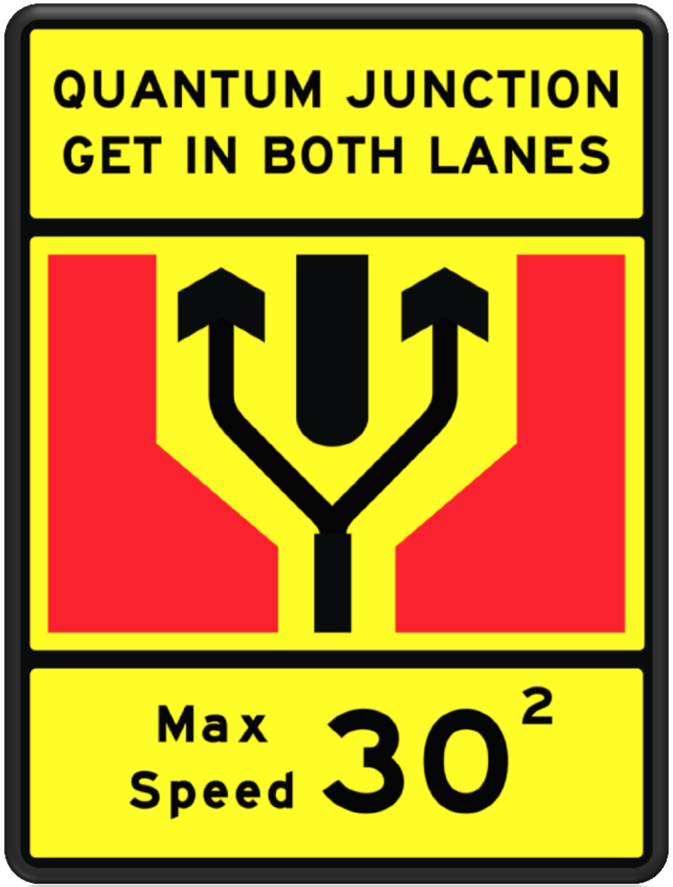




QUANTUM Superposition



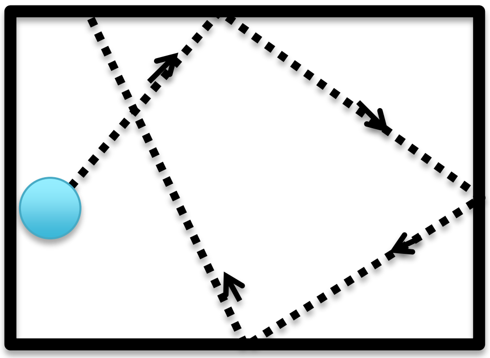


Quantum Interpretations

- Collapse
- Pilot Wave
- Many Worlds
- Copenhagen

- See D2L page

Classical Particle in a Box



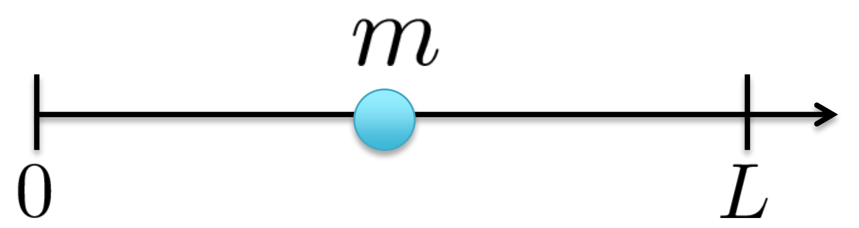
$$F = ma$$

Bounce in Perpetual Motion

But how does a quantum particle behave with this new quantum law $\lambda = \dfrac{h}{p}$?

Trap a Particle in a 1D Box

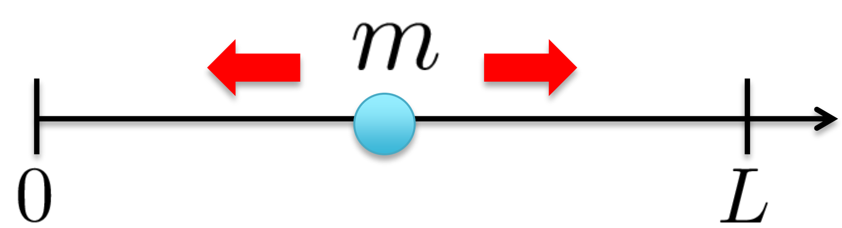
Suppose the particle as a definite energy E



What can be said about the particle's momentum?

Trap a Particle in a 1D Box

What can be said about the particle's momentum?



$$E = \frac{1}{2}mv^2 \quad \Longrightarrow \quad E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

$$p = \cancel{\sqrt{2mE}}$$

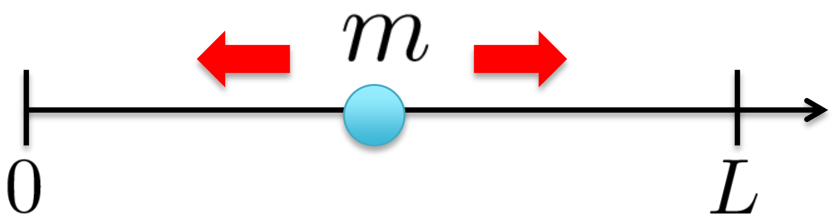
$$p = \pm\sqrt{2mE}$$

(right/left)

Classically, the particle behaves like a lump either moving left or right.

Trap a Particle in a 1D Box

What do we learn by using the de Broglie relation? $\lambda = \frac{h}{p}$



$$p = \pm\sqrt{2mE}$$

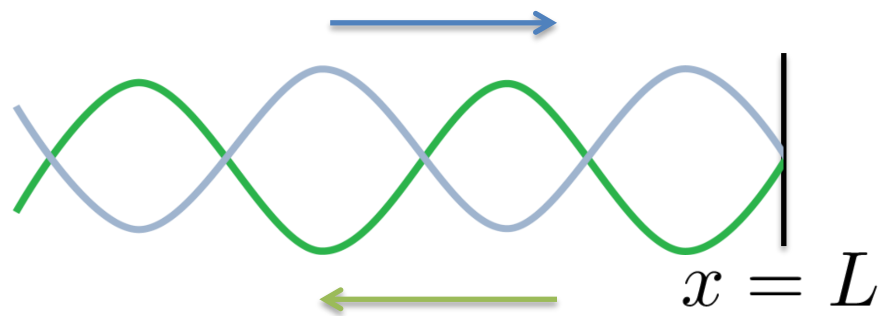
(right/left)

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$|p|$

What happens when an incident wave strikes a barrier?

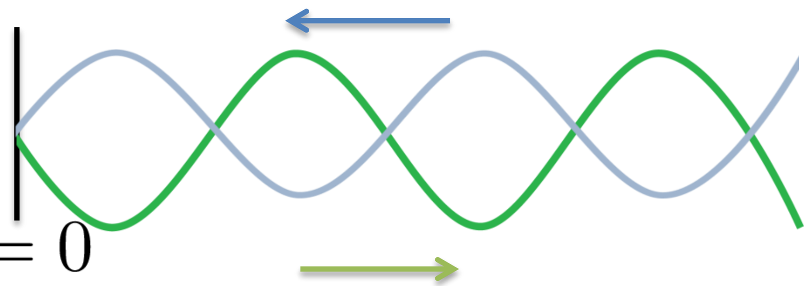
$$p = +\sqrt{2mE}$$



Reflected wave: $p = -\sqrt{2mE}$

What happens when an incident wave strikes a barrier?

$$p = -\sqrt{2mE}$$

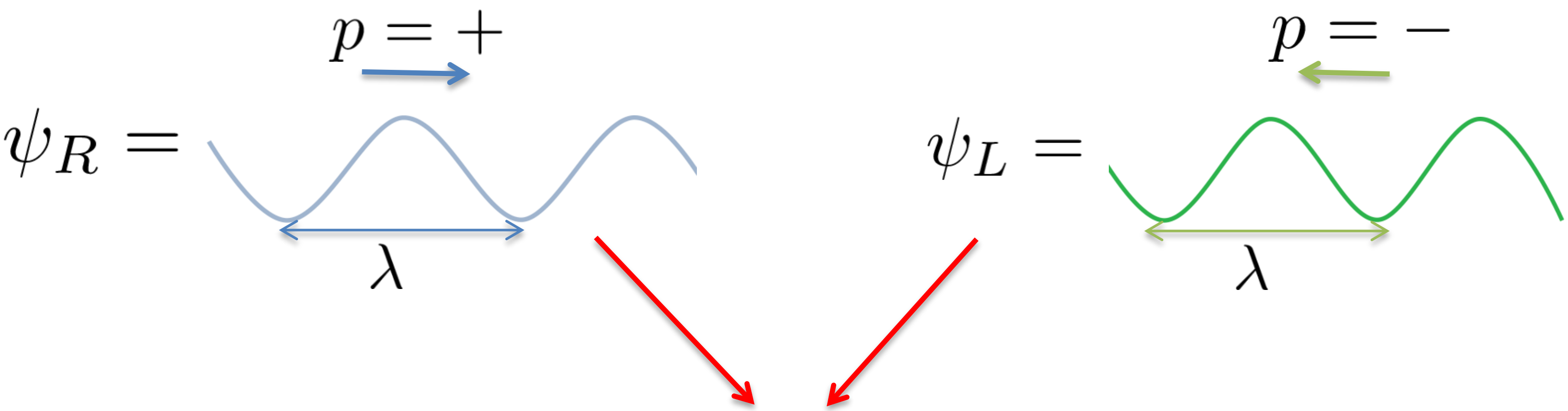


$$x = 0$$

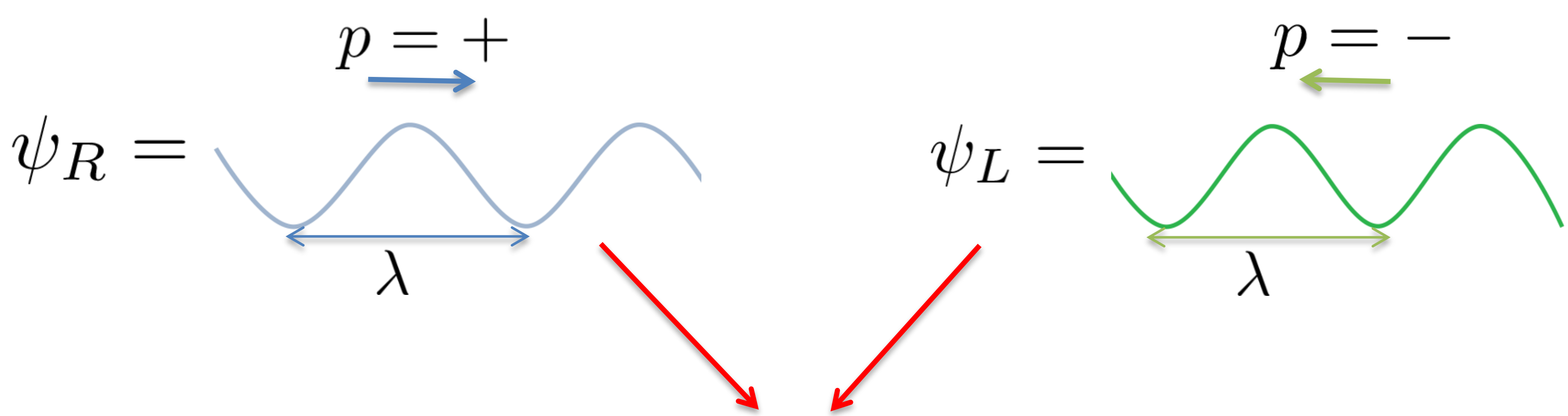
Reflected wave: $p = +\sqrt{2mE}$

The quantum view shows that the particle is not localized to one spot.

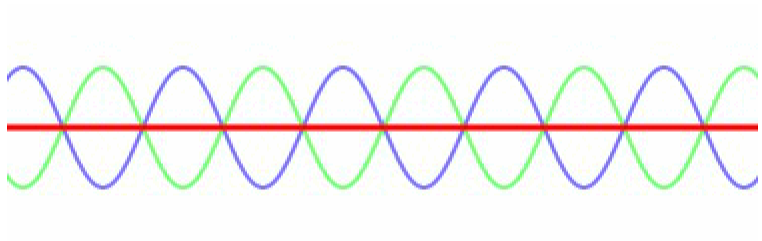
The wave spreads throughout the box with the right-moving wave being the source of the left moving wave and vice-versa.



$$\psi = \psi_L + \psi_R$$



$$\psi = \psi_L + \psi_R$$



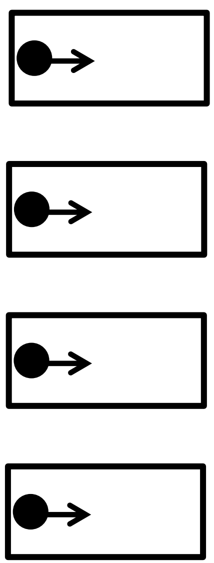
Standing Wave: Two traveling waves (left & right) which are present simultaneously in the same space. The two waves are in ***superposition***.

At any given instant the particle is neither moving left nor right. It is moving both ways at the same time!

$$\psi = \psi_L + \psi_R$$

Weird! ***At any given instant the particle is neither moving left nor right. It is moving <u>both</u> ways at the same time!***

<u>Classically</u> Lay out many boxes with particles all in the same initial state.

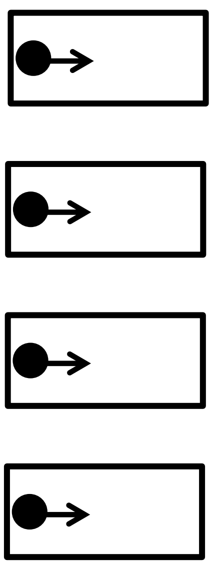


If we measure some time later they will all be in the same state or place.

$$\psi = \psi_L + \psi_R$$

Weird! ***At any given instant the particle is neither moving left nor right. It is moving both ways at the same time!***

Quantum Lay out many boxes with particles all in the same initial state.



If we measure some time later we get perfectly random result! 50/50 odds for either left or right moving particle.

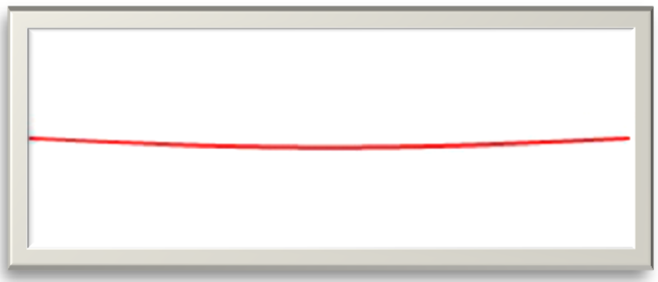
Collapse of the Wave Function ψ

- Double slit experiment: particle behaves like it is passing through both slits at once.
- If we measure we force it to decide where it is.
- Not a physical wave, but a mathematical wave that describes the *probability* we will observe the particle here or there.
- When we measure, the wave describing the state of the particle goes from spread out to *localized*.

Standing Waves

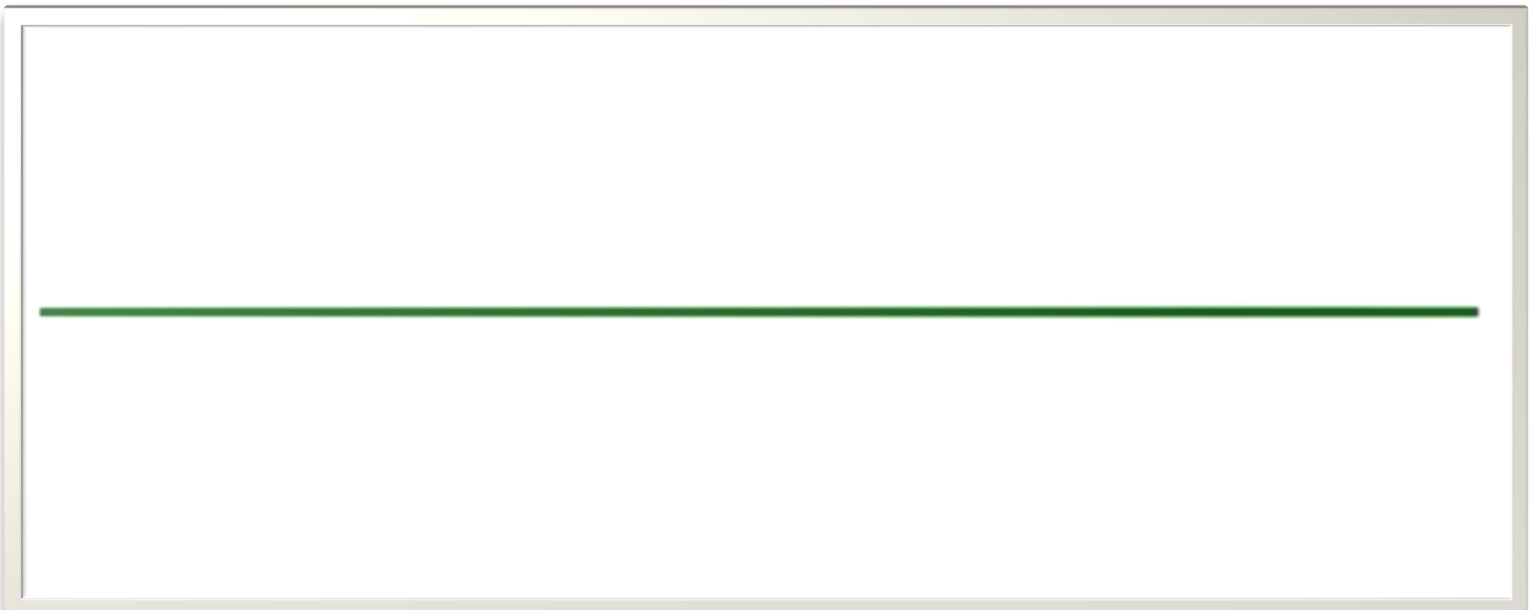
What is the *smallest* possible box?

What is the *smallest* possible box?



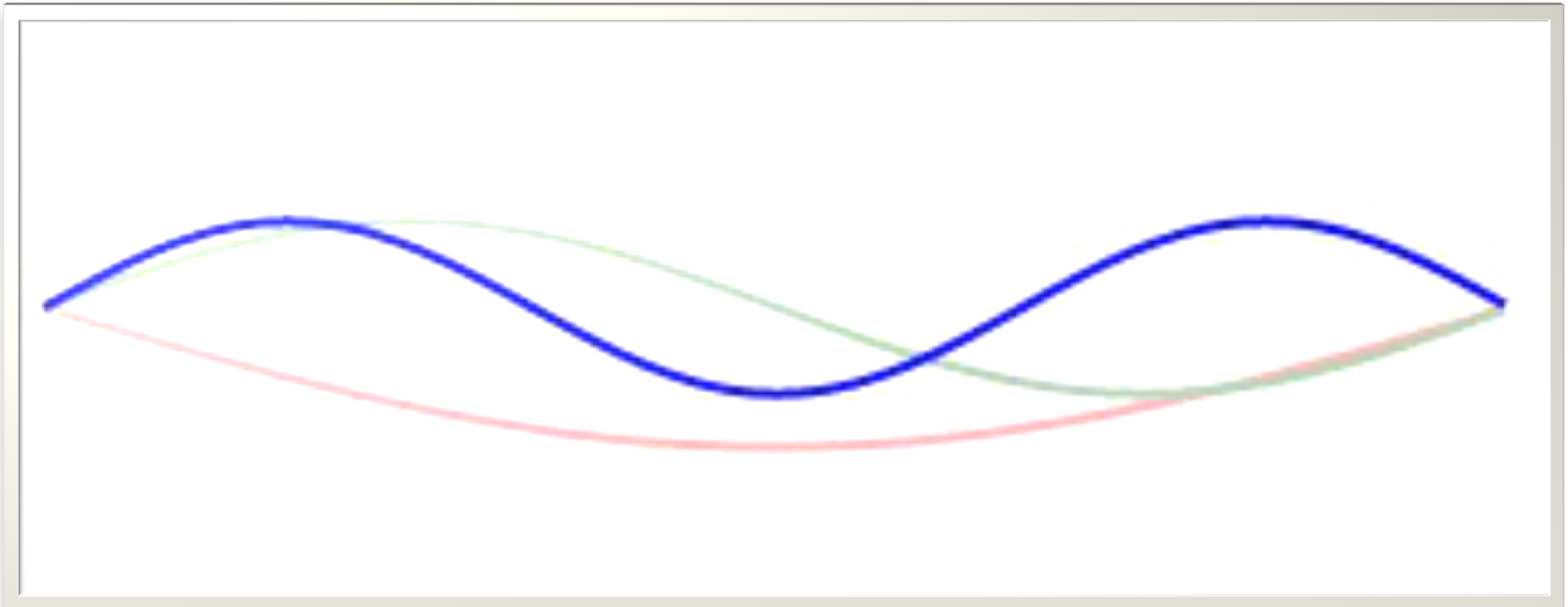
$$L = \frac{\lambda}{2}$$

What is the *next largest* box?



$$L = \frac{\lambda}{2} \qquad L = \lambda$$

What is the rule?



$$L = \frac{\lambda}{2} \qquad L = \lambda \qquad L = \frac{3\lambda}{2}$$

- Allowed box sizes: $L = \frac{n\lambda}{2}$ $\quad n = 1, 2, 3, ...$
- Or, the allowed wavelengths are: $\lambda = \frac{2L}{n}$
- This is the same as saying only certain values of momenta are possible:

$$p = \frac{hn}{2L}$$

- What does this mean for the energy?

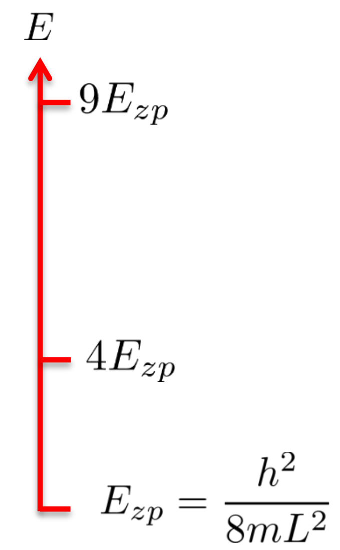
$$E = \frac{p^2}{2m} = \frac{h^2 n^2}{8mL^2}$$

Particle in a Box

Classical

- Continuum of possible energies
- Lowest energy is zero

Quantum



- Discrete set of energies
- Zero point energy

$$E = \frac{h^2 n^2}{8mL^2} = E_{zp} n^2$$

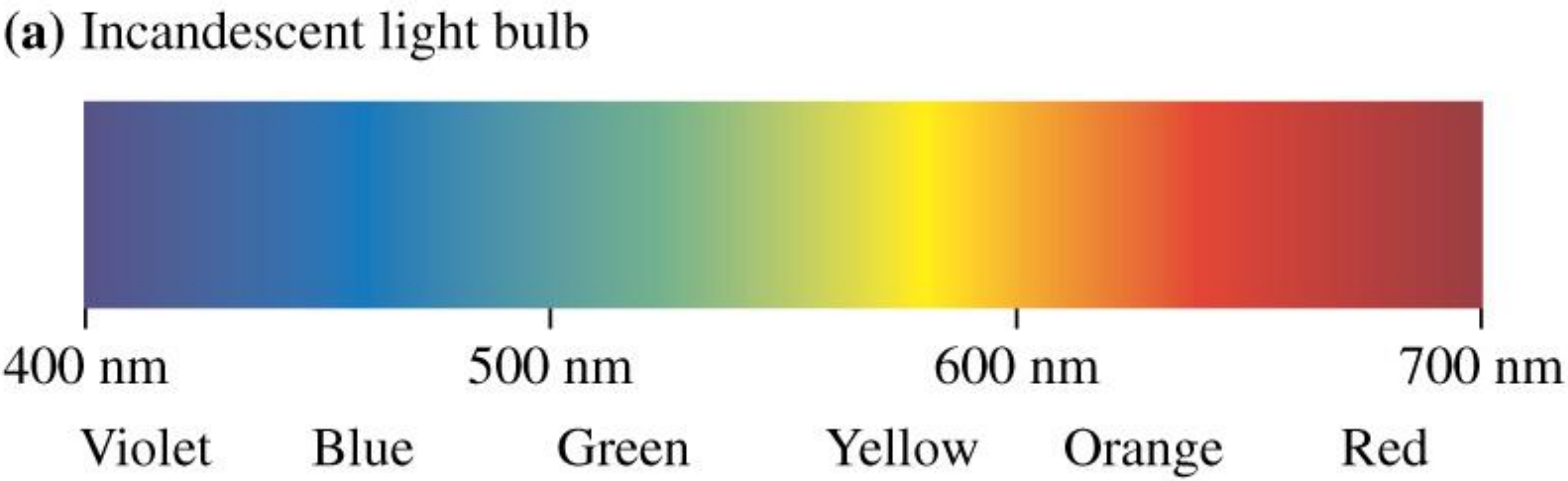
Quantization

- A quantity is quantized if its possible values are limited to a discrete set.

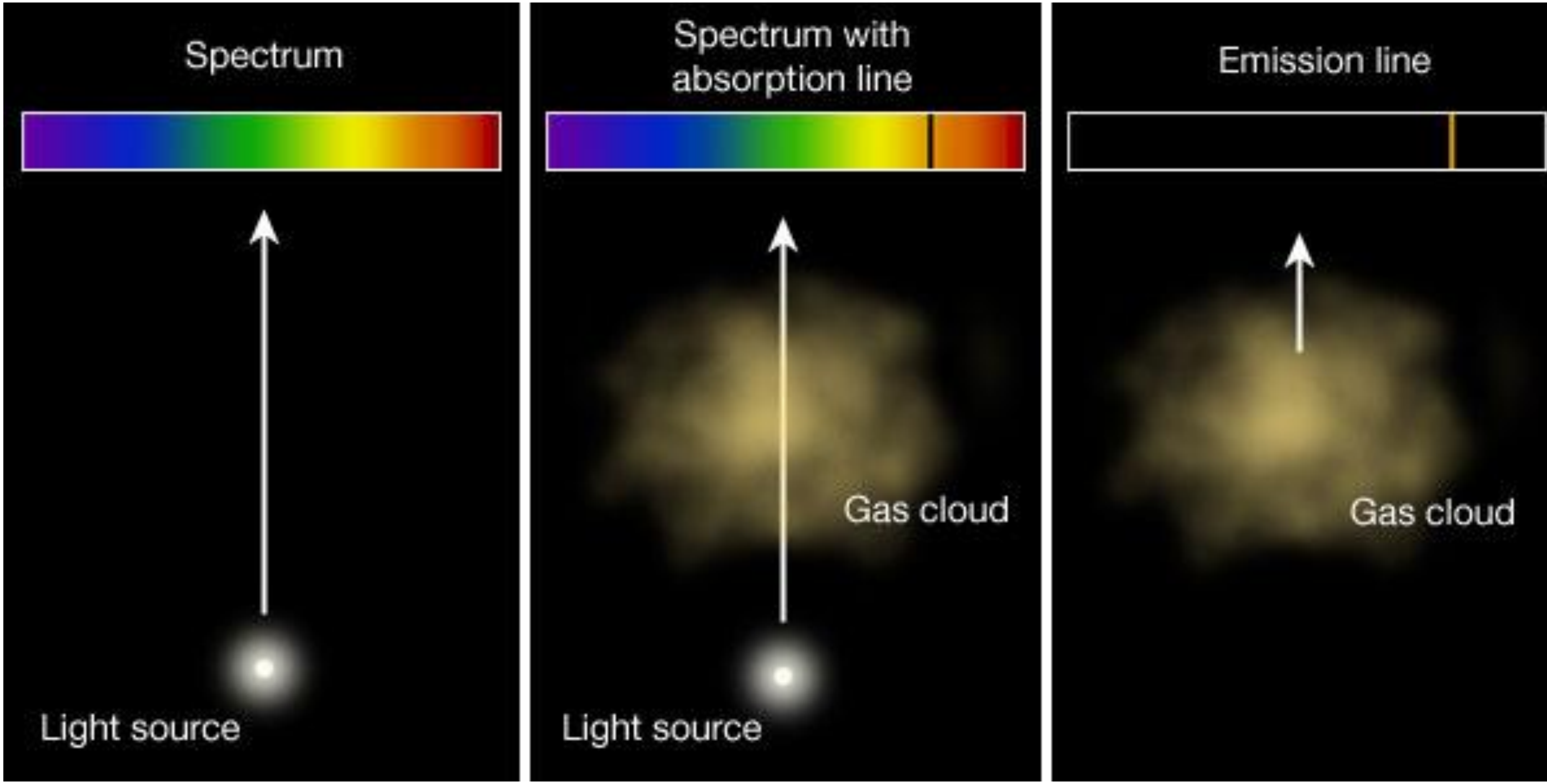
Examples:

- Number of chairs in the room.
- Frequency of standing wave on a stretched string.

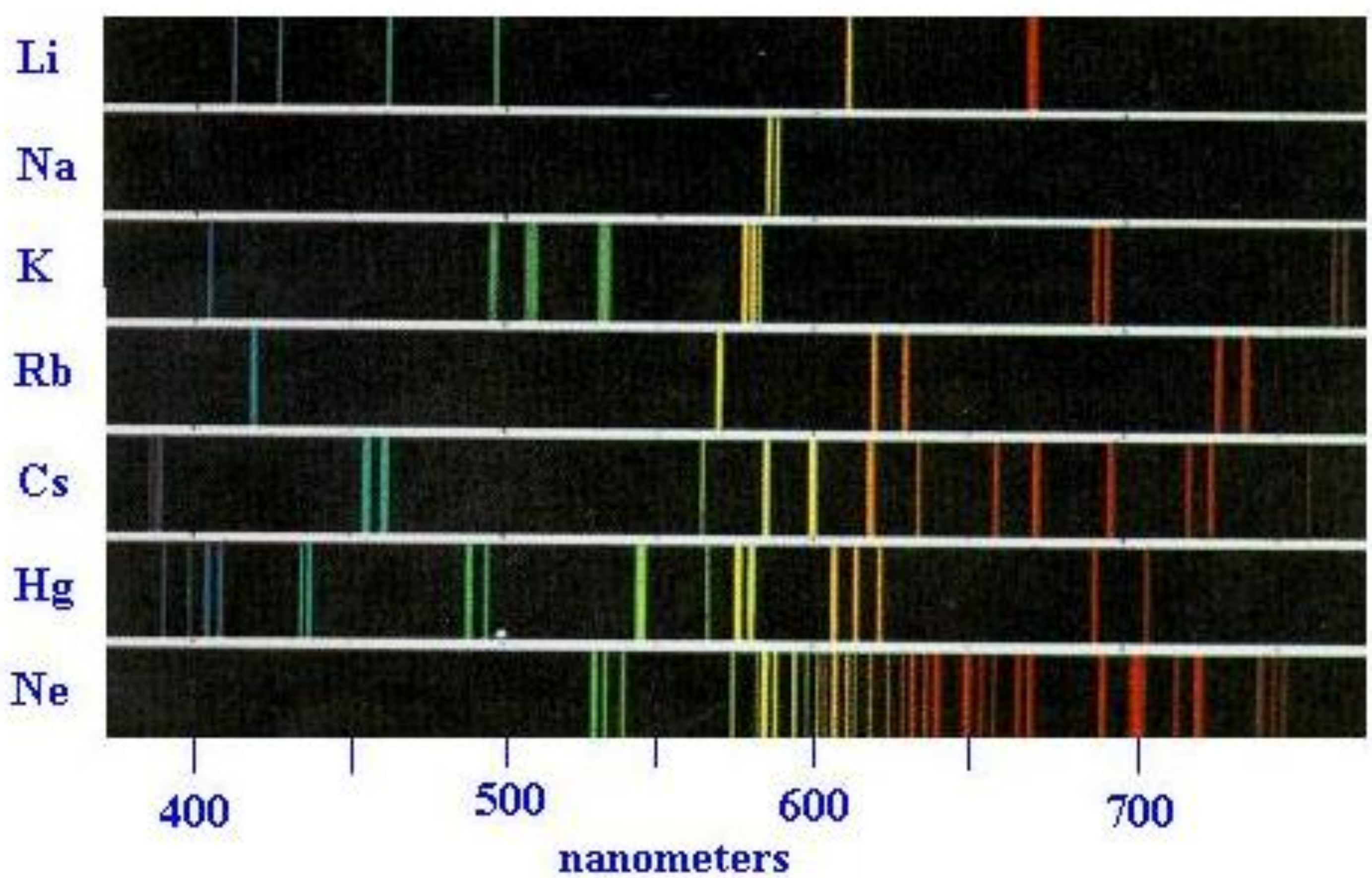
- A blackbody, such as the Sun or an incandescent light bulb, emits a ***continuous spectrum*** (some light at every wavelength)



Absorption & Emission



- Different emission pattern for different atoms.



Zero Point Energy

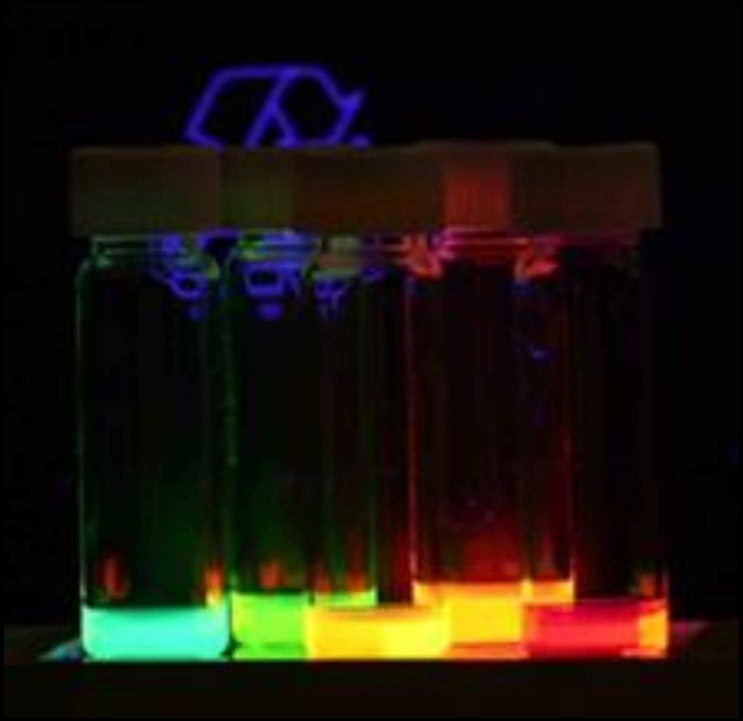
$$E_{zp} = \frac{h^2}{8mL^2}$$

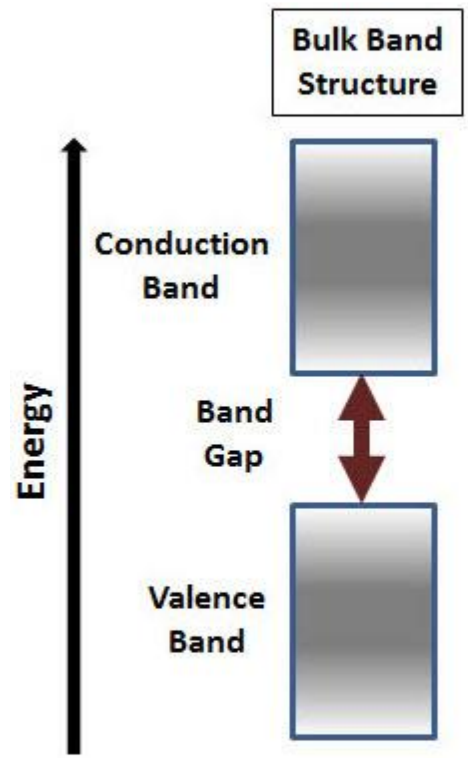
What happens when we squeeze the box?

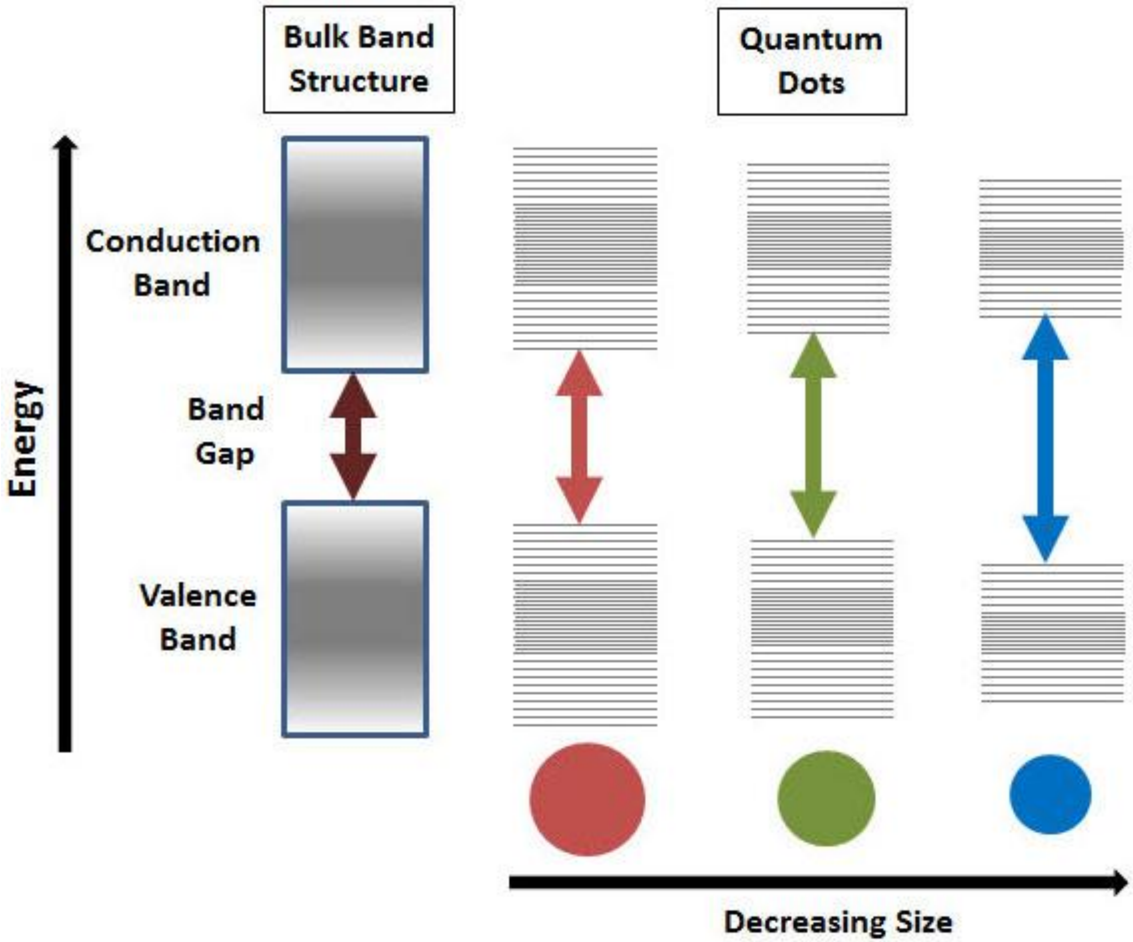
As we squeeze the box and make L smaller the zero point energy goes up!

Quantum Claustrophobia

Quantum Dots



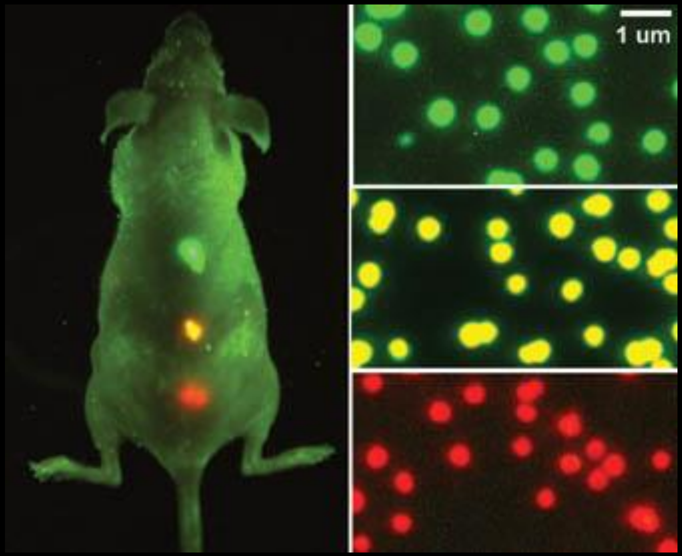

Bulk Band
Structure
Energy
Conduction
Band
Band
Gap
Valence
Band



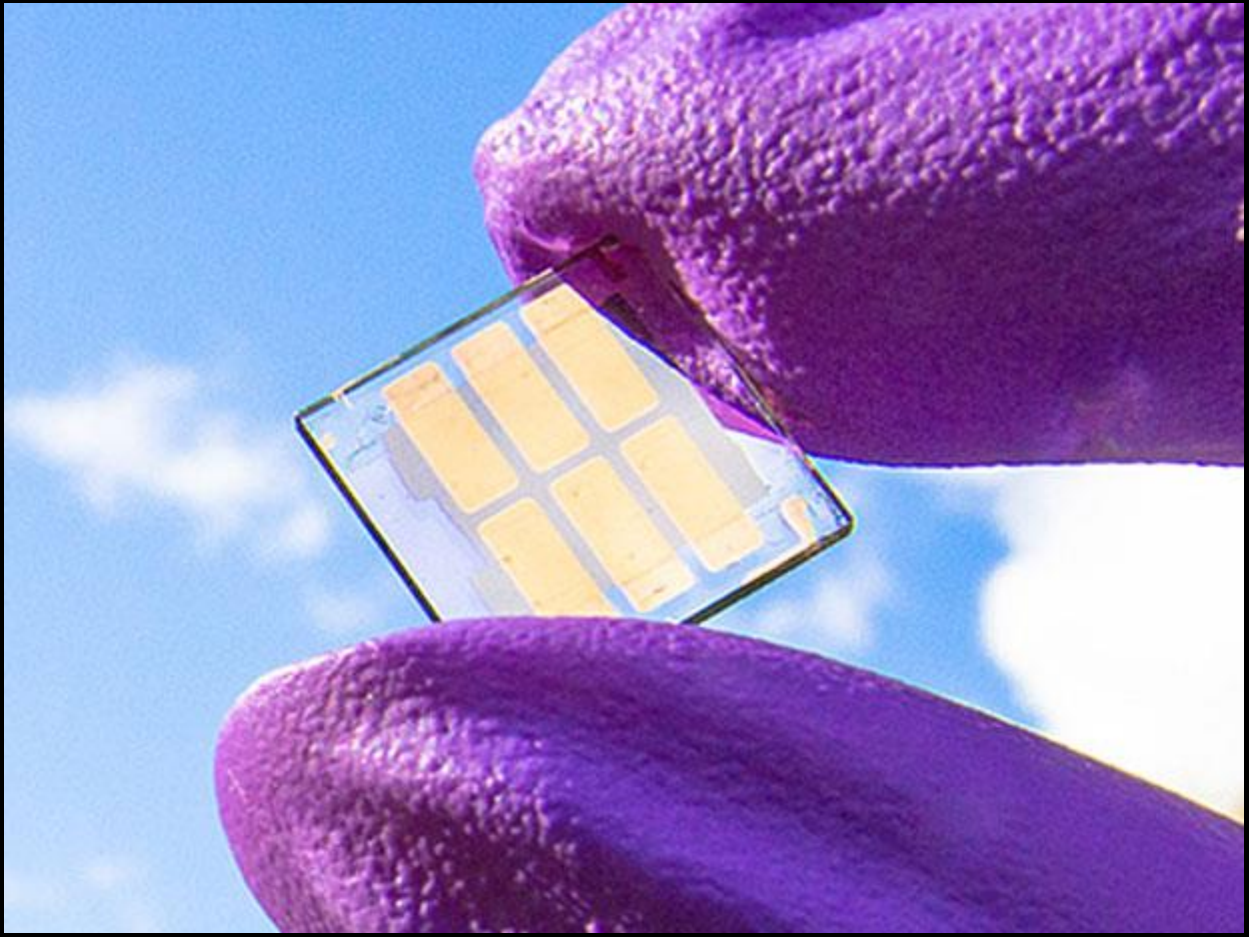
Bulk Band Structure
Quantum Dots
Energy
Conduction Band
Band Gap
Valence Band
Decreasing Size

EMERGING TECHNOLOGY- *Quantum Dots in Displays*

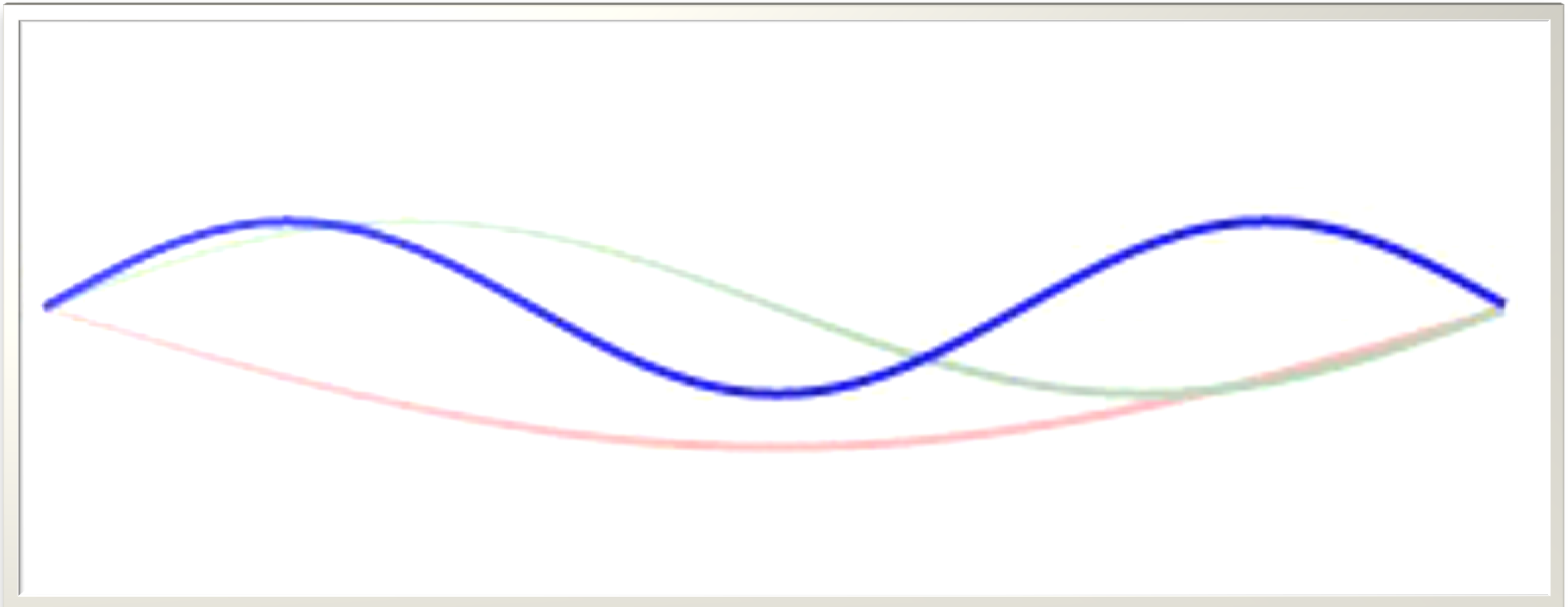
EMERGING TECHNOLOGY- *Quantum Dots in Medicine*



EMERGING TECHNOLOGY- *Quantum Dots in Solar Cells*



What is the rule?



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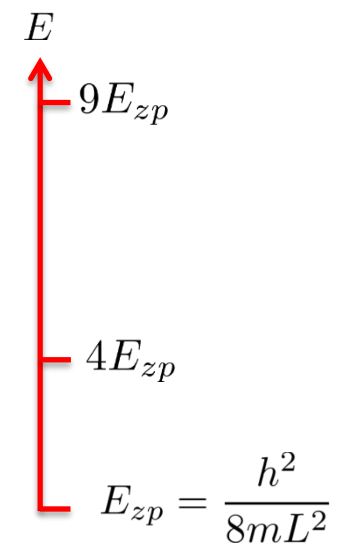
Particle in a Box

Classical

Quantum



- Continuum of possible energies
- Lowest energy is zero

- Discrete set of energies
- Zero point energy

$$E = \frac{h^2 n^2}{8mL^2} = E_{zp} n^2$$

Zero Point Energy

$$E_{zp} = \frac{h^2}{8mL^2}$$

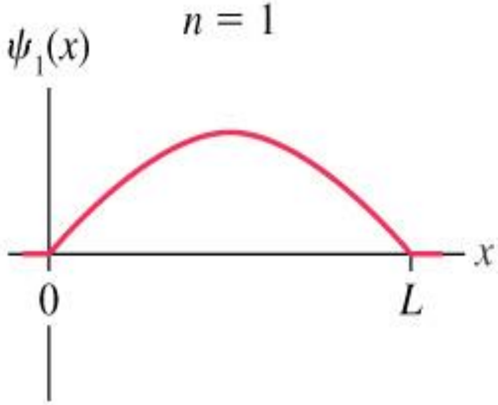
What happens when we squeeze the box?

As we squeeze the box and make L smaller the zero point energy goes up!

Quantum Claustrophobia

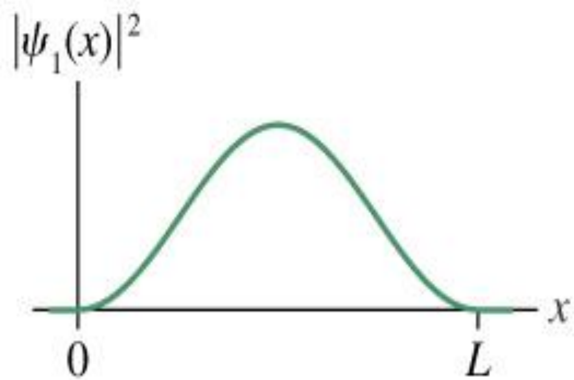
Allowed Standing Waves

Consider a particle in a 1D box at the lowest energy state (n=1).



$$\lambda = 2L$$

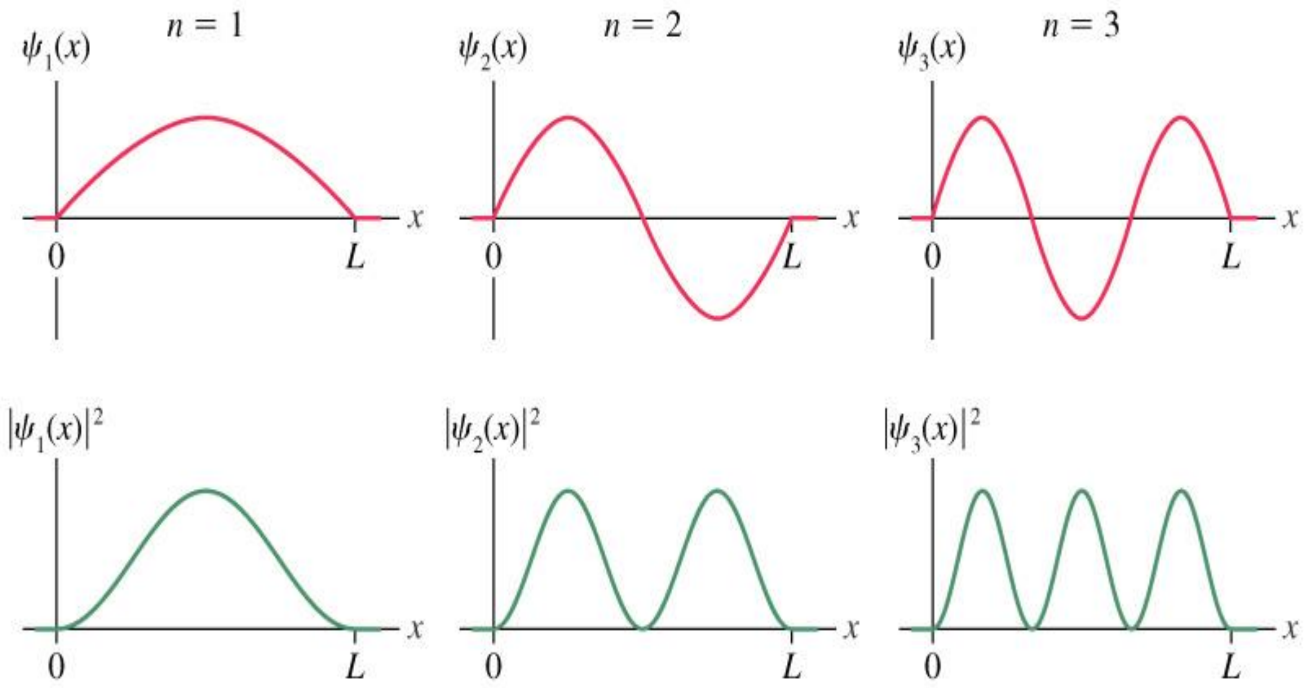
Recall that the square of the wave function gives the probability of finding the particle at x. Sketch the probability pattern.



$$P_1(x) = \psi_1^2(x)$$

Allowed Standing Waves

Sketch the wave function and the probability pattern for n=1, 2 and 3.



For n = 3, what is the probability of finding the particle between x = L/3 and x = 2L/3?

A. 0

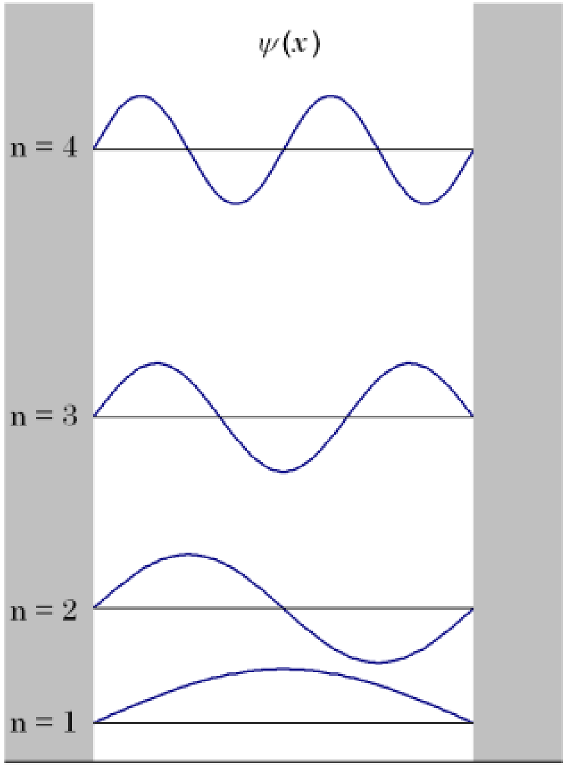
B. 1/3

C. 1/2

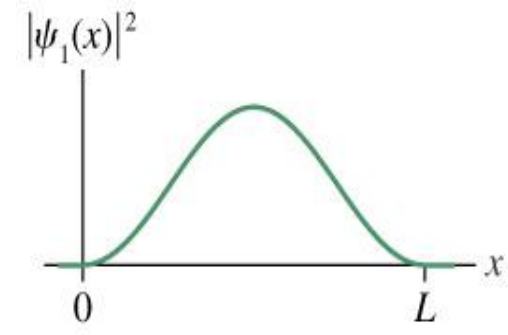
D. 2/3

E. 1

Wave functions



What does P(x) mean?

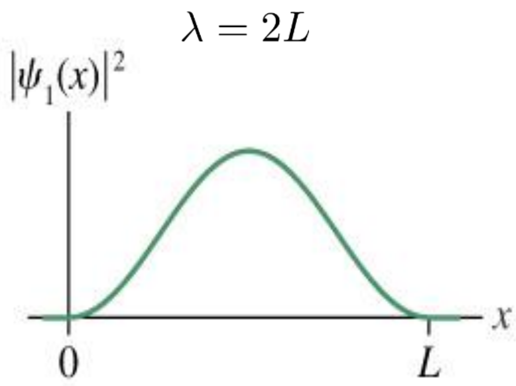


- Before we measure the particle it does not have a definite position.
- But! We know it is in the box somewhere between 0 and L.
- This is not an electron "cloud" distribution.
  - There would be repulsion between parts of the cloud
  - Not observed
- Over many measurements we would find:

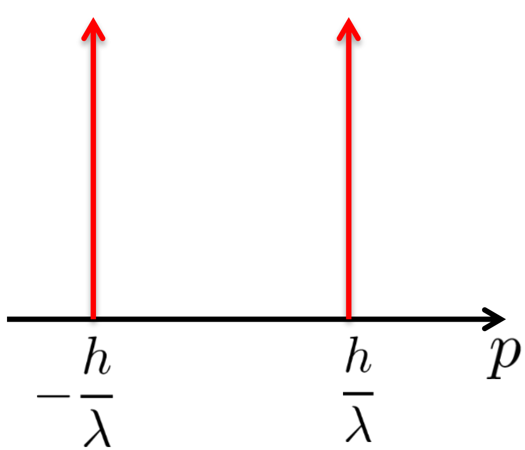
$$\frac{L}{2} \pm \frac{L}{2}$$

What is this?

Heisenberg's Uncertainty Principle



Uncertainty in position: $\Delta x = \dfrac{\lambda}{4}$



DISCRETE VALUES!!

What about the momentum?

$$\Delta p = \frac{h}{\lambda} = \frac{h}{2L}$$

But it could be moving left or right!

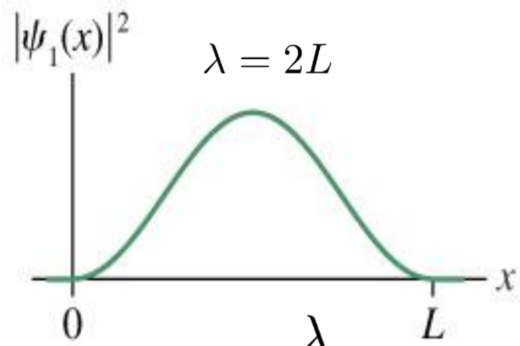
$$\Delta p = \pm\frac{h}{\lambda} = \pm\frac{h}{2L}$$

If we did many measurements half would be "+" and half would "–" so we get:

$$p_x = 0 \pm \frac{h}{\lambda}$$

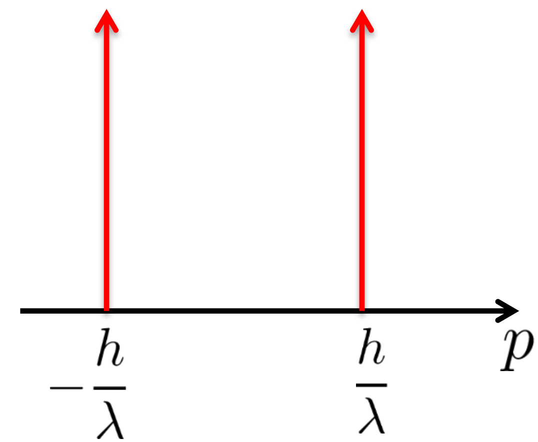
Heisenberg's Uncertainty Principle

POSITION

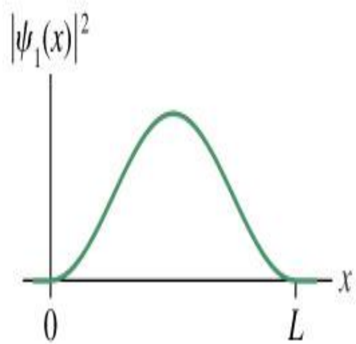


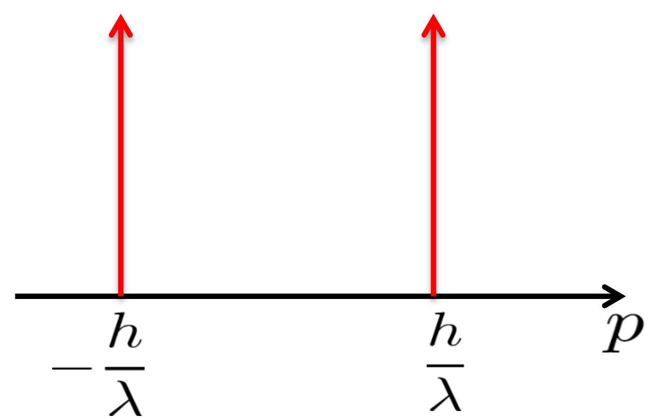
$$\Delta x = \frac{\lambda}{4}$$

MOMENTUM



What happens when we squeeze the box?





$$\Delta x = \frac{\lambda}{4}$$ is smaller!

$$\Delta p = \frac{h}{\lambda}$$ is larger!

Heisenberg's Uncertainty Principle

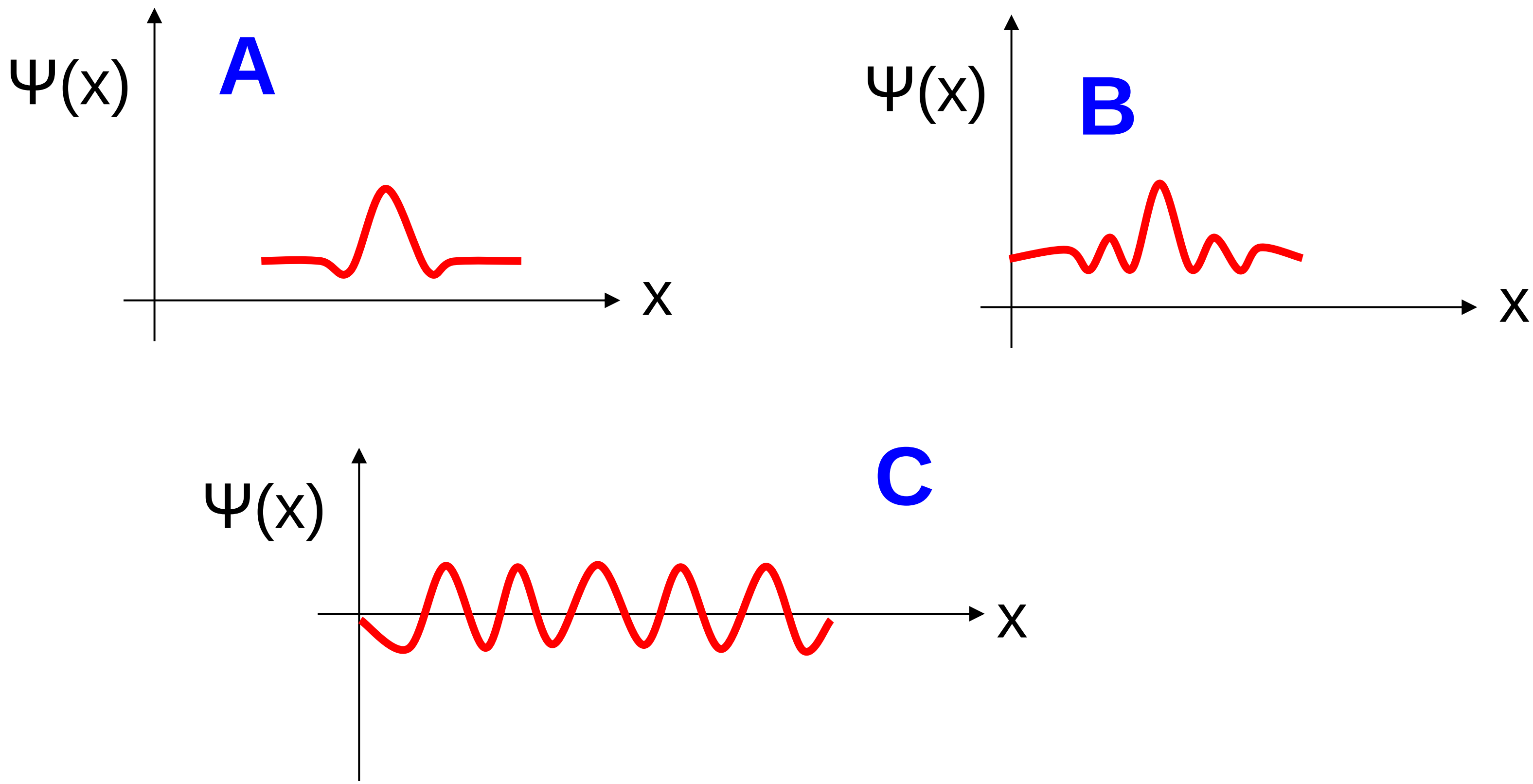
As we make the box smaller (decrease L) the uncertainty in position gets smaller.

But! As L decreases the uncertainty in the particle's momentum gets bigger!

The uncertainty in momentum and position are INVERSELY RELATED!

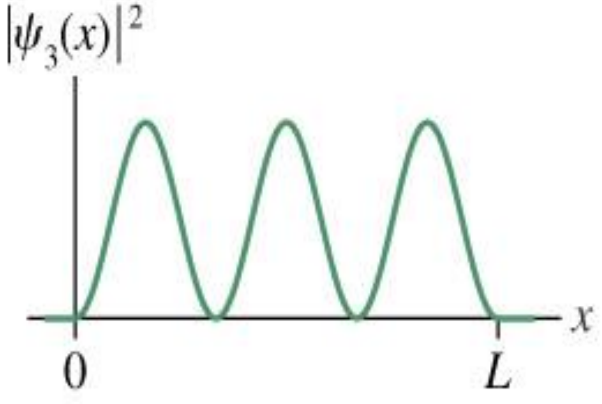
$$\Delta x \Delta p_x = \frac{L}{2}\frac{h}{2L} = \frac{\lambda}{4}\frac{h}{\lambda} = \frac{h}{4}$$

Which particle's speed can be determined most precisely?



Heisenberg's Uncertainty Principle

Repeat for n=3

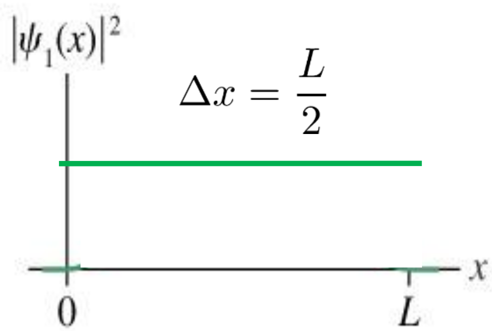


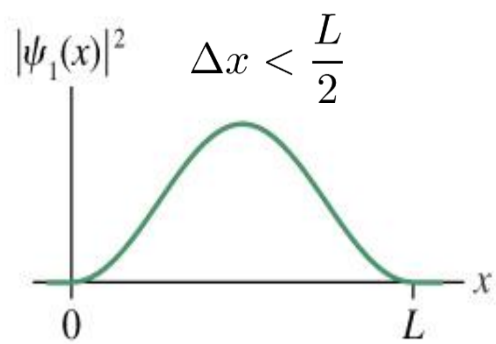
Heisenberg's Uncertainty Principle

In general we find the smallest (or minimum) is:

$$\Delta x \Delta p \geq \cancel{\frac{h}{4}} \qquad \Delta x \Delta p \geq \frac{h}{4\pi}$$

Why the π ?





HUP is Intuitive

$$\Delta p \uparrow \qquad \Delta x \downarrow$$

What is weird is that we can't have the ball at rest! There is a minimum energy!

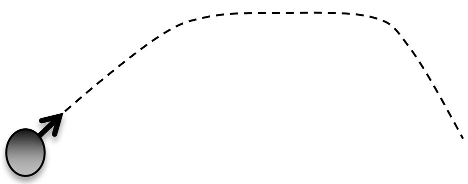
“Strong” HUP

- Particle cannot simultaneously possess a definite position and a definite momentum.

<u>Classical Question</u>

Given x(0) and p(0) what is x(t) and p(t)?

Particle is on a definite trajectory.



F=ma

<u>Quantum Question</u>

Given x(0), what is the probability of finding x(t)?

No such thing as a definite trajectory.

Given p(0), what is the probability of finding p(t)?

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

Recap

- Experiment showed that we need to replace $F = ma$ with the de Broglie relation.

$$\underset{\text{wave}}{\lambda}\,\underset{\text{particle}}{p} = h$$

- We applied this relation to a particle in 1d box.
  - Energy is discrete
  - Like harmonics on a violin
  - No definite trajectory just a probability

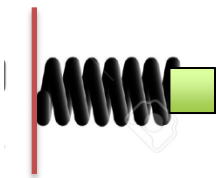
Harmonic Oscillators

- Any kind of oscillation whose amplitude is a simple sine wave function of time.

Spring

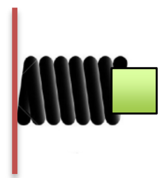
Frequency is independent of amplitude

$$F = 0$$



$$x = 0$$

$$F \rightarrow$$



$$x < 0$$

$$F \leftarrow$$

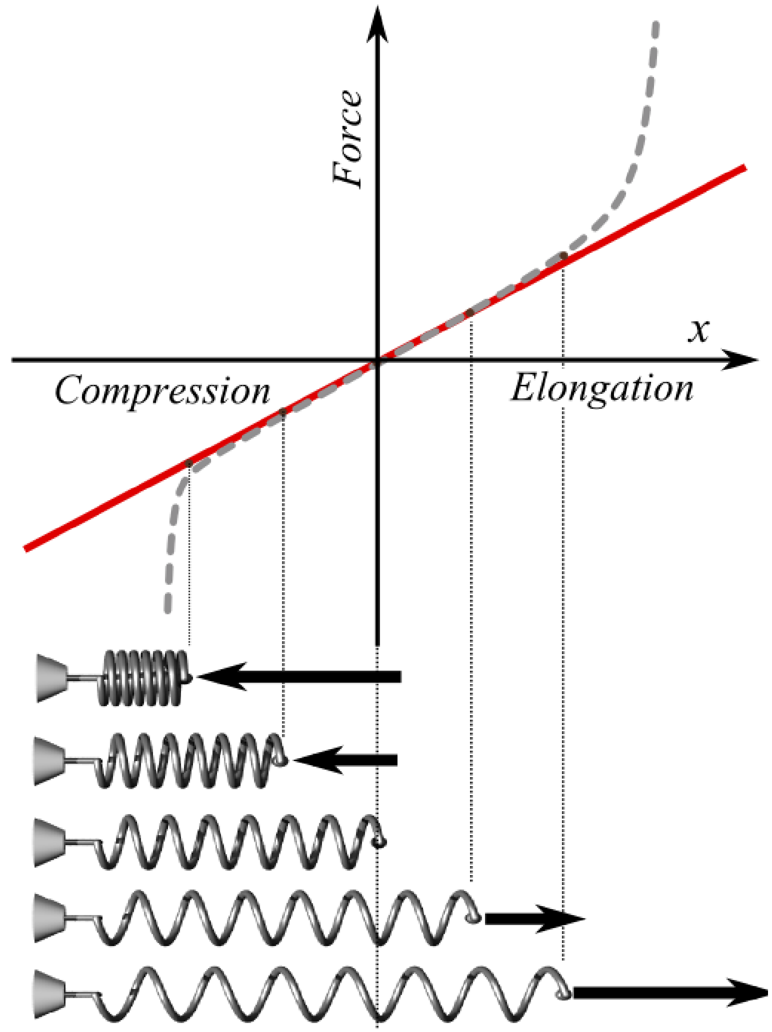
$$x > 0$$

$$F = -kx$$

What does the frequency depend on?

- k – the spring constant
- m – the mass

$$f = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$



Energy H.O.

Two kinds of energy $KE + PE$

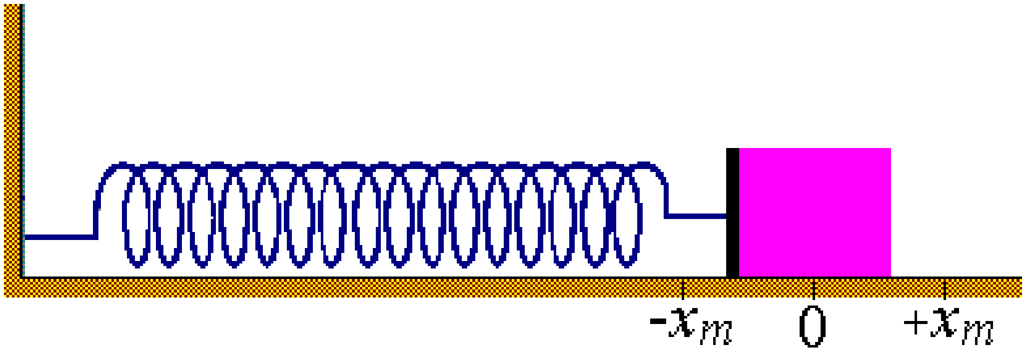
motion

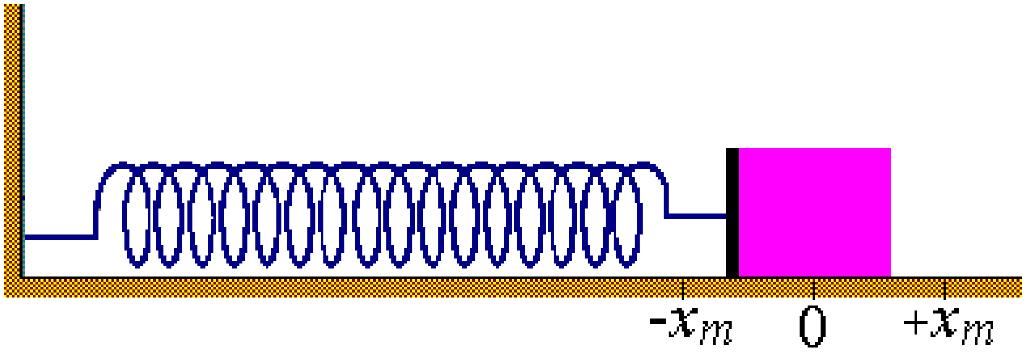
Electrostatic field of molecules in spring

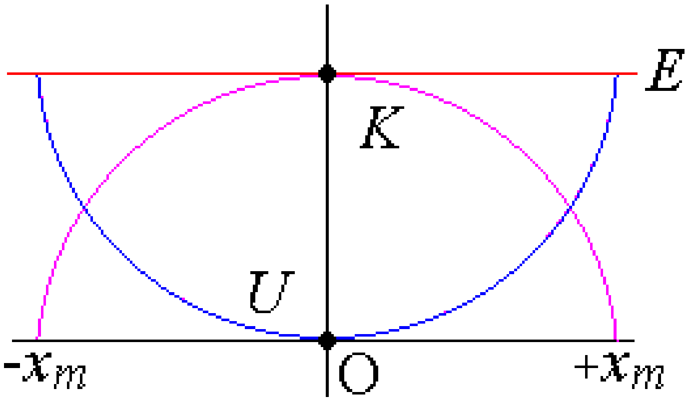
$$E = KE(t) + PE(t) = \text{constant}$$

Draw KE(t), PE(t) and E(t) on one plot.

How does the energy ‘slosh’ back and forth?

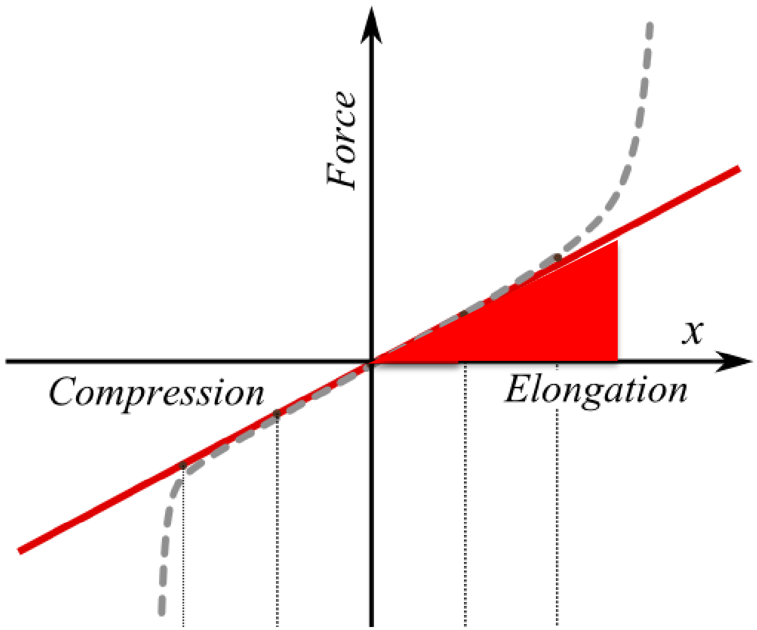






How does the energy ‘slosh’ back and forth?

$$\Delta W = \text{Force x Distance} = kx\Delta x$$



$$\Delta W = \frac{1}{2}hb = \frac{1}{2}kx^2$$

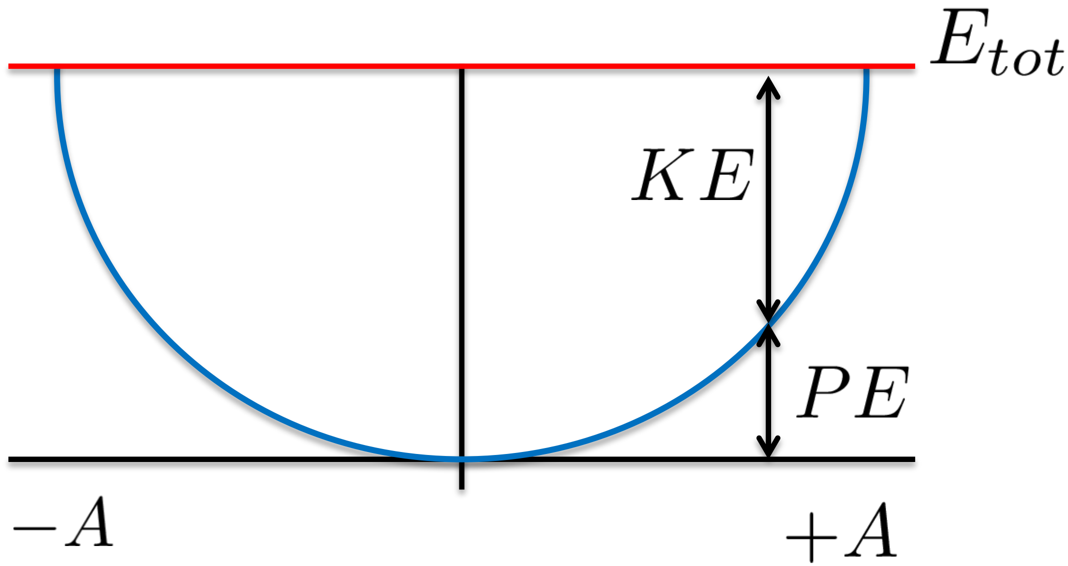
The total energy transferred from KE to PE as mass moves from eq to any position x.

$$PE(x) = \frac{1}{2}kx^2$$

$$W = \int_{x_i}^{x_f} \vec{F} \cdot d\vec{r} = \int_0^{x_f} (kx\vec{i}) \cdot (-dx\vec{i}) = \int_0^{x_f} -kxdx$$

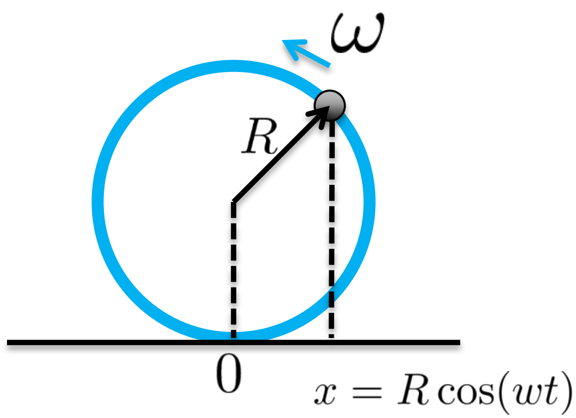
$$W = -\frac{1}{2}kx_f^2$$

$$E_{total} = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}kA^2$$



$$v = \sqrt{\frac{k}{m}(A^2 - x^2)} \qquad v_{max} = \sqrt{\frac{kA^2}{m}}$$

Circular & Harmonic Motion



$$v_x$$

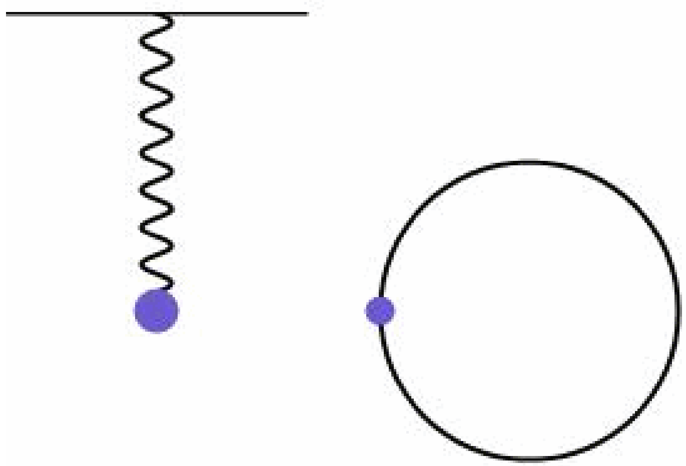
$$v_x = -v_t \sin(\omega t) = -R\omega \sin(\omega t)$$

$$\omega^2 x^2 + v_x^2 = R^2 \omega^2$$

$$v_x = \sqrt{\omega^2 (R^2 - x^2)}$$

Very Similar!

$$v = \sqrt{\frac{k}{m}(A^2 - x^2)}$$



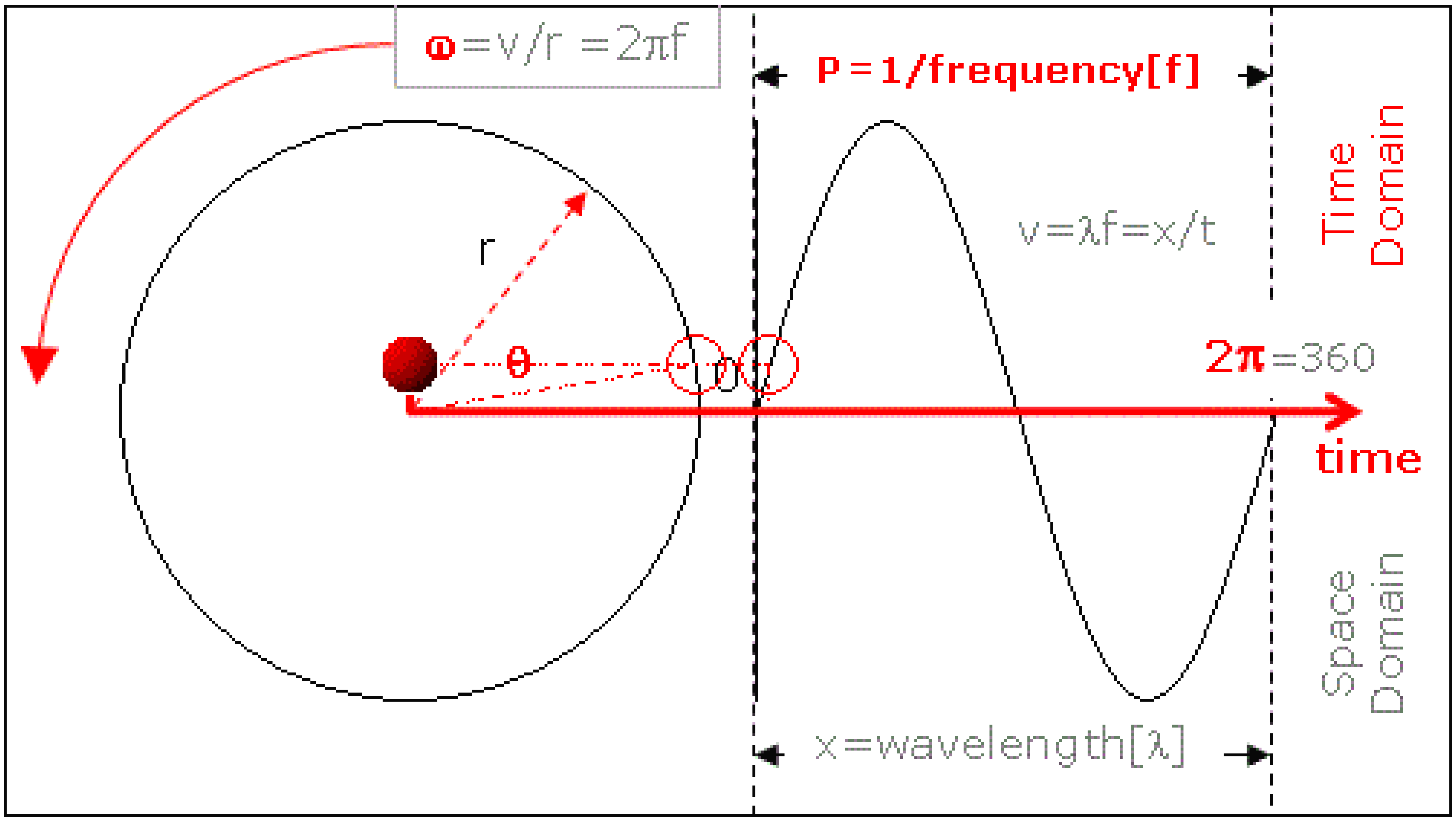
For circular motion:

$$T = \frac{2\pi}{\omega} \qquad f = \frac{1}{T}$$

$$T = \frac{1}{f} = 2\pi\sqrt{\frac{m}{k}}$$

$$x = R\cos(wt) \longrightarrow x = A\cos(\sqrt{\frac{k}{m}}t) = A\cos(2\pi f t)$$

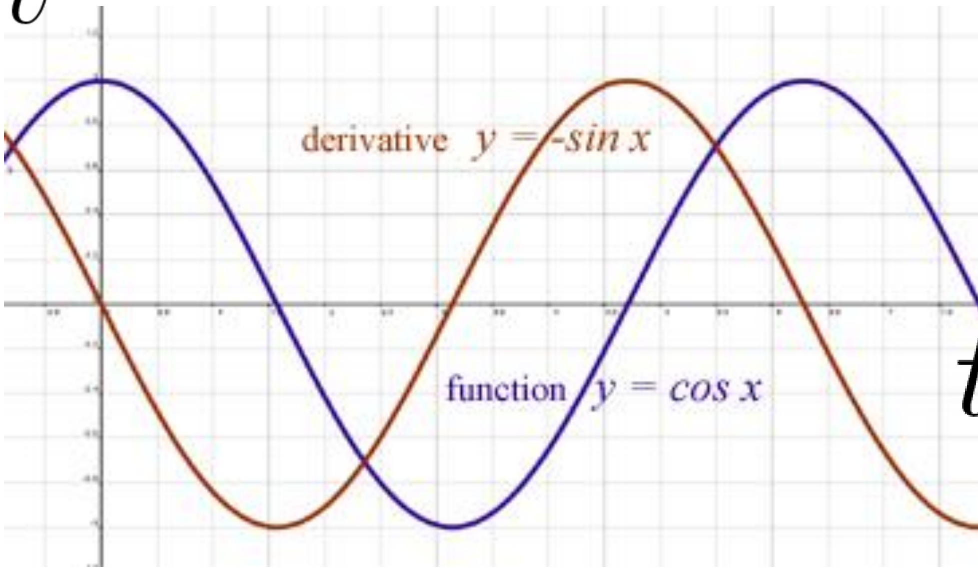
$$v = -R\omega\sin(\omega t) \longrightarrow v = -A\sqrt{\frac{k}{m}}\sin(\sqrt{\frac{k}{m}}t) = -A\sqrt{\frac{k}{m}}\sin(2\pi f t)$$



ω=v/r =2πf
P=1/frequency[f]
r
θ
v=λf=x/t
Time Domain
2π=360
time
Space Domain
x=wavelength[λ]

Position & Momentum

x, v



t

$$x = A\cos(2\pi f t)$$

$$v = -A\sqrt{\frac{k}{m}}\sin(2\pi f t)$$

$$E = \frac{1}{2}mv^2(t) + \frac{k}{2}x^2(t)$$

$$\sin^2(\theta) + \cos^2(\theta) = 1$$

$$E = \frac{kA^2}{2}$$

Energy is constant!

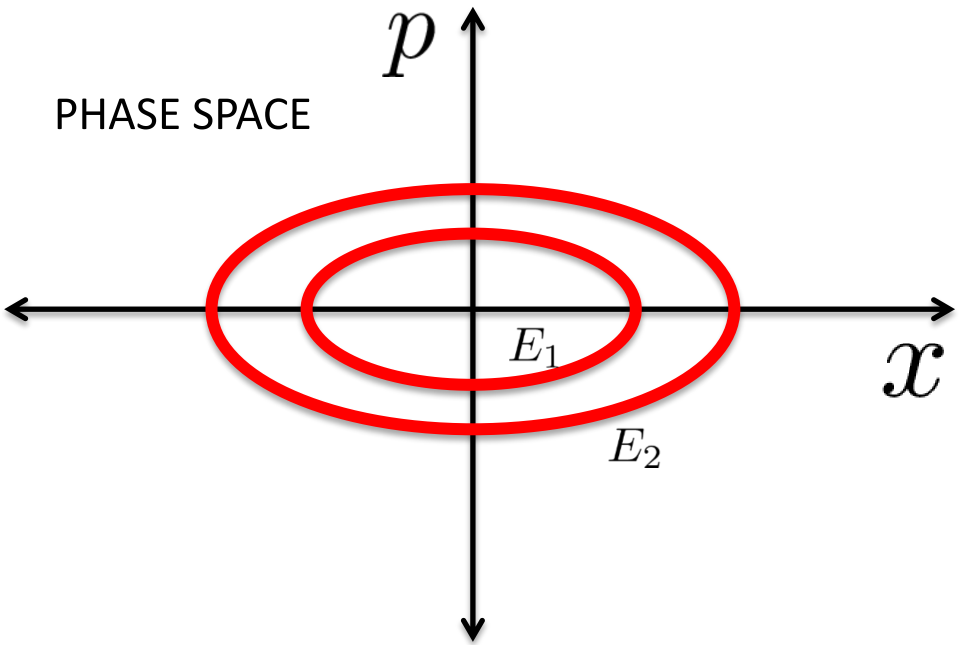
Energy

What kind of equation is this? Equation of an Ellipse

$$\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 = 1$$

$$E = \frac{1}{2}\frac{p^2(t)}{m} + \frac{k}{2}x^2(t)$$

PHASE SPACE



As time ranges over one full period the point x(t) and p(t) traces an ellipse in the clockwise direction.

The size of the ellipse depends on the energy.

Phase Space

$$E = \frac{1}{2}\frac{p^2(t)}{m} + \frac{k}{2}x^2(t)$$

Use the equation of an ellipse and the area of an ellipse to show that:

$$E = A \times f$$

$$\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 = c^2$$

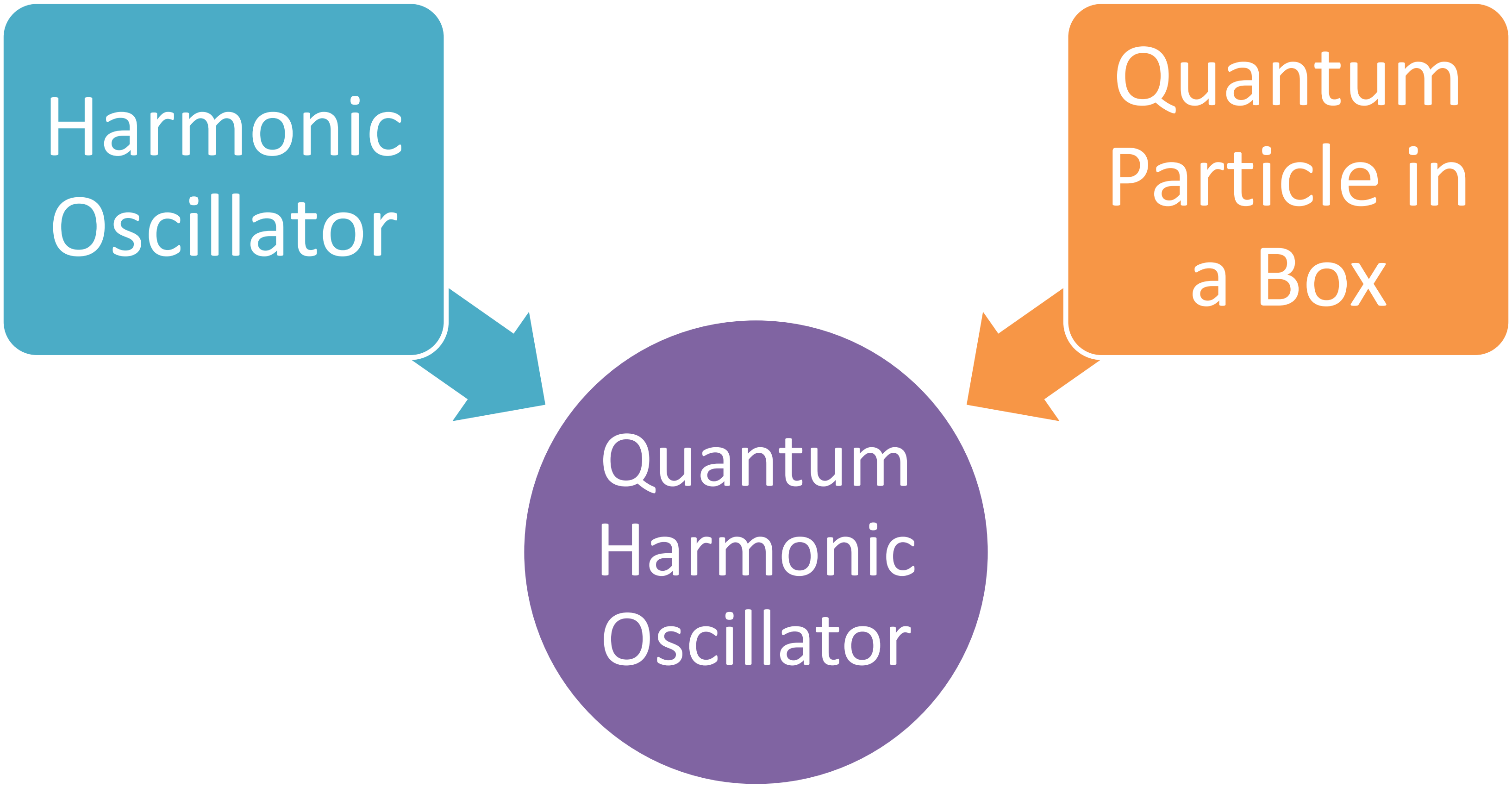
$$\left(\frac{x}{ac}\right)^2 + \left(\frac{y}{bc}\right)^2 = 1$$

$$Area = \pi AB$$

$$Area = \pi AB = \pi c\sqrt{2m}\sqrt{\frac{2}{k}} = 2\pi\sqrt{\frac{m}{k}}c = \frac{E}{f}$$

The importance of phase space in classical physics is that a point in phase space represents *everything* you need to know about the system to predict what it will do in the future.

Quantum Harmonic Oscillators



- Recall that for a harmonic oscillator when:

$$x = A \longrightarrow PE = E_{tot}$$

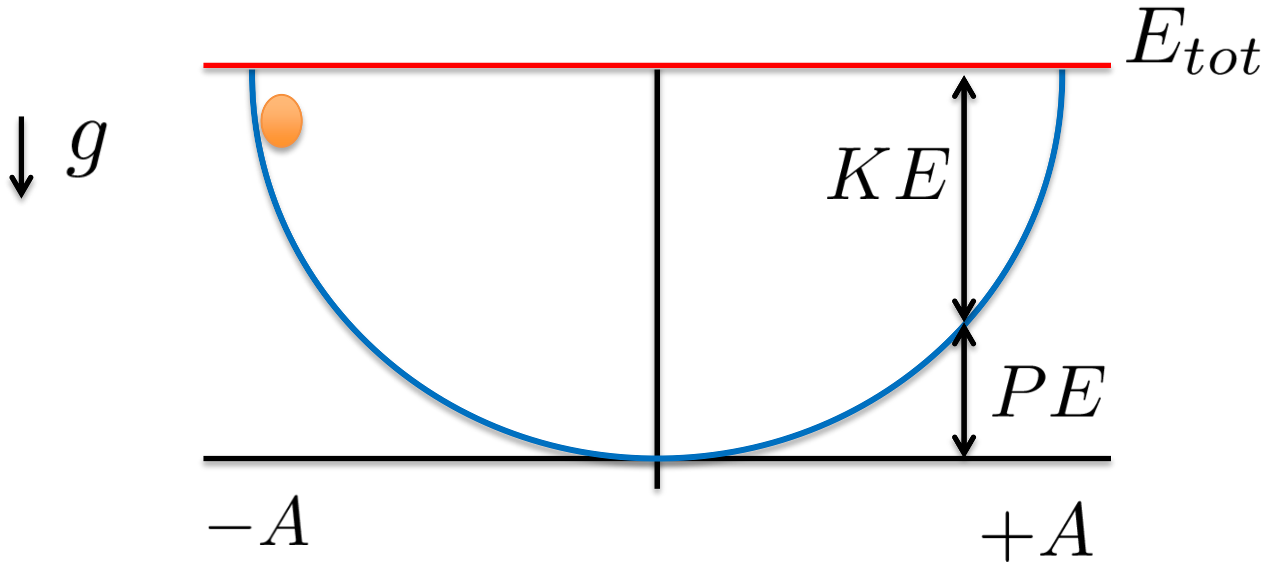
- This means that $E = \dfrac{kA^2}{2}$ and $A = \sqrt{\dfrac{2E}{k}}$

- This tells us that for given energy E, the mass is bound between

$$x = \pm\sqrt{\frac{2E}{k}}$$

- For the particle in a box, the mass was bound as well, but it did not depend on energy!

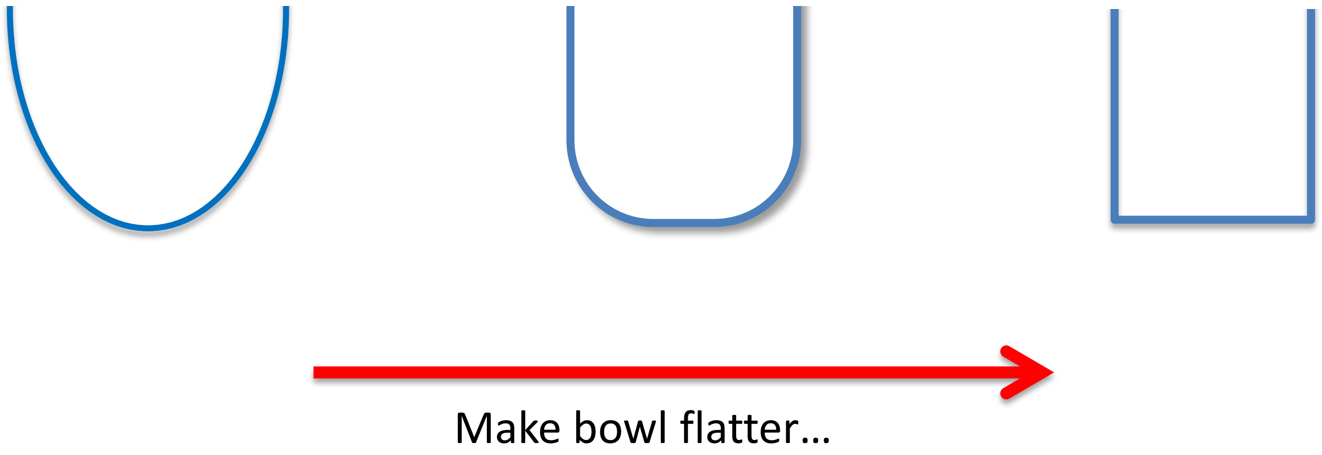
Size of “Box” Depends on Energy



$$y \propto x^2$$

Where we release the mass the size determines the energy!

Qualitatively Similar to P.B.

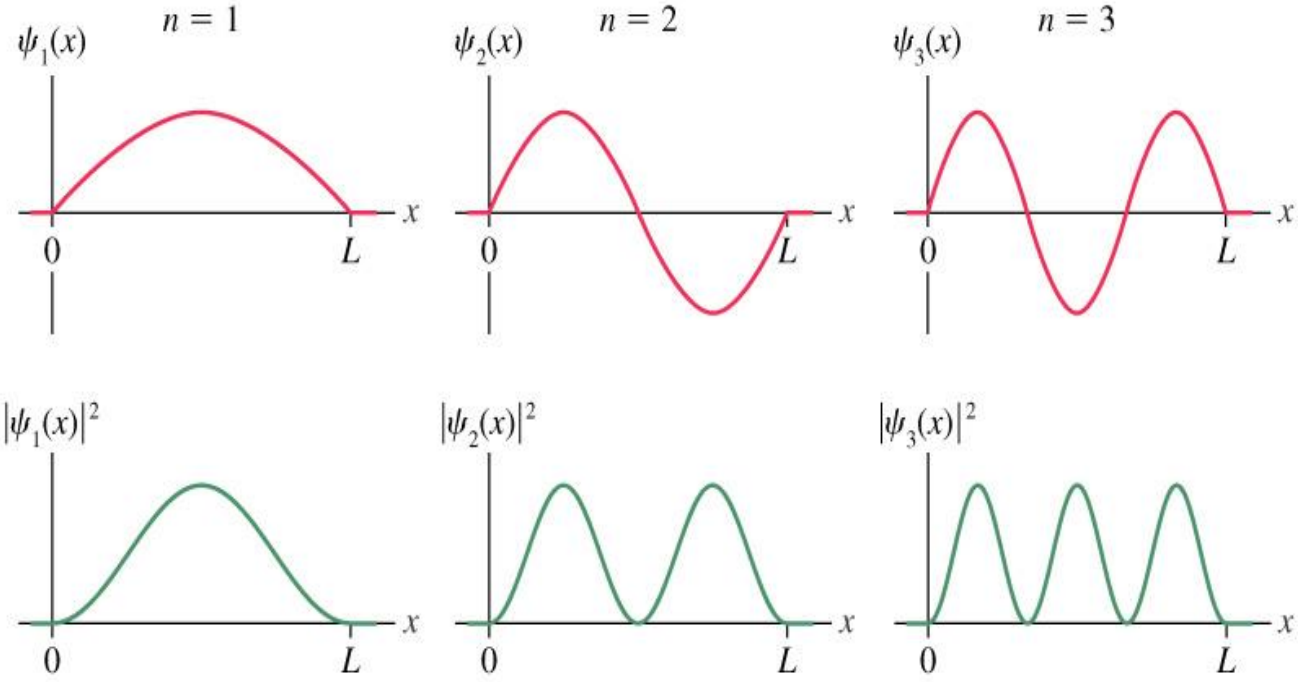


Key Difference between HO and PB: A depends on E!

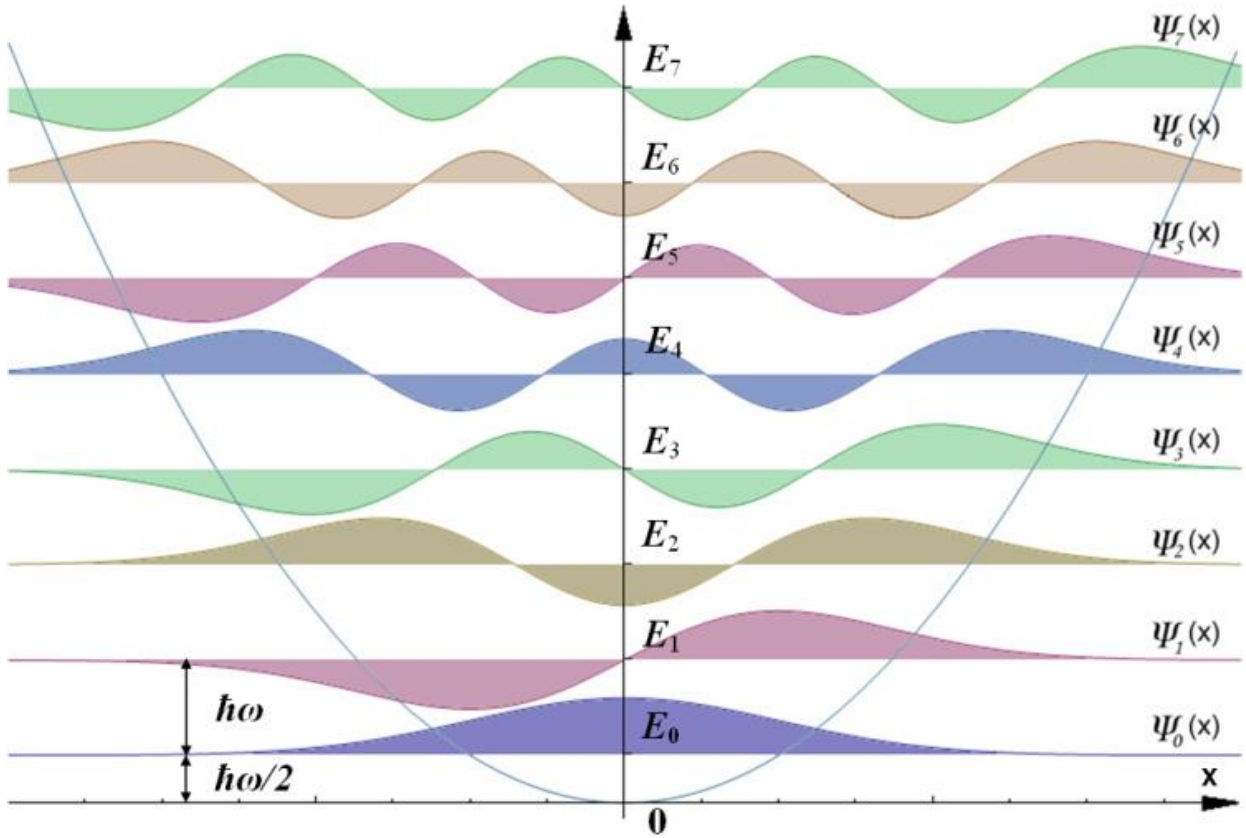
HO is a Bound System like PB

- Allowed energy levels will be discrete
- Lowest Energy level will not be zero (zero point energy)
- Nodes at each end or integer # of $\frac{\lambda}{2}$

Repeat this Sketch for HO

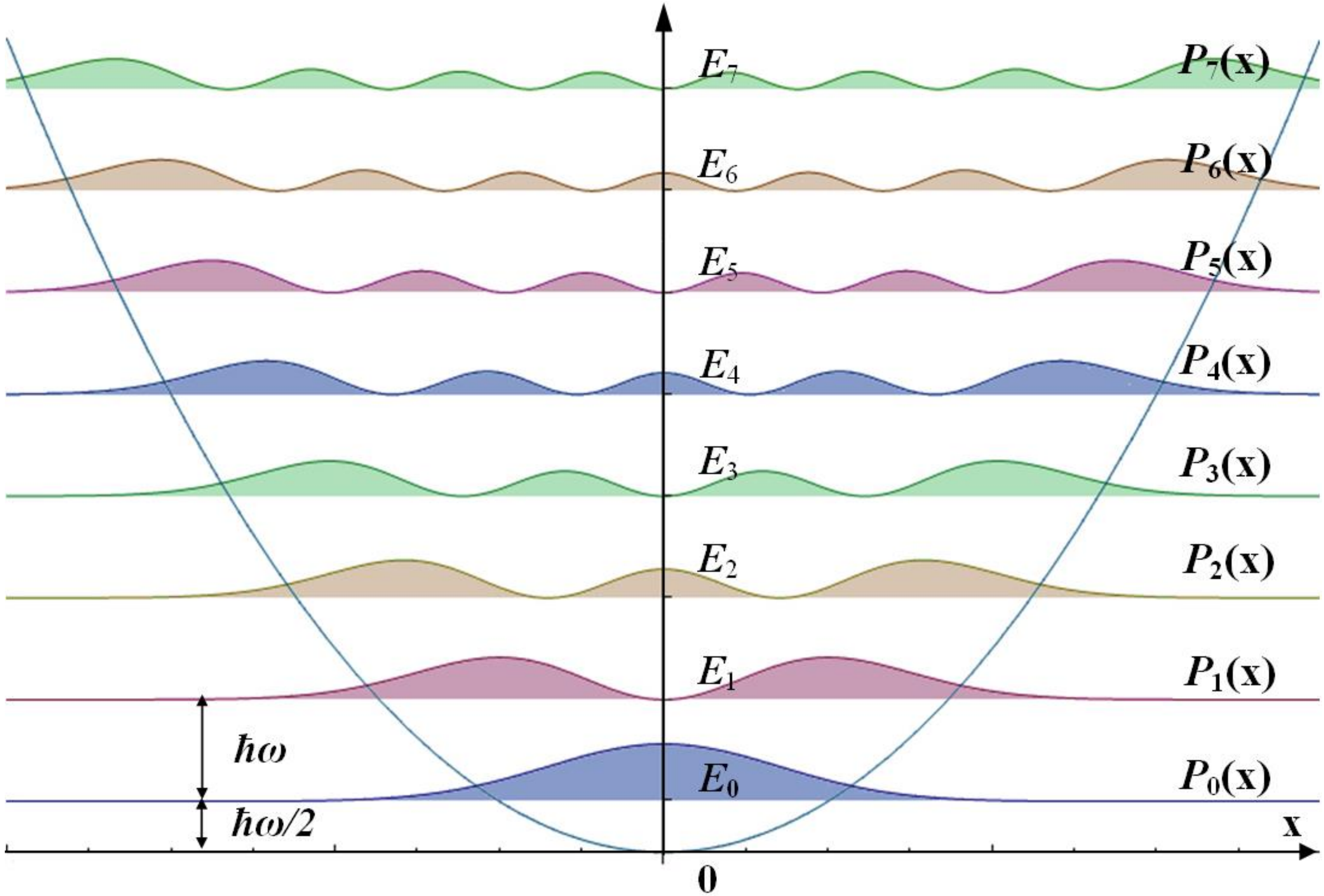


QHO



$$\hbar = \frac{h}{2\pi} \qquad \omega = 2\pi f$$

QHO



E_7
$P_7(x)$
E_6
$P_6(x)$
E_5
$P_5(x)$
E_4
$P_4(x)$
E_3
$P_3(x)$
E_2
$P_2(x)$
E_1
$P_1(x)$
$\hbar\omega$
E_0
$P_0(x)$
$\hbar\omega/2$
x
0

QHO

- Allowed energy levels are evenly spaced:

$$E_n = (n + \frac{1}{2})hf$$

- The zero point energy is given by:

$$E_{zp} = \frac{hf}{2}$$

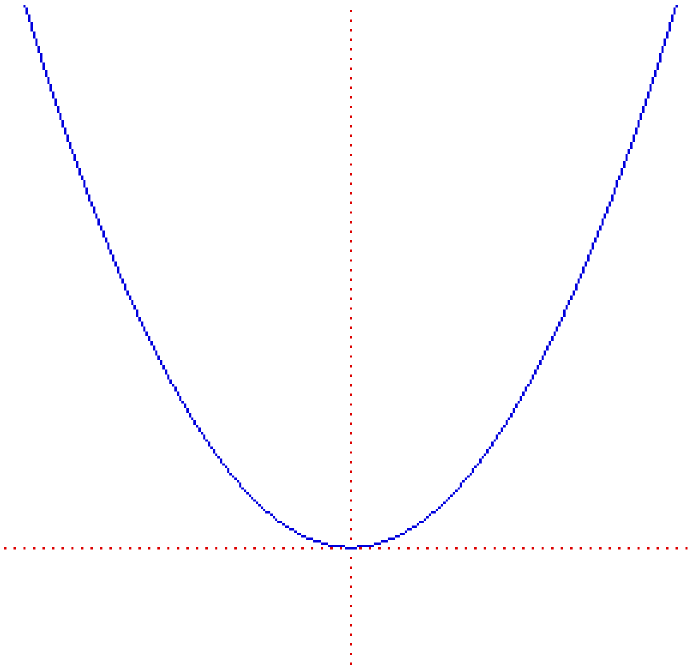
- As the size of box goes up so does the energy

Take Snapshots of a Child on Swing

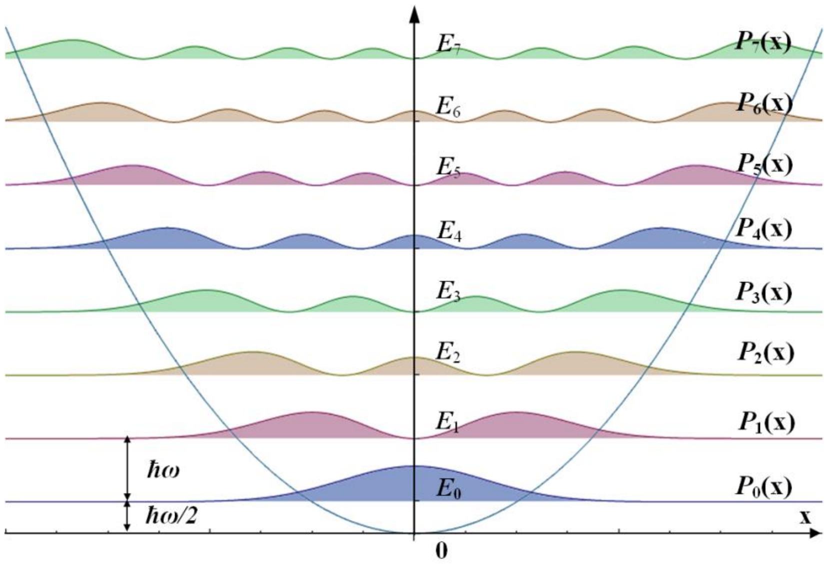
Where is most time spent? Where is the probability highest of finding the child?

Weird!

Probability of Classical HO



Probability of QHO



Let's try a calculation!

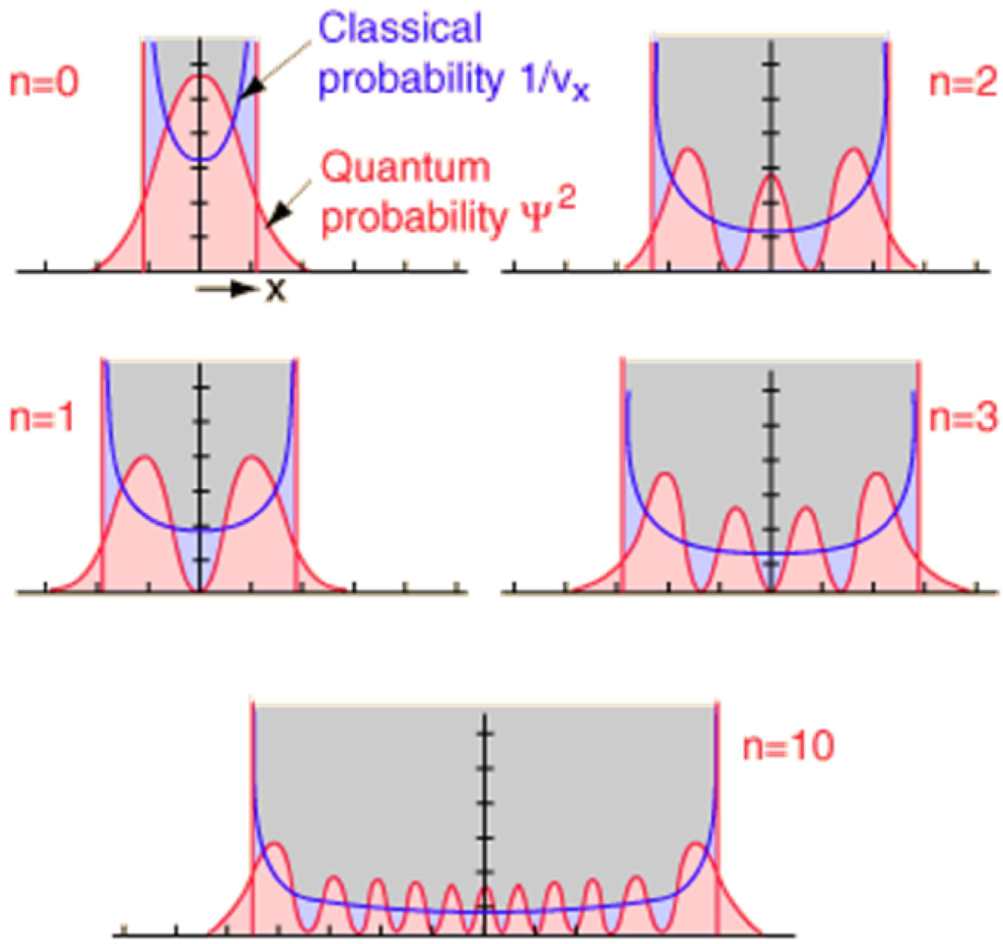
Consider a 30 kg child swinging at frequency of f=1 /s. What is the spacing between quantum energy levels? If her height is 1m, what is the total energy and what is n?

$$E = hf \approx 10^{-33} \text{ J}$$

$$E = mgh = 30 \cdot 10 \cdot 1 = 300 \text{ J}$$

$$n = \frac{E}{hf} \approx 10^{35}$$

This is very big!
Try sketching the probability of the QHO!



- As n increases the curves look more similar
- As n gets smaller behaviour diverges from what we expect

Why Are the Energy Levels Evenly Spaced?

Particle in a Box

$$E_n = \left(\frac{h^2}{8mL^2}\right) n^2$$

Not evenly spaced.

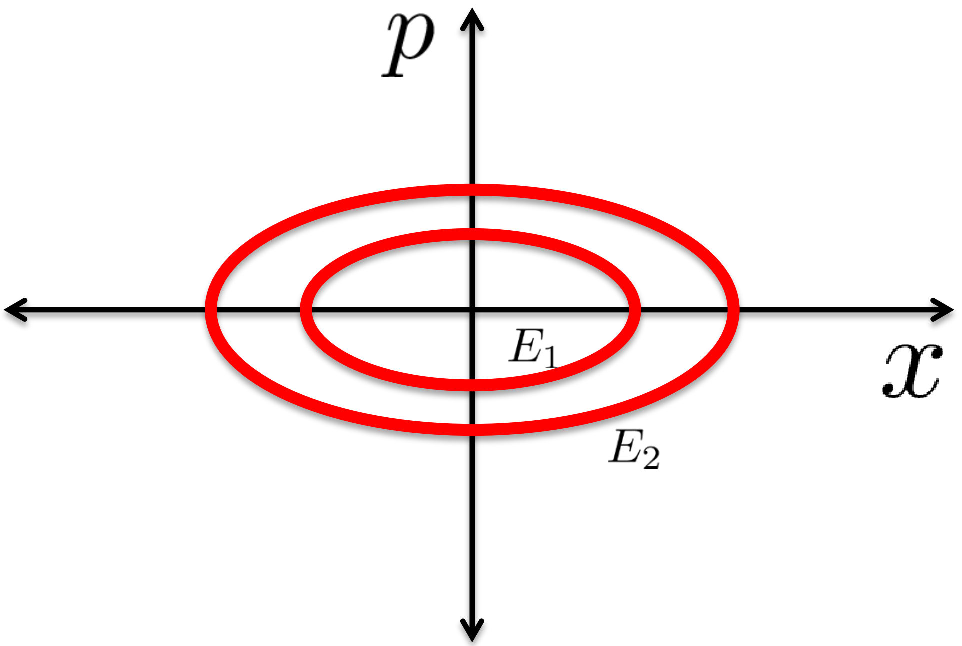
QHO

$$E_n = (n + \frac{1}{2})hf$$

Linear with n.

- Energy of harmonic oscillator is proportional to an area inside a so-called ***phase space***
- In QM, area in phase space must be integer multiples of Planck's constant.

Classical HO



At any point in space the particle has a ***definite position*** and subsequent ***trajectory***.

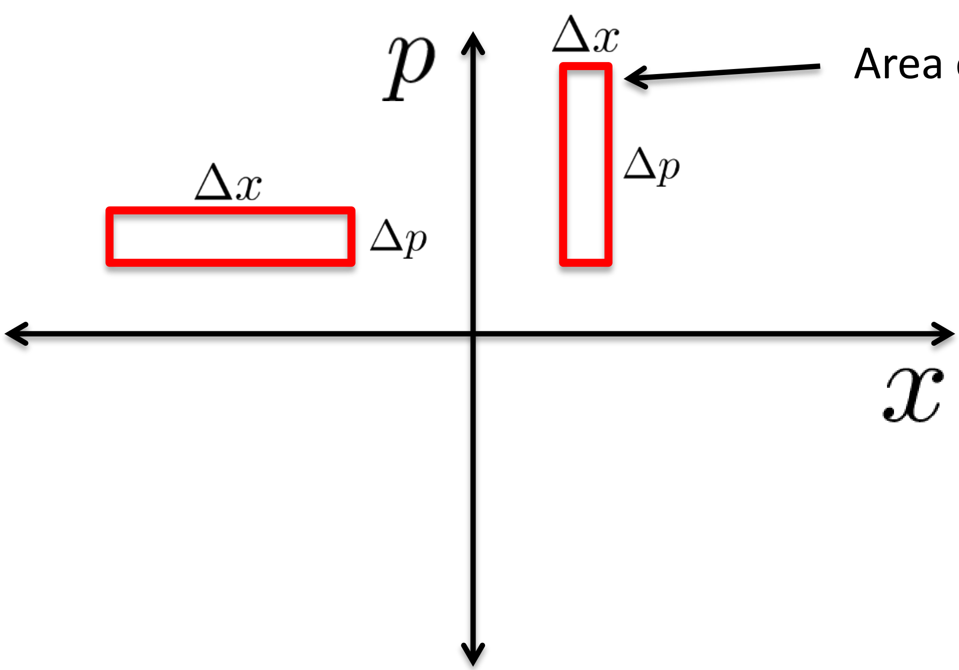
Not the case in QM!

HUP

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

From HUP we learned that the uncertainty in position and momentum cannot be smaller than a certain size.

$$\Delta p \uparrow \quad \Delta x \downarrow$$



Area of rectangle is: $\frac{h}{4\pi}$

We can play with the shape of the rectangle, but the area must remain the same!

Classical State = Point in Space

Quantum State = Region in Space

- It is as though phase space is “granular” or discrete at the ultramicroscopic scale of QM.
- The smallest grain as an area proportional to h (***Planck grain***)
- The smallest change in a quantum state must involve a change in the area of the region equivalent to adding or subtracting a Planck grain.

What is the area of a Planck Grain?

- We might guess $\frac{h}{4\pi}$ but it is actually h
- It is “fuzzier” than we have drawn (not a sharp-edged rectangle).
- Area is given by: $Area = nh$
- Using what we learned before gives:

$$E_n = Area \times h = nhf$$

- It is actually: $E_n = (n + \frac{1}{2})hf$

Particle in a Box

- Repeat this for a particle in a box. *Hint: Orbits will be rectangles instead of an ellipse with fixed length (not height).*

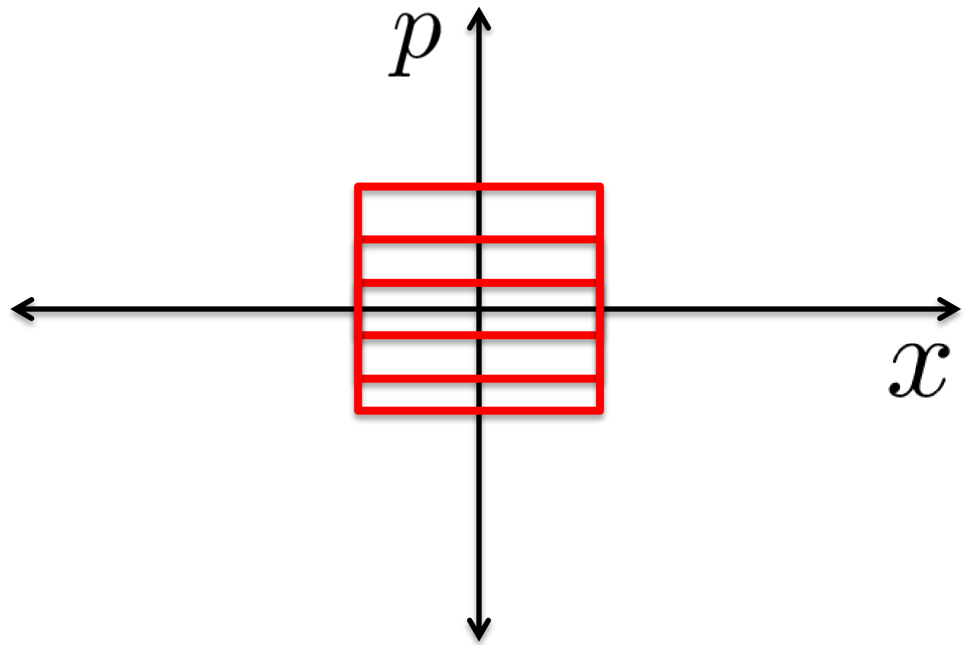
$$A = L \cdot p = L \cdot \sqrt{2mE}$$

$$E = \frac{A^2}{2L^2 m}$$

$$A = nh$$

$$E_n = \frac{n^2 h^2}{2L^2 m}$$

Off by a factor of 4.



Why is the Zero Point Energy ½ hf?

Recall the classical HO $$E = \frac{1}{2}mp^2(t) + \frac{k}{2}x^2(t)$$

p and x oscillate as sine and cosine functions of t. We see that E=0 requires that both p=0 and x=0

From QM, E=0 is impossible

- ***Argue based on HUP:*** If x=0 then Δx = 0. This means Δ p = ∞ (not 0!).
- ***Argue based on de Broglie:*** If E=0 then p=0 and this means λ = ∞. This is not possible for a bound particle!

Probabilities

- We know that QM deals in probabilities so let's set up many oscillators each at E_{min} and take a snapshot of their positions and take the average.

$$\langle x^2 \rangle$$

- Do the same for the momentum

$$\langle p^2 \rangle$$

- Together this gives:

$$\langle E \rangle = \frac{1}{2m}\langle p^2 \rangle + \frac{k}{2}\langle x^2 \rangle$$

The average of the square of the positions will not be zero!

- The larger $\langle x^2 \rangle$ the wider the scattering (like uncertainty!).
- Mathematically for HUP: $\sqrt{\langle x^2 \rangle} = \Delta x$
- Like a “standard deviation”
- Rename: $\Delta x \longrightarrow A_q$ (Quantum Amplitude)
- The quantum amplitude is not a “classical” amplitude. It describes the size of the quantum fuzziness.

- Follow the same line of reasoning for the momentum:

$$\sqrt{\langle p^2 \rangle} = \Delta p \geq \frac{h}{4\pi \Delta x} = \frac{h}{4\pi A_q}$$

- Let's go back to the energy equation:

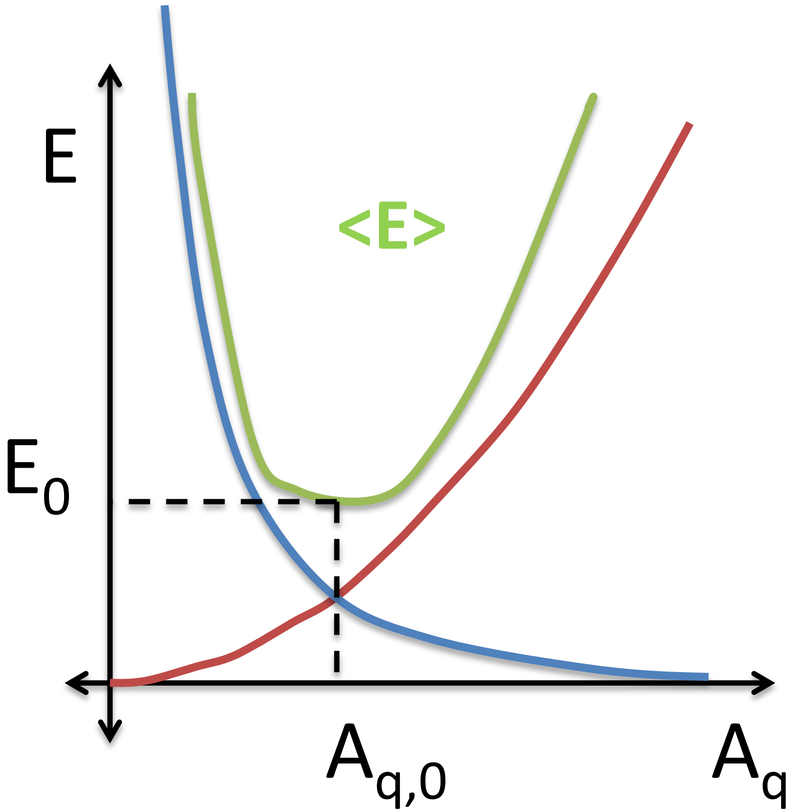
$$\langle E \rangle = \frac{1}{2m}\langle p^2 \rangle + \frac{k}{2}\langle x^2 \rangle \geq \left(\frac{h^2}{32\pi^2 m}\right)\frac{1}{A_q^2} + \left(\frac{k}{2}\right) A_q^2$$

QUANTUM TERM CLASSICAL TERM

Classical Term $\propto A_q^2$ If it was just this term then E = 0 when A_q =0

Quantum Term $\propto \frac{1}{A_q^2}$ Prevents A_q =0 because E blows up when A_q =0

$$\left(\frac{h^2}{32\pi^2 m}\right)\frac{1}{A_q^2} + \left(\frac{k}{2}\right)A_q^2$$



Classical Term $\propto A_q^2 \quad PE_q$

The total energy stored in the oscillator decreases as the quantum amplitude gets smaller.

Quantum Term $\propto \dfrac{1}{A_q^2} \quad KE_q$

The total energy stored in the oscillator *increases* as the quantum amplitude gets smaller (claustrophobia!).

What is the minimum energy?

$$\langle E \rangle = \left(\frac{h^2}{32\pi^2 m} \right) \frac{1}{A_q^2} + \left(\frac{k}{2} \right) A_q^2$$

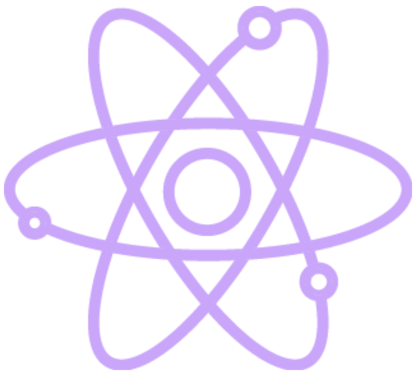
If you know calculus differentiate <E> as a function of A_q and set derivative to zero.

$$A_{q,0}^2 = \frac{h}{4\pi\sqrt{mk}}$$

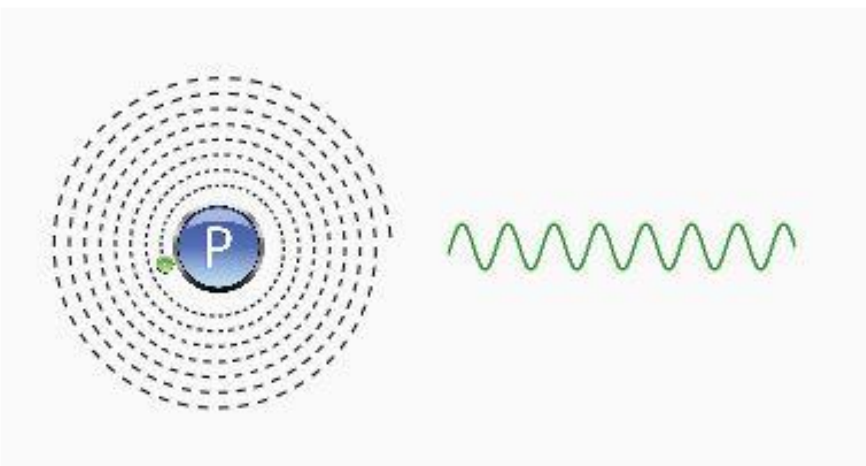
If you don't know calculus, sub the result into <E> and solve for E_0

$$E_0 = \frac{h}{4\pi}\sqrt{\frac{k}{m}} \qquad f = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \longrightarrow E_0 = \frac{1}{2}hf$$

The Hydrogen Atom

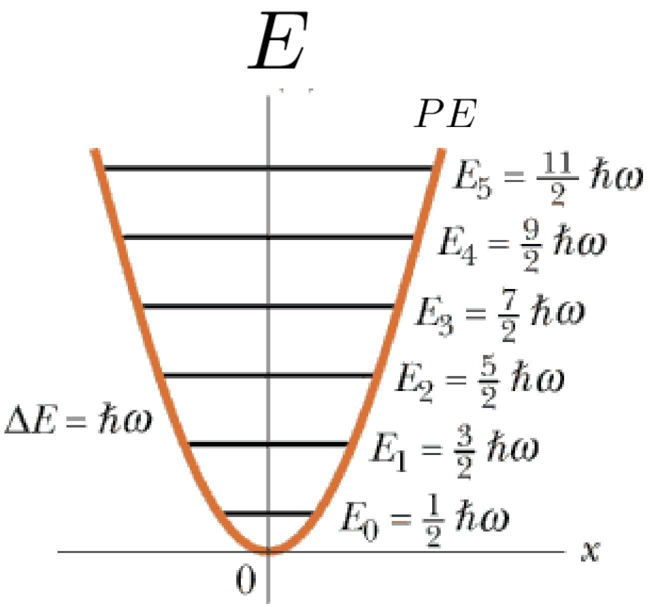


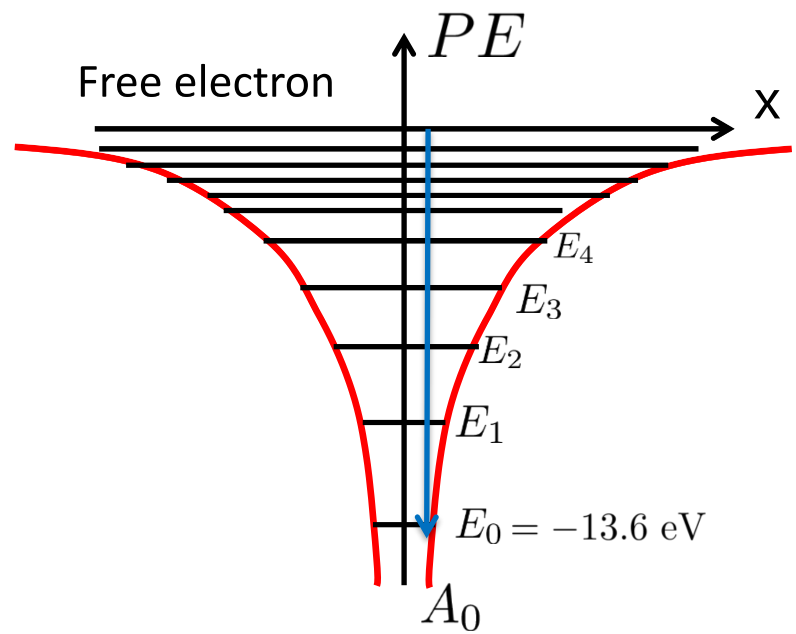
What is wrong with the classical model of the atom?



- Lower energy for smaller orbits
- No limit
- Loss of energy via E/M-radiation
- Unstable!

Electron in a Bowl versus an Atom





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

What is the PE or "bowl" for the atom?

$$PE = -\frac{ke^2}{r}$$

H-Atom

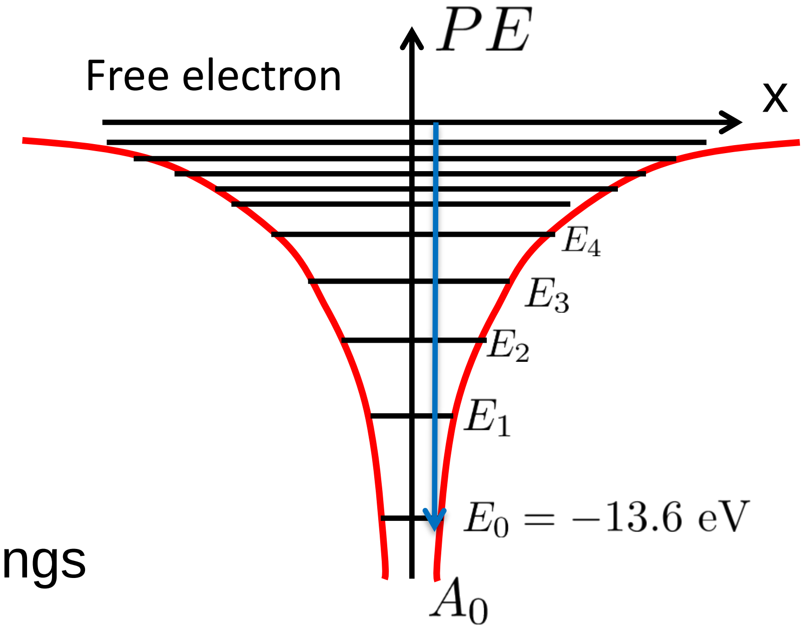
- Large R -> E->0
- Small R -> E-> ∞

- Ground State of electron is -13.6 eV

- The electron is “bound”
- “Bound Particle” = “Standing Wave”

- The PE determines the E- level spacings

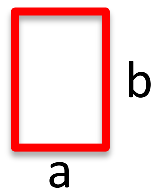
- A_o is the quantum fuzziness -> Bohr Radius



Stability of Atom

- Recall, there is a general property of any bound particle in any number of dimensions:

$$KE_{min} = \frac{h^2}{2mS^2}$$



$$\frac{1}{S^2} = \frac{1}{2a^2} + \frac{1}{2b^2}$$

- S is a number characteristic of the "size" of the region the particle is bound to (i.e. particles are claustrophobic)

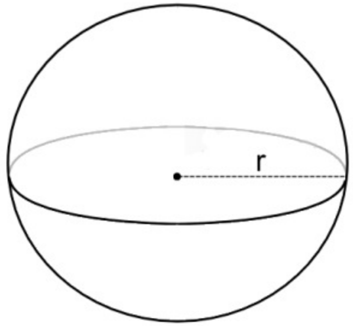
What is the Shape & Size of Bound Region?

- If we make repeated measurements of the electron’s position we find:
  - All angles are equally likely (spherically symmetric)
  - R = average(r1, r2, r3)
  - Electron is bound to a ***ball*** of radius R

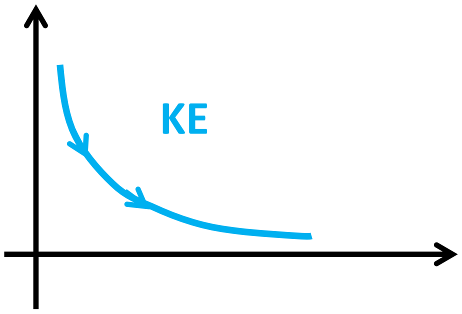
Zero Point Energy

- Minimum KE: $$KE_{min} = \frac{h^2}{2mS^2}$$

- S is a number characteristic of the size of the ball of radius R



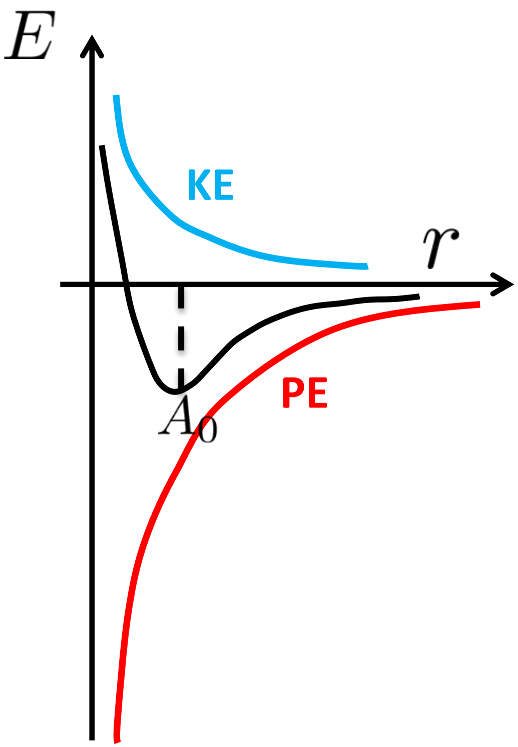
$$S = 2\pi R$$ Length of great circle



$$KE_{min} = \frac{h^2}{8\pi^2 mR^2}$$

- Tendency to lower energy states, which leads to an expansion of the atom. ***Opposes the tendency to collapse!***

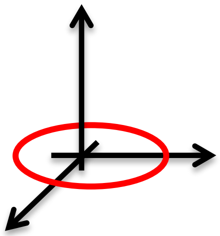
Atom is Stabilized by HUP



- As photons are emitted (higher-> lower orbital jumps), the atom gets smaller (same as classical)
- But there is a limit! If enough energy is emitted, it cannot get smaller without re-gaining energy again.
- ***HUP is necessary for atoms to exist***.

Problems with Bohr Model

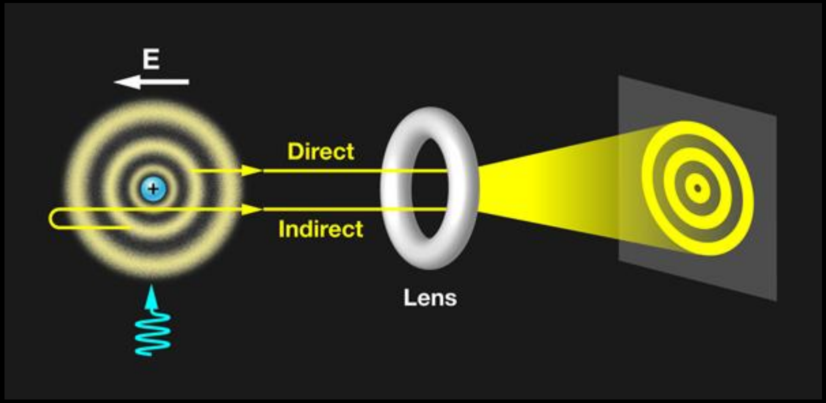
- “Orbits” in plane simply can’t exist

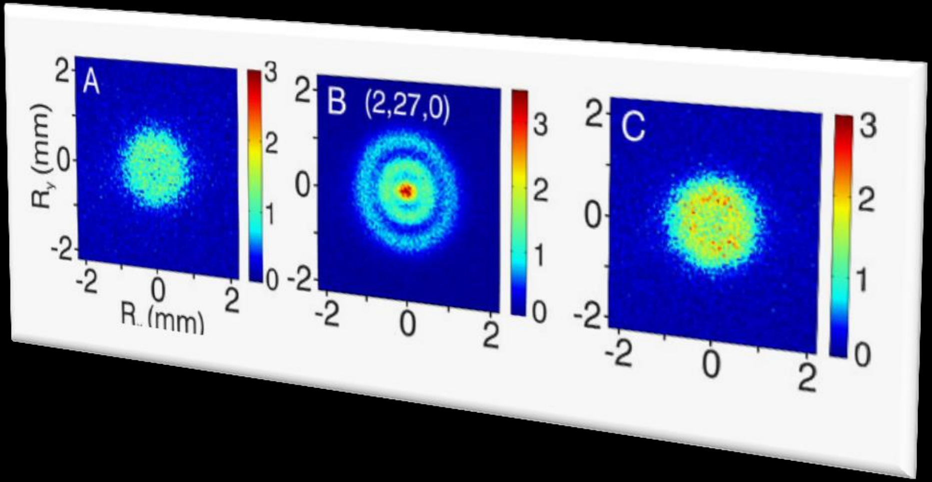


$$\Delta z = 0 \rightarrow \Delta p_z = \infty$$

- Ground state is spherically symmetric.

IMAGING THE HYDROGEN ATOM

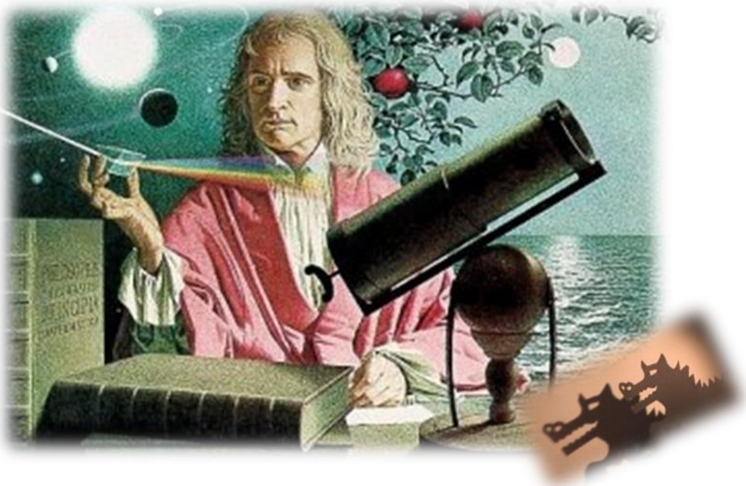


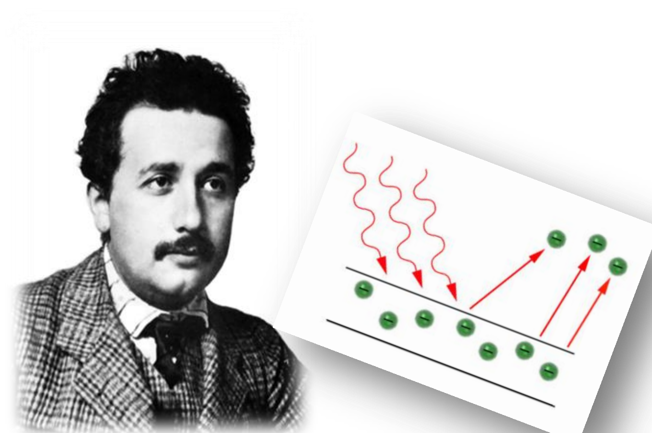


Photons

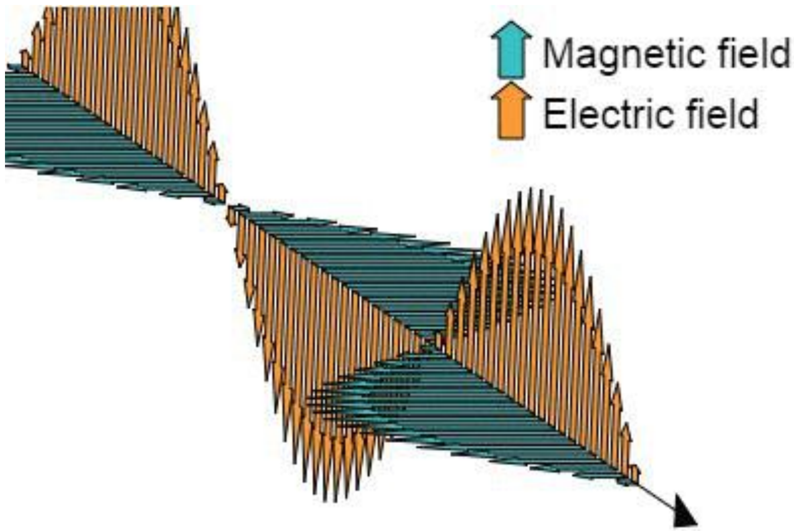
$$E = hf$$

We see waves behaving like particles!





MAXWELL – Electromagnetic Wave



$$\nabla \cdot \mathbf{E} = \frac{1}{\epsilon_0}\rho$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial \mathbf{t}} = 0$$

$$\nabla \times \mathbf{B} - \mu_0\epsilon_0\frac{\partial \mathbf{E}}{\partial \mathbf{t}} = \mu_0\mathbf{J}$$

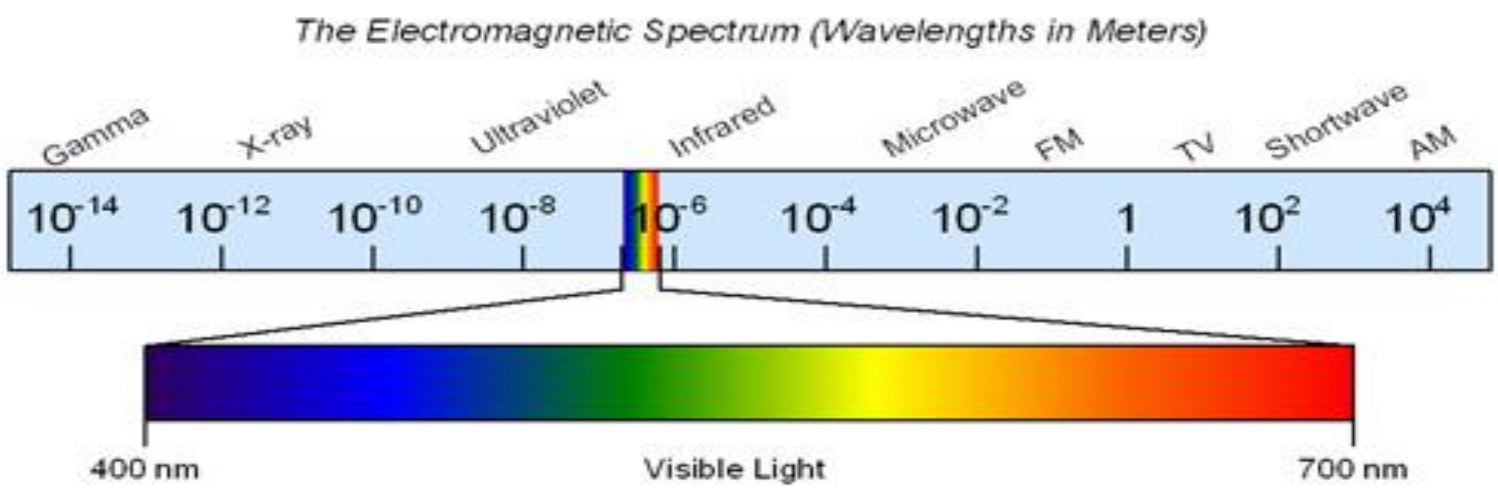
Light is an E/M Field

- Electric and Magnetic Fields store energy (i.e. capacitor)

- E and M energy can be interconverted.
  - Changing an M-field induces an E-field
  - Changing an E-field induces an M-field
  - This continuous process allows the wave to propagate through space.

The Electromagnetic Spectrum

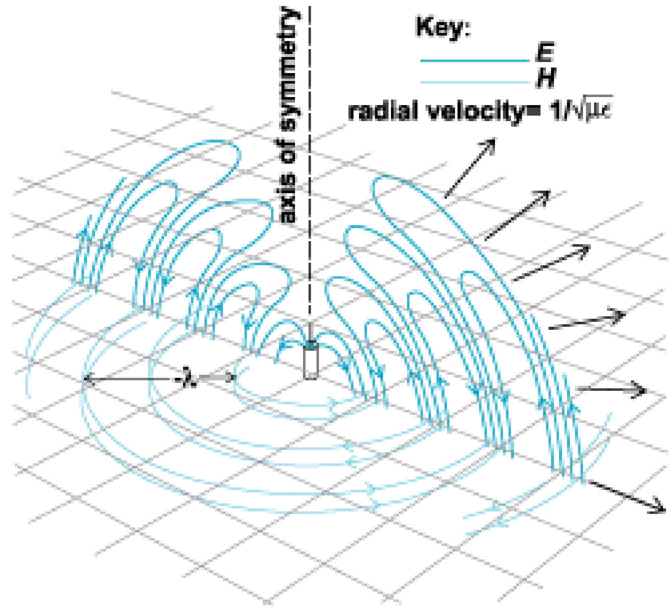
- Electromagnetic waves can have an infinite range of frequencies (or wavelengths)
- Some frequencies (wavelengths) are visible to the unaided human eye, which interprets different frequencies as different colours
- Most of the frequencies are not visible to the human eye



How are electromagnetic waves created?

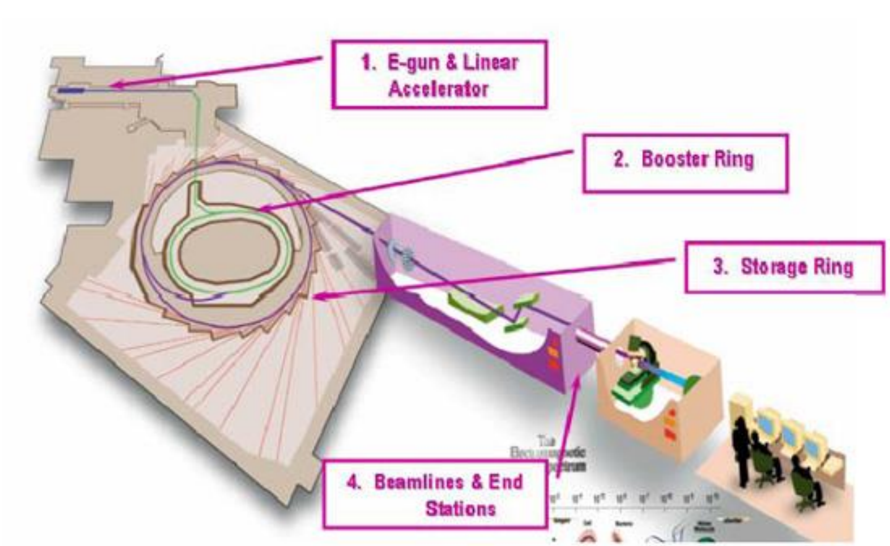
• Electromagnetic waves are created by the acceleration of charged particles.

• Radio-waves are created by the motion of electrons in antennae. The frequency of the periodic motion of the electrons determine the frequency of the wave.



Electric and magnetic field created by a small antenna

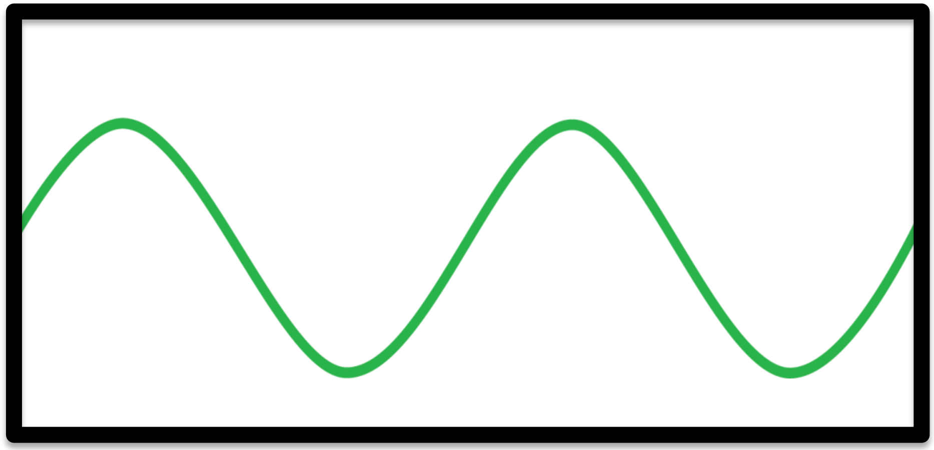
http://www.answers.com/topic/electromagnetic-wave-transmission



http://www.lightsource.ca/education/whatis.php

• At the other end of the spectrum, x-ray can be produced by accelerating electrons in synchrotrons.

Trap Light in a Box with Mirrors



- Trapping light is like trapping energy
- We get a standing wave!
- It sloshes back and forth between E-field and M-field energy
- Looks like a Harmonic Oscillator!

Discrete Energy

- QM says energy is discrete!

n is the # of photons!

- For the QHO we saw that $E_n = (n + \frac{1}{2})hf$

- Imagine populating an oscillator with some # of photons:
  - 7 photons of hf_1
  - 4 photons of hf_2
  - What is the total energy of the box?

$$E = 7hf_1 + 4hf_2 + \dots$$

Laser

A 200 W infrared laser emits photons of wavelength 2.0 x 10^{-6} m. What is the photon energy? How many photons are emitted?

$$E = hf = \frac{hc}{\lambda} = \frac{6.626 \times 10^{-34} \cdot 3 \times 10^{8}}{2 \times 10^{-6}} = 10 \times 10^{-20} \text{ J}$$

$$n = \frac{200 \text{ J/s}}{10 \times 10^{-20} \text{ J/photon}} = 2 \times 10^{21} \text{ photons/s}$$

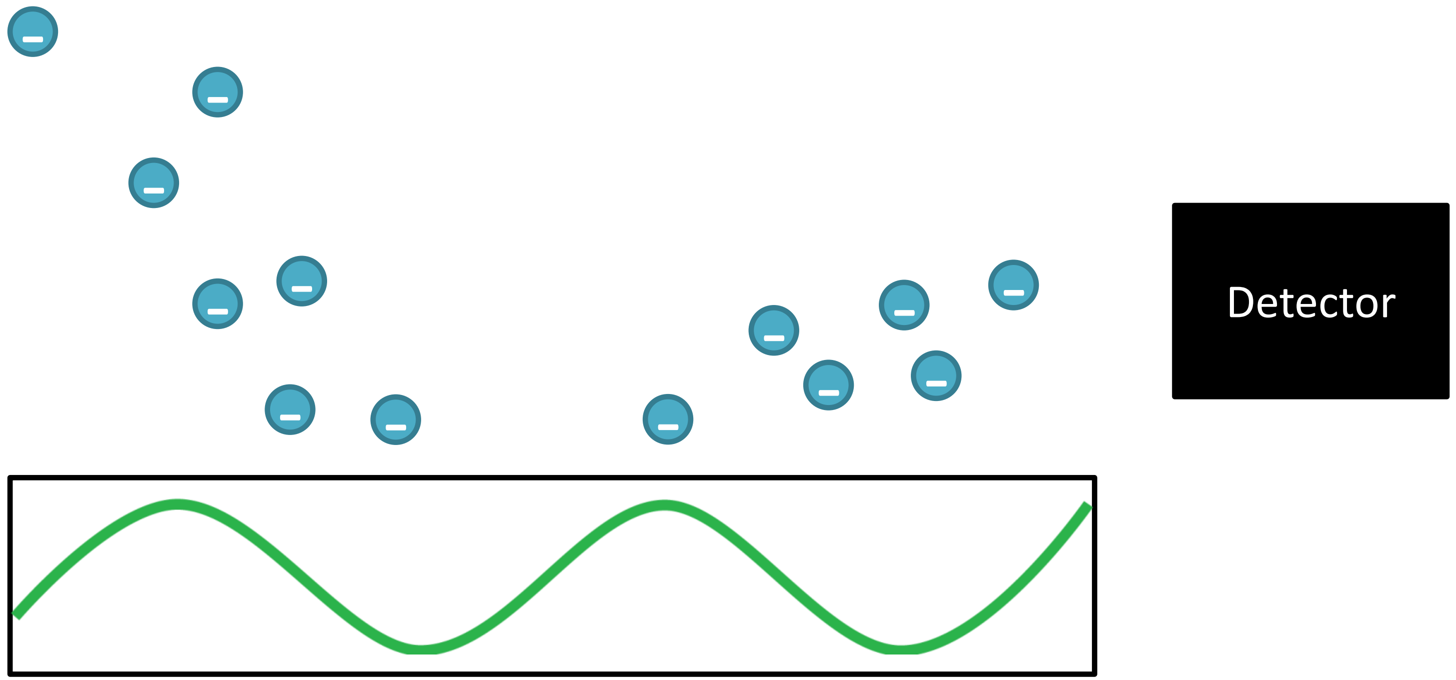
Is the photon a particle? Is it *localized*?

- It appears like light is non-local (spreads out)
- But light deposits energy in tiny localized bundles
- When we measure energy, photons are localized. When we don’t measure, they are non-local.
- Behaves like a wave, but acts like a particle when we measure it!

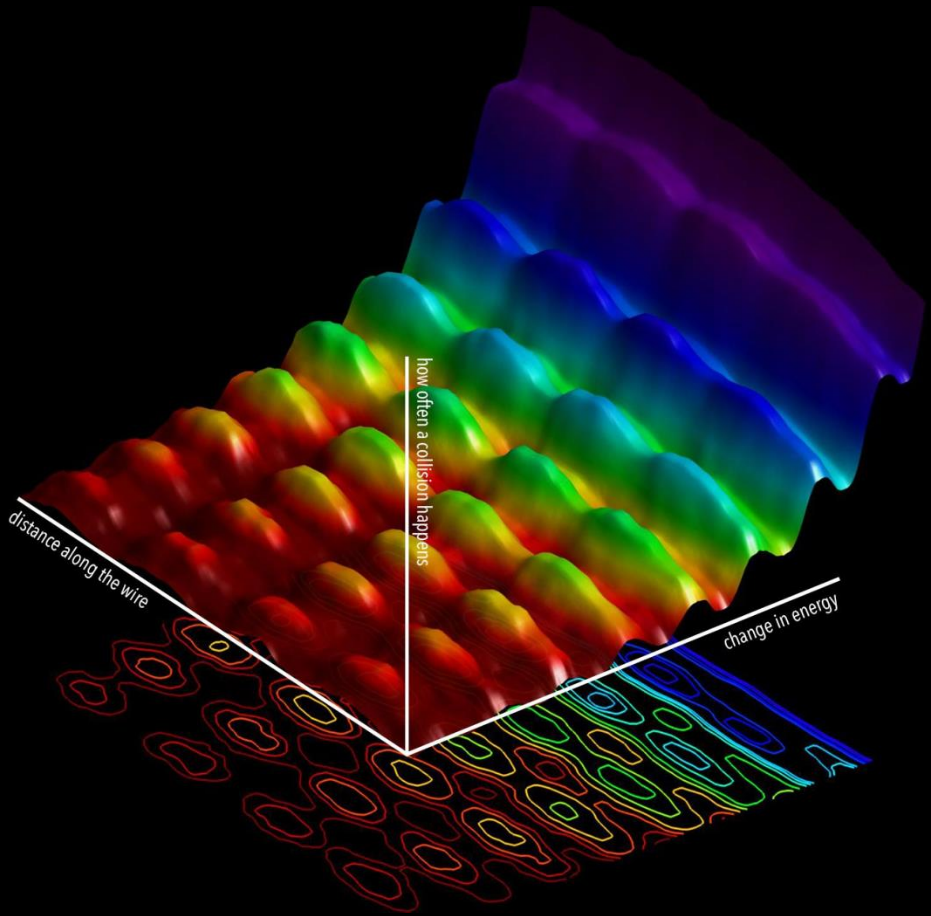
The Wavefunction

- The square of ψ tells us the probability that if we do measure the photon we will find it there.
- Classically ψ^2 is the square amplitude of the EM-field in that volume.
- This means the EM energy in a small volume of space is proportional to the probability of finding a photon in that volume.

CAN YOU TAKE A PICTURE OF LIGHT?


Detector

LIGHT'S FIRST PHOTOGRAPH!



Particle in a Box

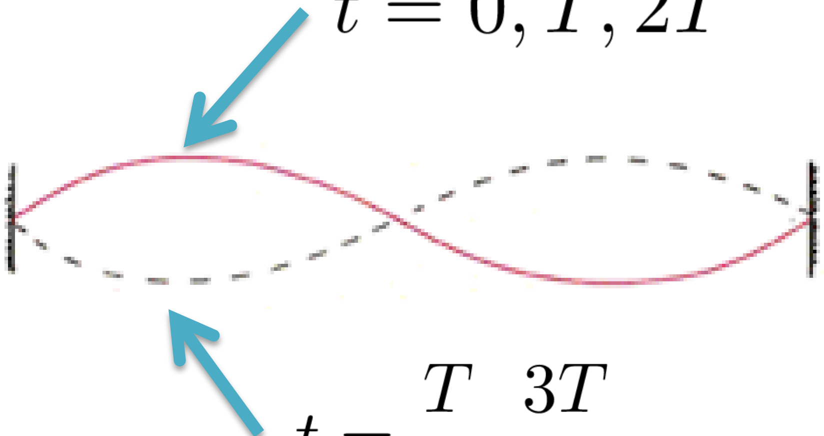
$$\psi = \psi_L + \psi_R$$

Sketch the standing wave at different moments in time.

Snapshots

What does it look like at T/4?

$$t = 0, T, 2T$$

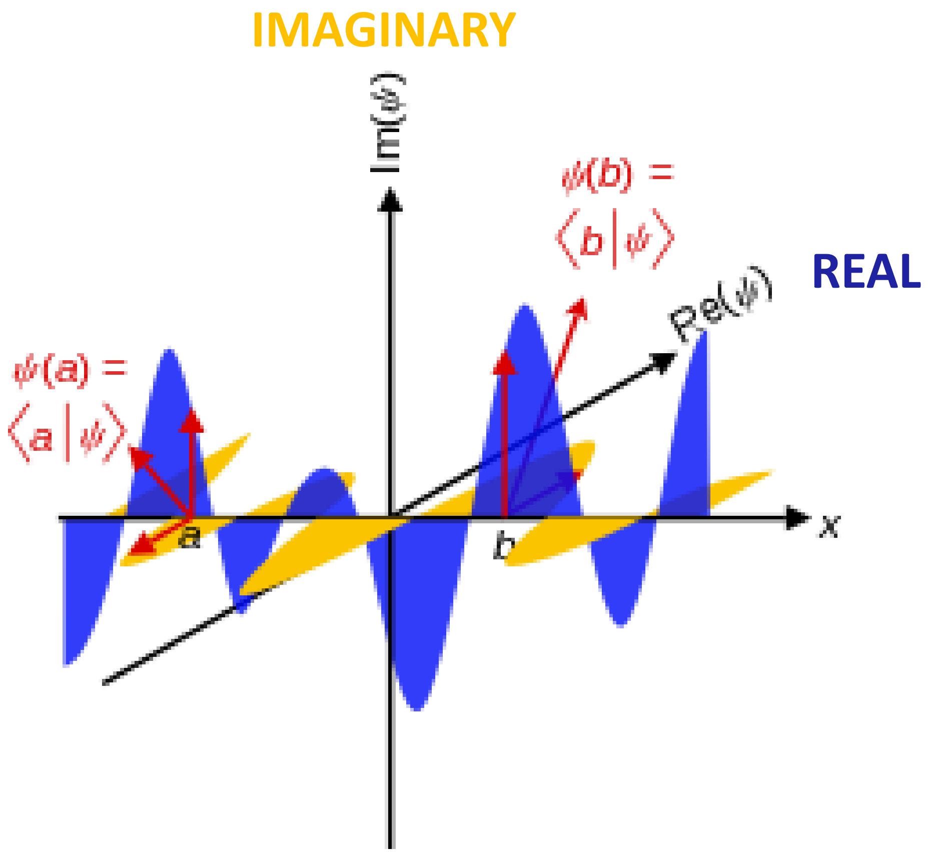


$$t = \frac{T}{2}, \frac{3T}{2}$$

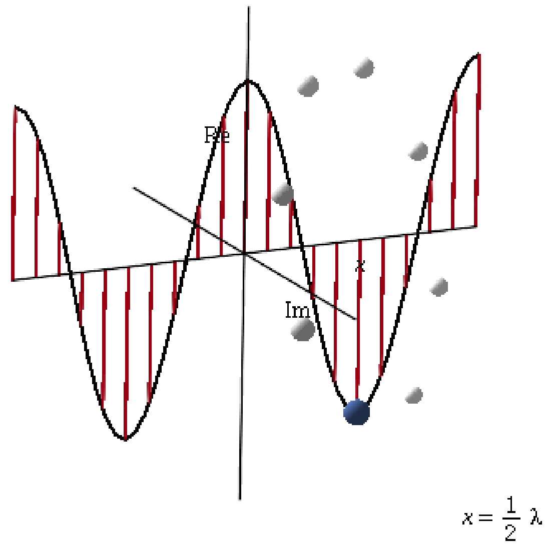
$$P = \psi^2 = 0$$

- No probability of finding the particle anywhere!!
- Does that mean it blinks in out of existence?

Complex Waves

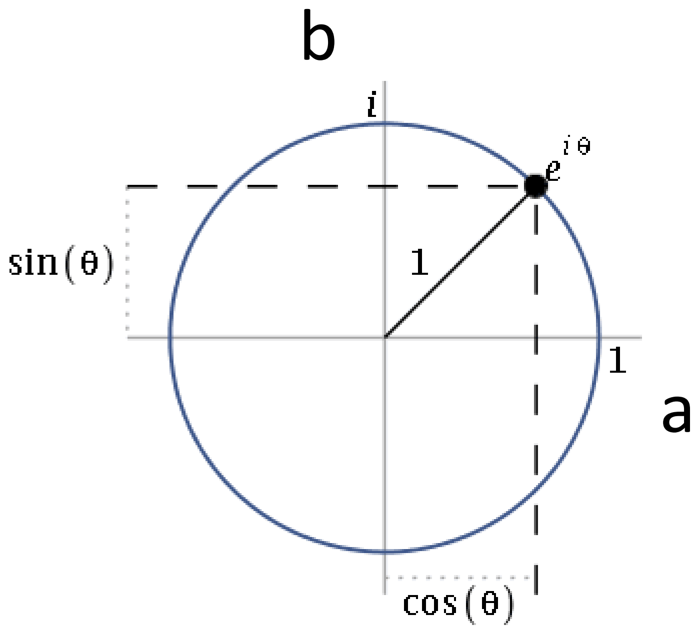


Complex Standing Wave



At a fixed time	**At a fixed position**
$t = T$	$x = \frac{1}{2}\lambda$
How the wave **looks through space** *at that time*:	How the wave **varies with time** *at that position*:
$\psi(x) = 2\cos\left(2\,\frac{\pi x}{\lambda}\right)$	$\psi(t) = -2e^{\left(-2i\frac{\pi t}{T}\right)}$
$x =$	$t =$
$-\lambda \quad -\frac{\lambda}{2} \quad 0 \quad \frac{\lambda}{2} \quad \lambda$	$0 \quad \frac{T}{4} \quad \frac{T}{2} \quad \frac{3T}{4} \quad T$

Complex Numbers



$$x = a + ib$$

$$\psi = \cos(k\theta) + i\sin(k\theta)$$

$$\psi = \cos\left(\frac{1}{\hbar}(px - Et)\right) + i\sin\left(\frac{1}{\hbar}(px - Et)\right)$$

$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$\psi = e^{i\frac{1}{\hbar}(px - Et)}$$

Taking the Square of a Complex Number

$$x = a + ib$$

$$|x|^2$$

$$|x|^2 = (a + ib)(a - ib) = a^2 + b^2$$

Solution

$$\psi = \cos(\frac{1}{\hbar}(px - Et)) + i\sin(\frac{1}{\hbar}(px - Et))$$

At T/4

$$P = |\psi|^2 > 0$$

- Probability pattern is static
- Particle does not disappear!
- P does not depend on time (it is a stationary state!)
- Particle is always present with the same constant probability pattern!

Quantum Field Theory

- MATTER (e-, p, n) are ***quantum particles***

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

- FORCES (EM) are also ***quantum particles***

$$\lambda = \frac{h}{p} \longrightarrow E = hf$$

Quantum seems to be suggesting a **UNIFICATION** of matter and forces.

QFT

Box of Photons
Box of H.O.s

=

Box of Electrons
Box of Q.H.O.s

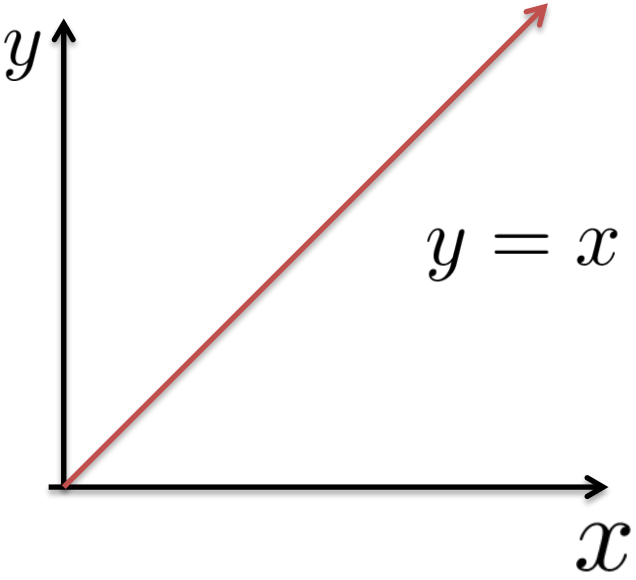
- Putting electrons on the same footing as photons leads us to QFT
- A single theory that encompasses all known types of matter and forces in the Universe
- This leads us to the standard model (experimentally a success)
- Except gravity!

What is Schrödinger's Equation?

- The most general and fundamental postulate in quantum mechanics

- Differential equation

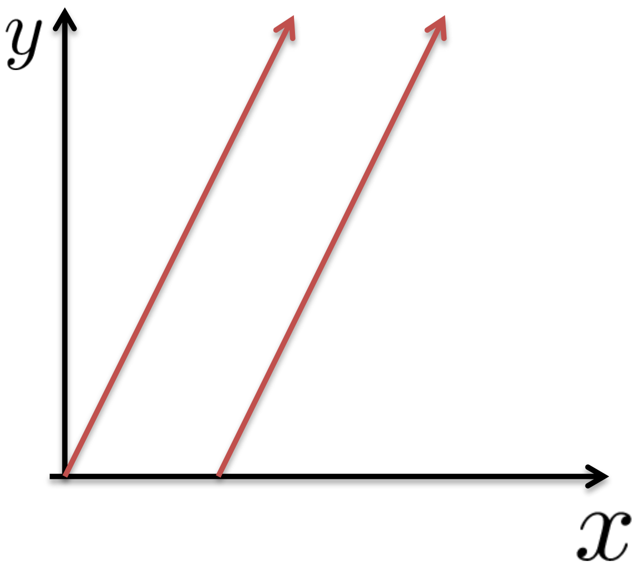
- Derivative -> slope



Differential Equation

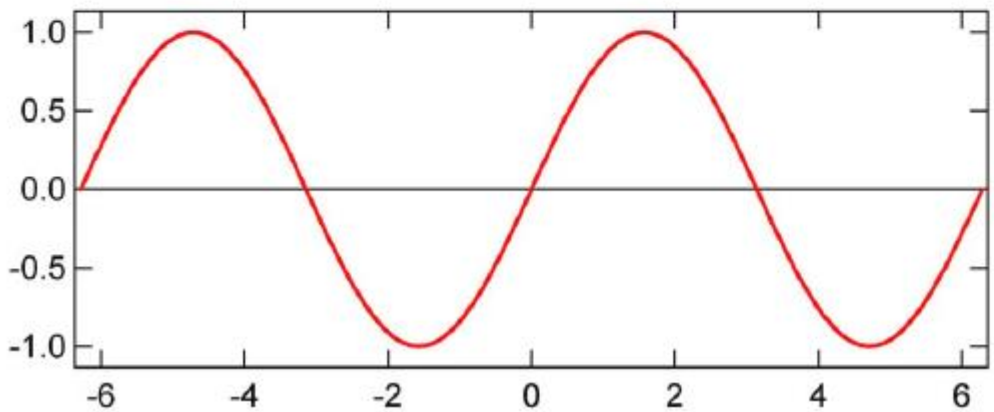
$$\frac{dy(x)}{dx} = 2$$

Which functions y(x) have a derivative of 2?

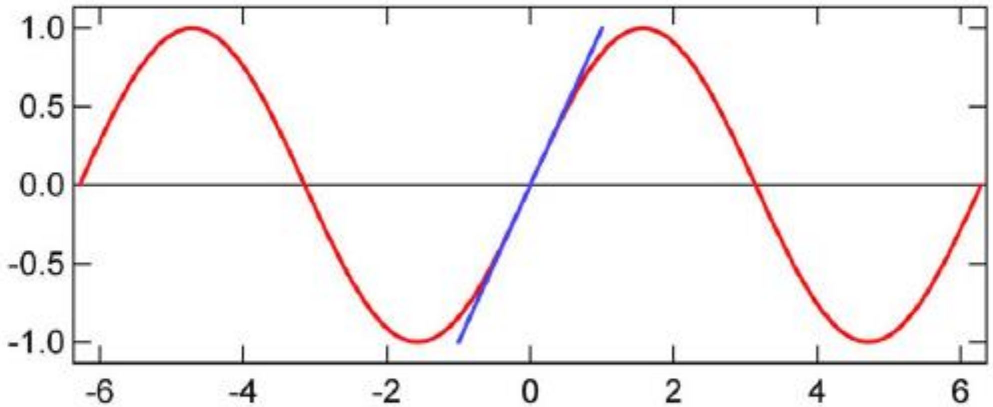


$$y(x) = 2x + b$$

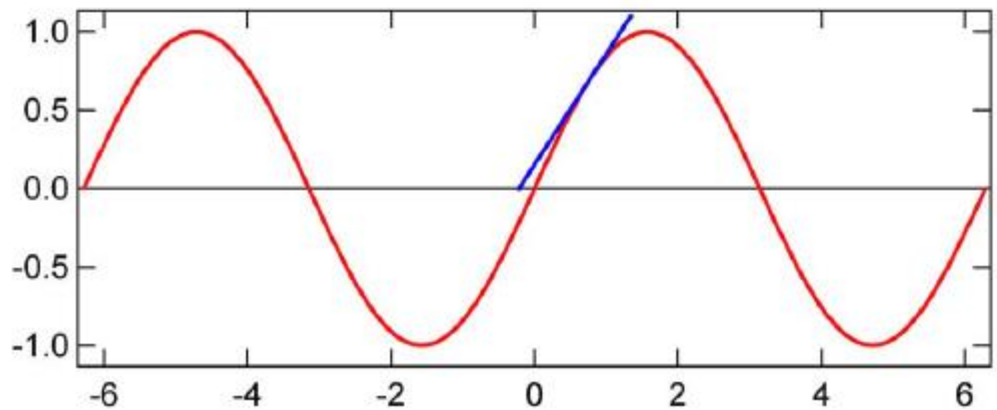
$$y = \sin(x)$$



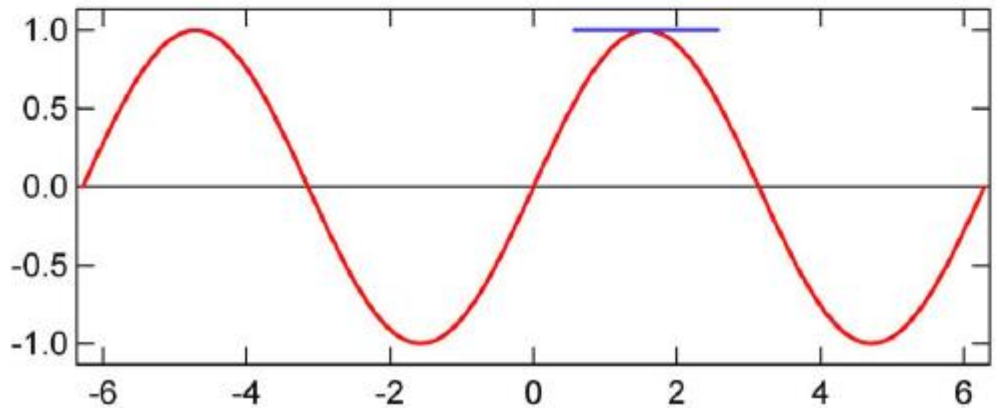
$$\text{slope} = 1$$



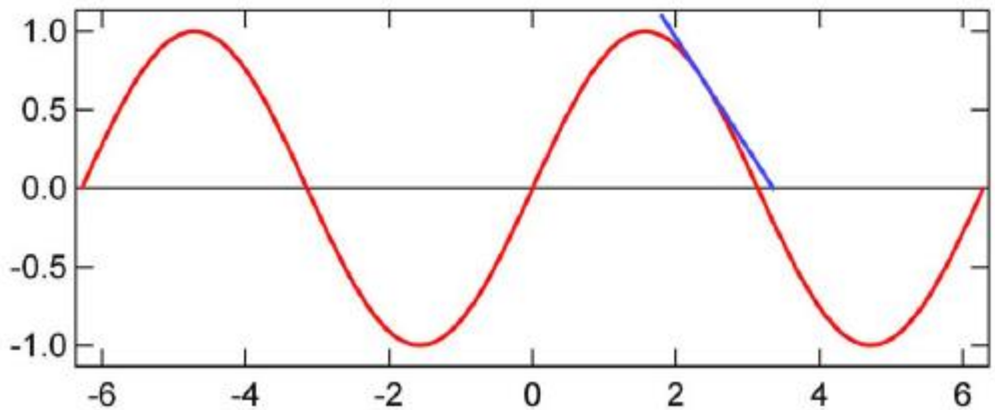
$$\text{slope} = \frac{1}{\sqrt{2}}$$

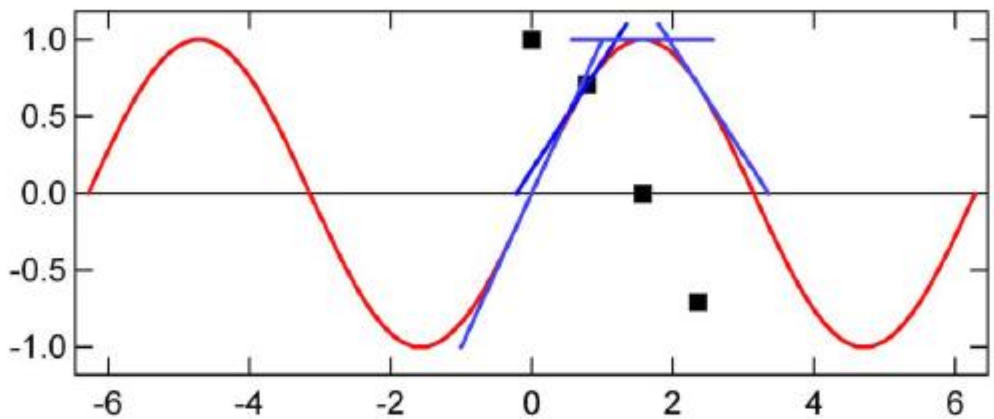


$$\text{slope } = 0$$

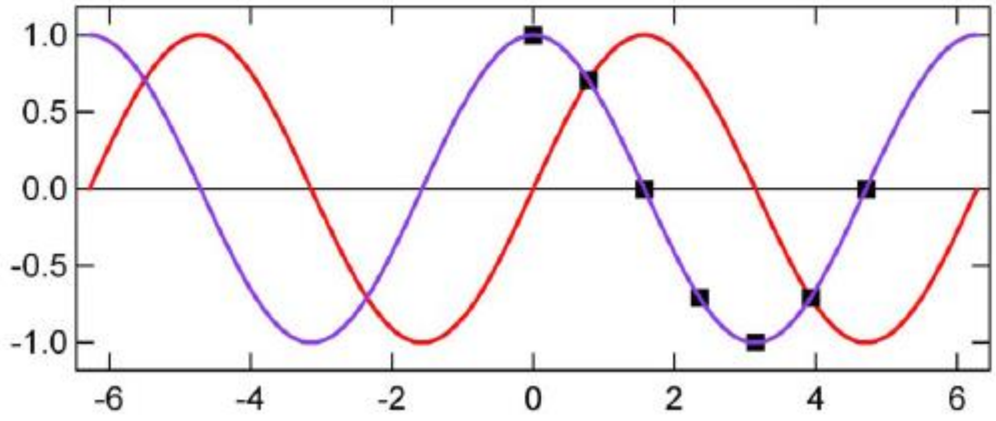


$$\text{slope } = \frac{-1}{\sqrt{2}}$$



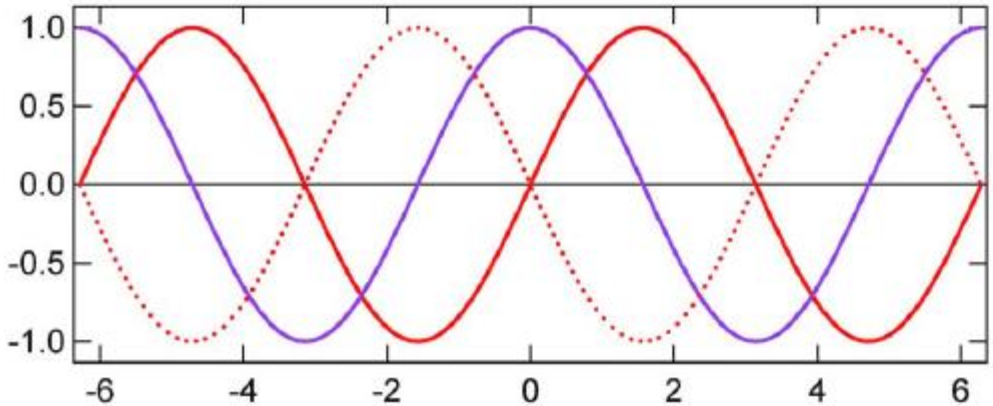

1.0
0.5
0.0
-0.5
-1.0
-6
-4
-2
0
2
4
6

The derivative of sin(x) is cos(x)!



$$\frac{d}{dx}\sin(x) = \cos(x)$$

The derivative of cos(x) is -sin(x)!



$$\frac{d}{dx}\cos(x) = -\sin(x)$$

What is the derivative of the derivative of sin(x)? (This is called the second derivative!)

$$\frac{d}{dx}\frac{d}{dx}\sin(x) \longrightarrow \frac{d^2}{dx^2}\sin(x) = -\sin(x)$$

Time-Independent Schrödinger's Equation

How to derive?

$$KE + PE = E$$

$$\frac{p^2}{2m}$$

Stationary wave function

energy

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

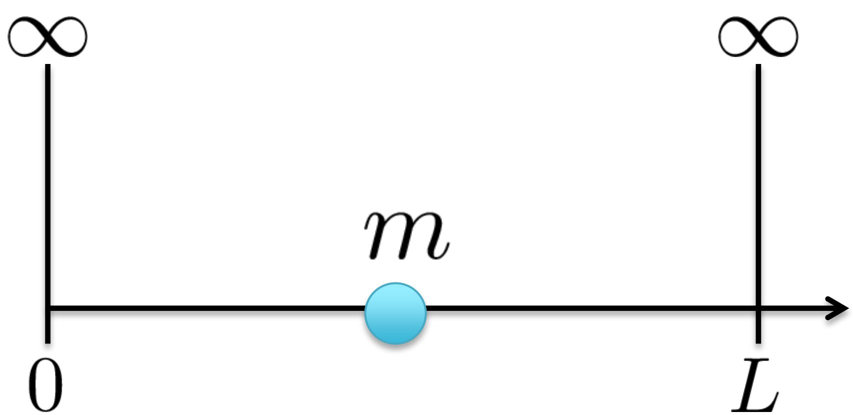
Mass of particle

Potential energy

TISE for Particle in a Box

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

$$\psi(x) = A\sin(kx) + B\cos(kx)$$



In this case PE=0

TISE for Particle in a Box

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

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

We know that the probability of finding the particle at x=0 or x=L is 0.

This means B=0!

$$\psi(x) = A\sin(kx)$$

What is k?

$$\psi(x) = A\sin(kx)$$

$$\frac{d\psi}{dx} \qquad\qquad \frac{d\psi}{dx} = kA\cos(kx)$$

$$\frac{d^2\psi}{dx^2} \qquad\qquad \frac{d^2\psi}{dx^2} = -k^2 A\sin(kx)$$

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

$$k = \left(\frac{8\pi^2 mE}{h^2}\right)^{1/2}$$

What is A?

$$\psi = A\sin\left(\frac{8\pi^2 mE}{h^2}\right)^{1/2} x$$

To find A we will use the boundary conditions again. The probability of finding the particle at x=0 or x=L is zero.

$$0 = A\sin\left(\frac{8\pi^2 mE}{h^2}\right)^{1/2} L$$

$$\left(\frac{8\pi^2 mE}{h^2}\right)^{1/2} L = n\pi$$ where n = 1, 2, 3

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

What is A? $$\psi = A \sin \frac{n\pi}{L} x$$

To determine A remember that the total probability of finding the particle in the box is 1.

$$\int_0^L \psi^2 dx = 1$$

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

$$A = \sqrt{\frac{2}{L}}$$

Solution

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right) x$$

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

$$E = \frac{h^2 n^2}{8mL^2} = E_{zp} n^2$$

Schrödinger's Equation

- Classical Harmonic Oscillator
  - Energy Conservation $\frac{1}{2}mv^2 + \frac{1}{2}kx^2 = E$
  - Newton's Laws $F = ma = -kx$

- Quantum Harmonic Oscillator
  - Energy Conservation $\frac{p^2}{2m} + \frac{1}{2}kx^2$
  - Schrödinger's Equation

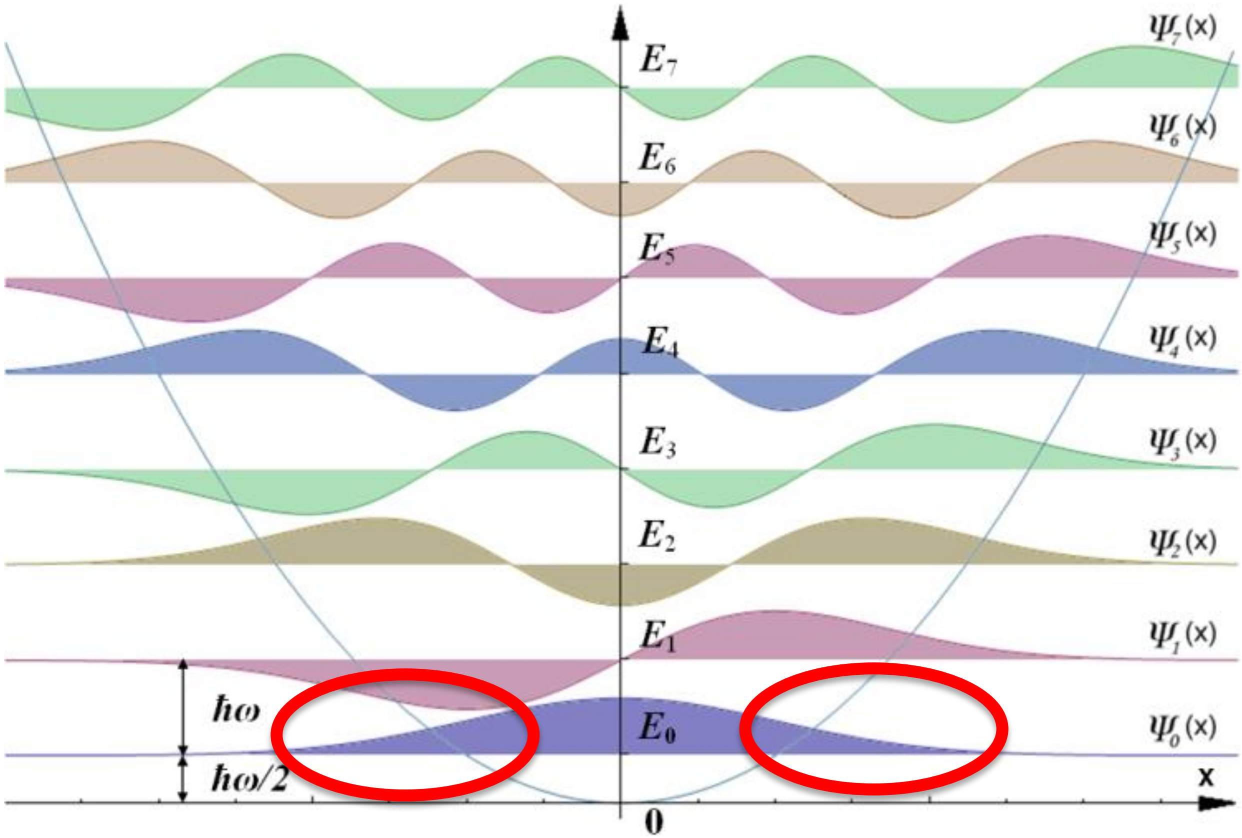
$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{2m}{\hbar^2}\left[E - U(x)\right]\psi(x)$$

Quantum Recipe

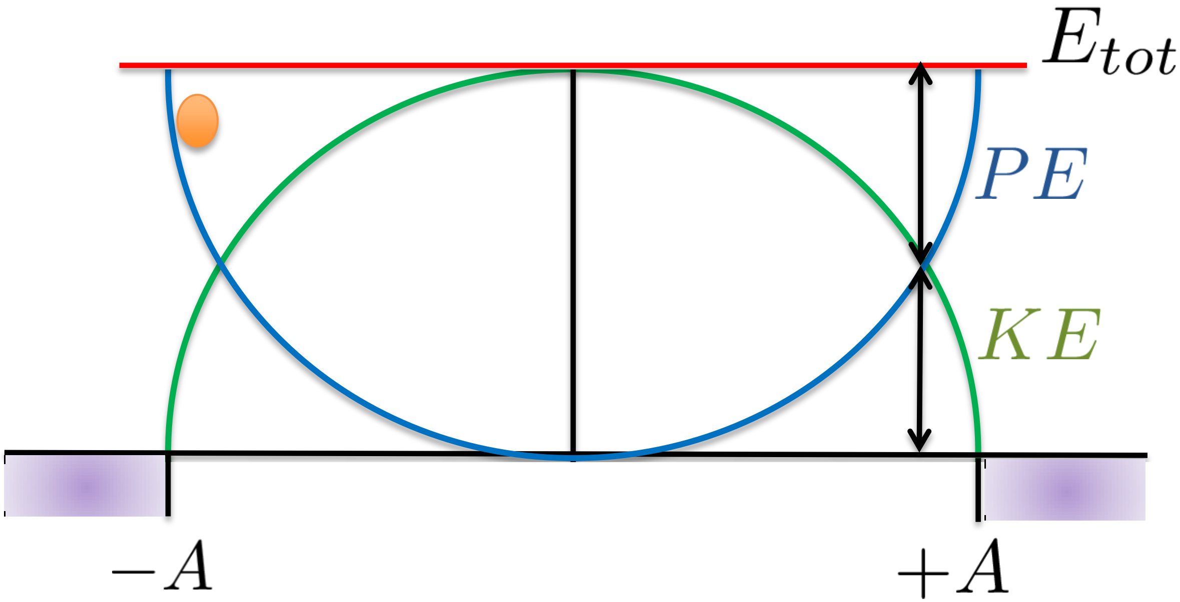
- How does a quantum system change with space and time?
  - What is my bowl or box? (ie. What is the PE?)
  - Apply my boundary conditions
  - Solve the TISE or the TDSE
  - Find the wavefunction
  - Find the allowed energies

- Sounds easy, but differential equations are actually really hard to solve most of the time!

How can a mass move into a classically forbidden region?

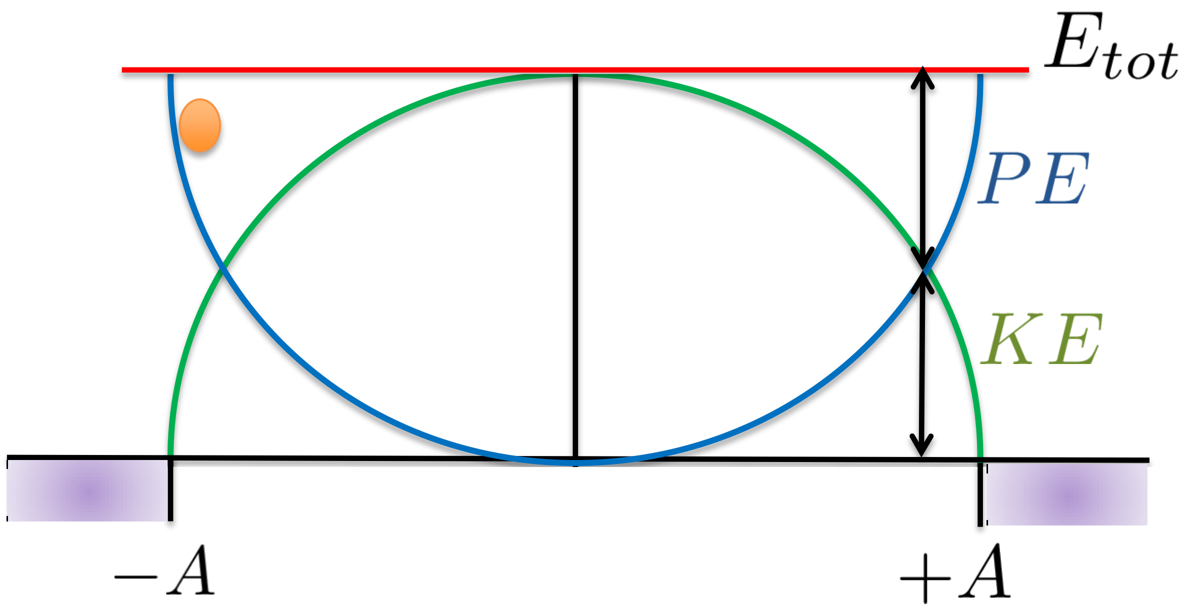


$$E_{total} = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}kA^2$$

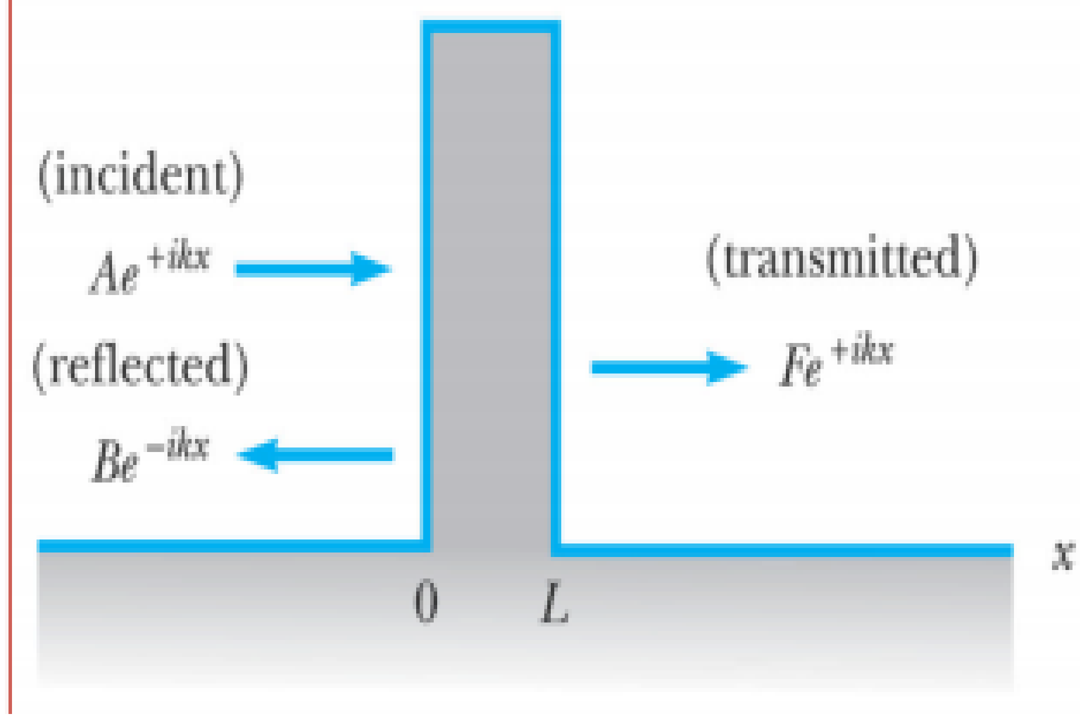


- Classically the turning points are $\pm A$
- As x approaches A the KE goes to zero. This why the mass stop!

$$E_{total} = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}kA^2$$



- How could the mass go past $\pm A$?
- This would mean: $PE > E_{tot}$
- This would require KE to be negative (i.e. $p^2 < 0$)
- p is an imaginary number!



$$(x<0) \qquad \psi = Ae^{ikx} + Be^{-ikx}$$

$$(0<x<L) \qquad \psi = Ce^{\kappa x} + De^{-\kappa x}$$

$$(x>L) \qquad \psi = Fe^{ikx}$$

$$y(x) = y_{edge} e^{-\frac{x}{h}}$$

$$h = \frac{\hbar}{\sqrt{2m(U - E)}}$$

- Sun shines via nuclear fusion
  - 4 protons stick together to form He
  - These protons need energy to overcome the Coulomb Barrier

Temperature: 15 000 000 000 degrees

Sun: 10 000 000 000 degrees

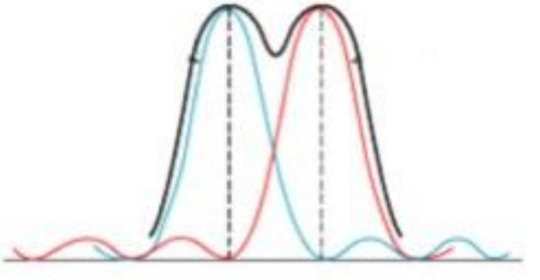
Solution: Tunneling!

There is a small probability of particles passing through impenetrable barriers!

This is what powers the sun!

Electron microscopy vs. Light microscopy

• The <u>resolution</u> of a microscope corresponds to the shortest distance between two points that can still be distinguished by the observer as separate entities.

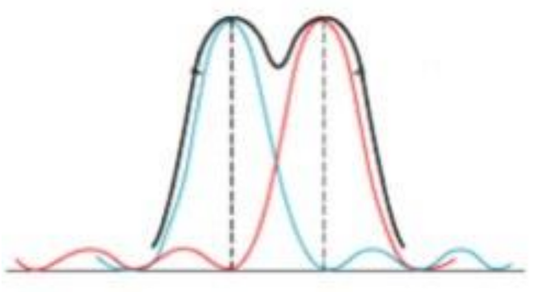


Electron microscopy vs. Light microscopy

• Because of HUP, the best resolution that can be achieved using radiation or particles with wavelength λ is ~λ/2.

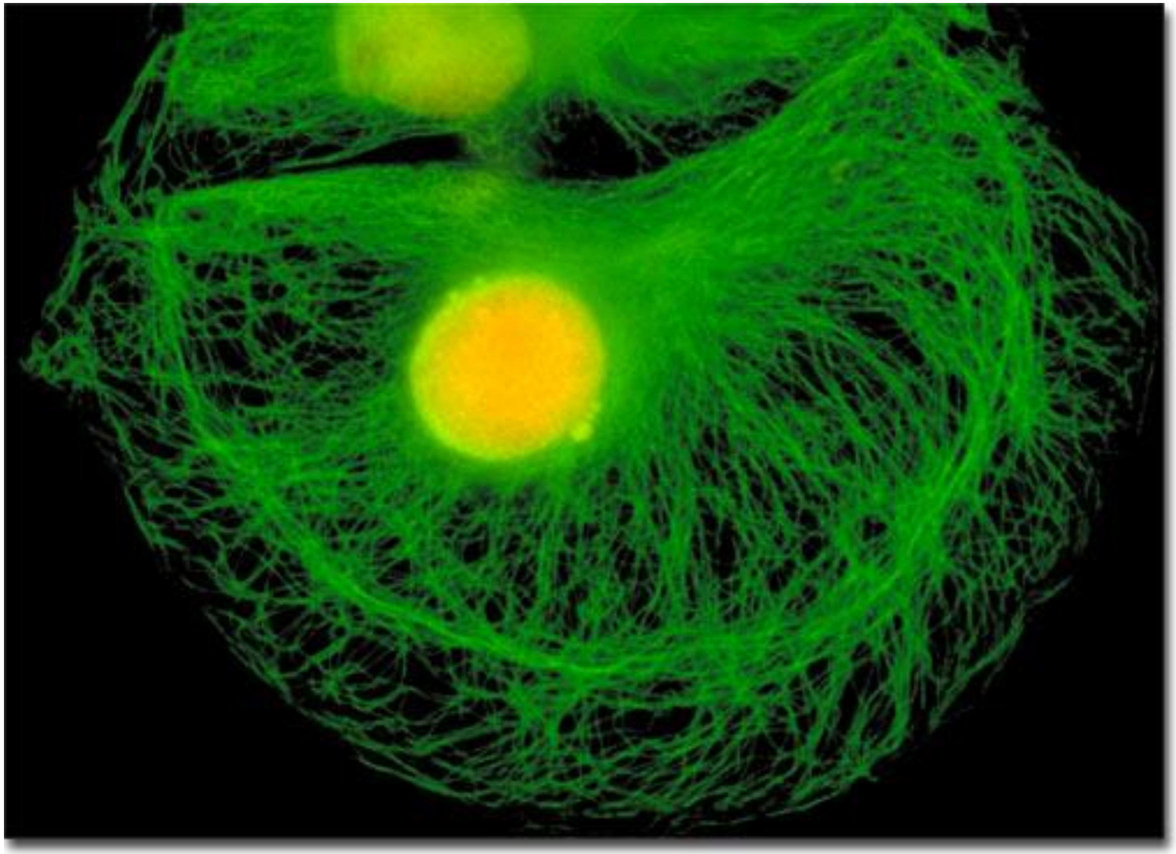
• Visible light microscope the best resolution is ~200 nm

• Electron microscopes on the order of ~0.2 nm



Light Microscopy

- This means that light microscopy is useful to visualize eukaryotic cells (size: 10 – 100 µm).

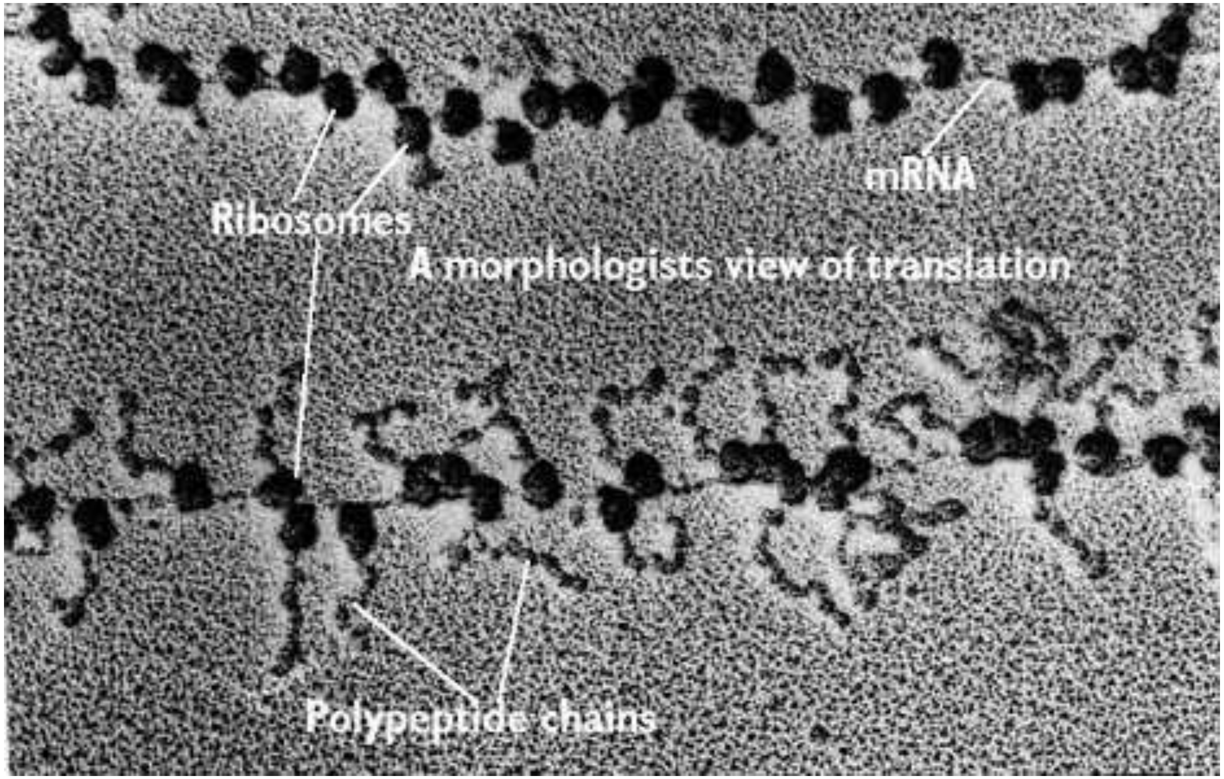


The size of a cell nucleus is ~10 µm.

http://www.olympusmicro.com/galleries/fluorescence/images/p2k2microtubulescellnuclarge.jpg

Electron microscopy

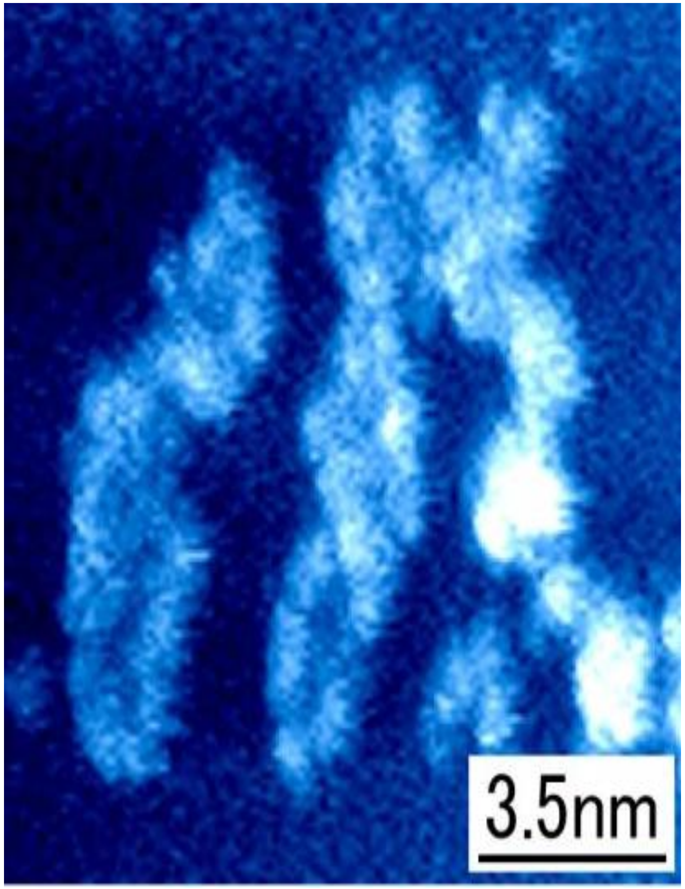
• But smaller cells (e.g. bacteria, size ~1-2 μm), or the inside structure of cells can only be seen well using electron microscopy.



The size of a ribosome is ~11 nm.

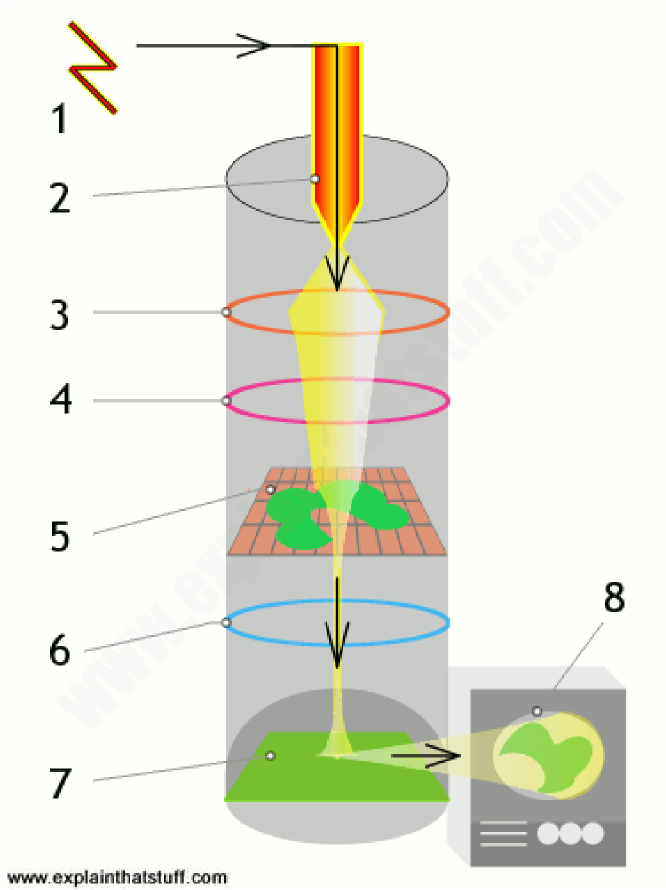
http://nanobiologynotes.blogspot.com/

- Direct imaging of single DNA molecules

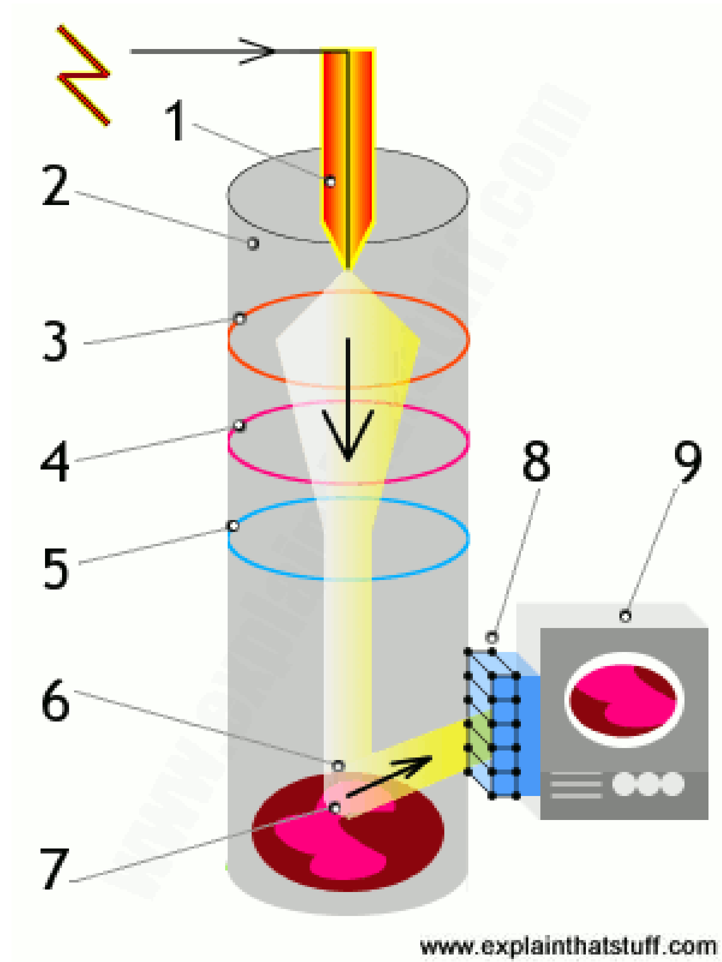


Electron Microscopy

TEM: Transmission Electron Microscope

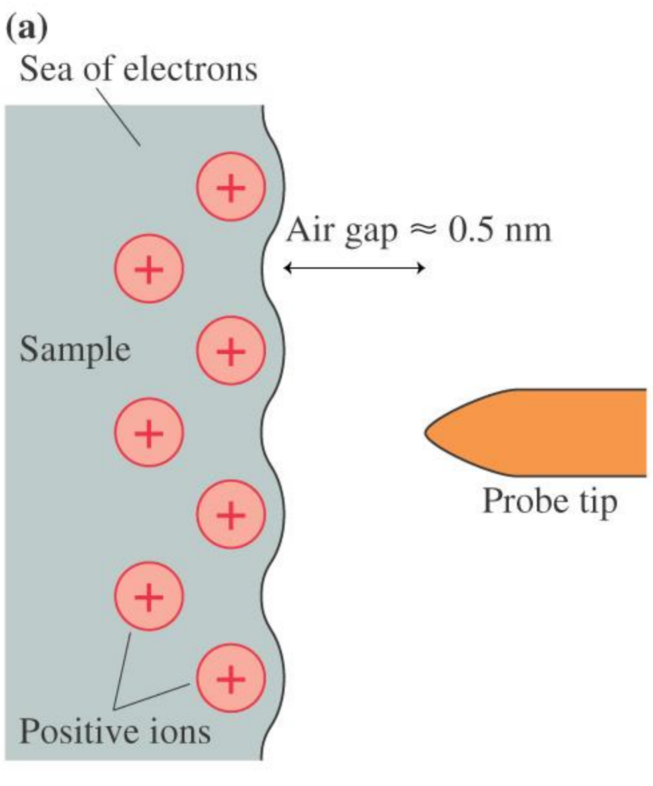


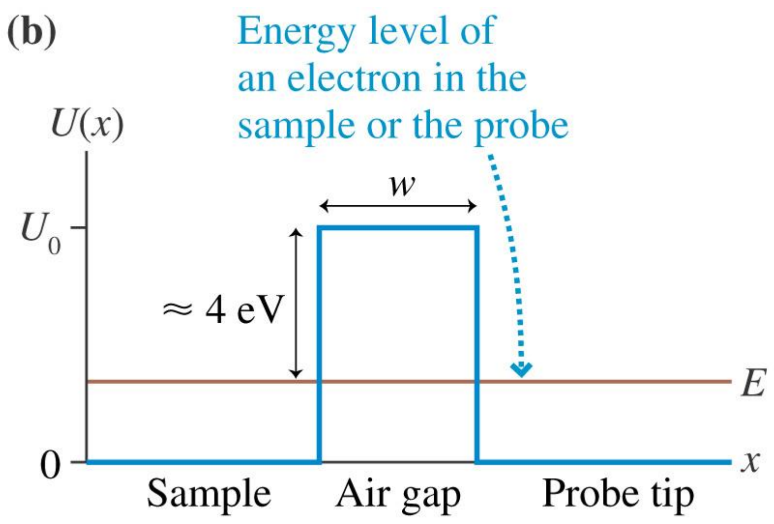
SEM: Scanning Electron Microscope



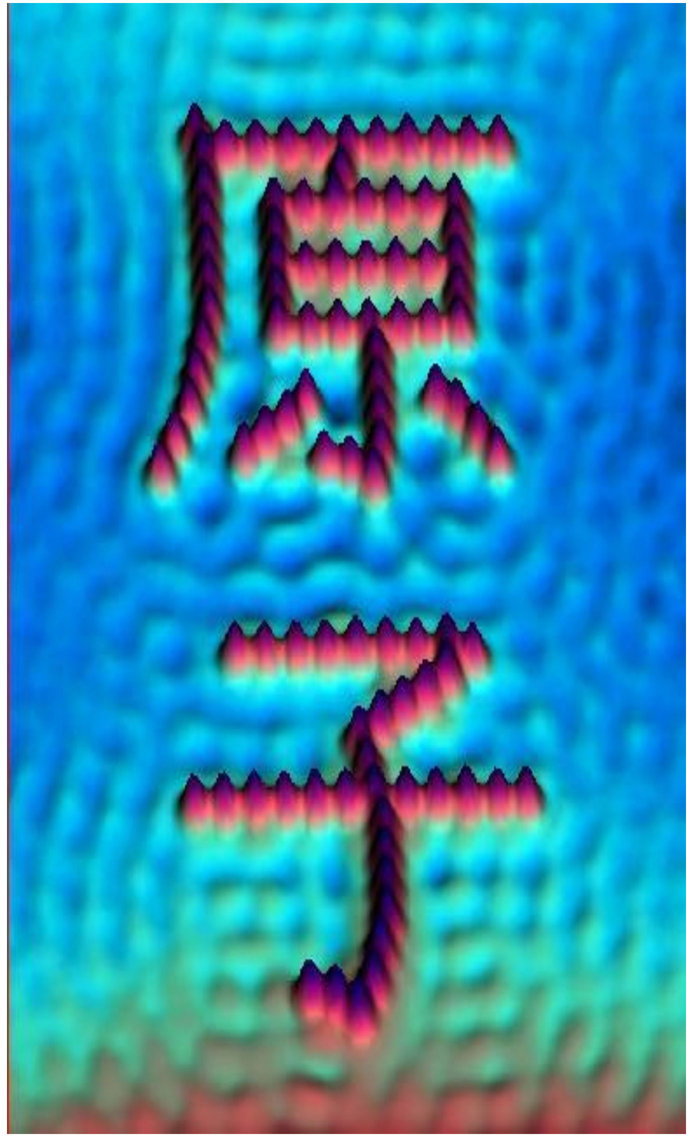
Scanning Tunneling Microscopy

• STM (developed in 1981) makes use of the tunneling effect to achieve 0.01 nm resolution or better.

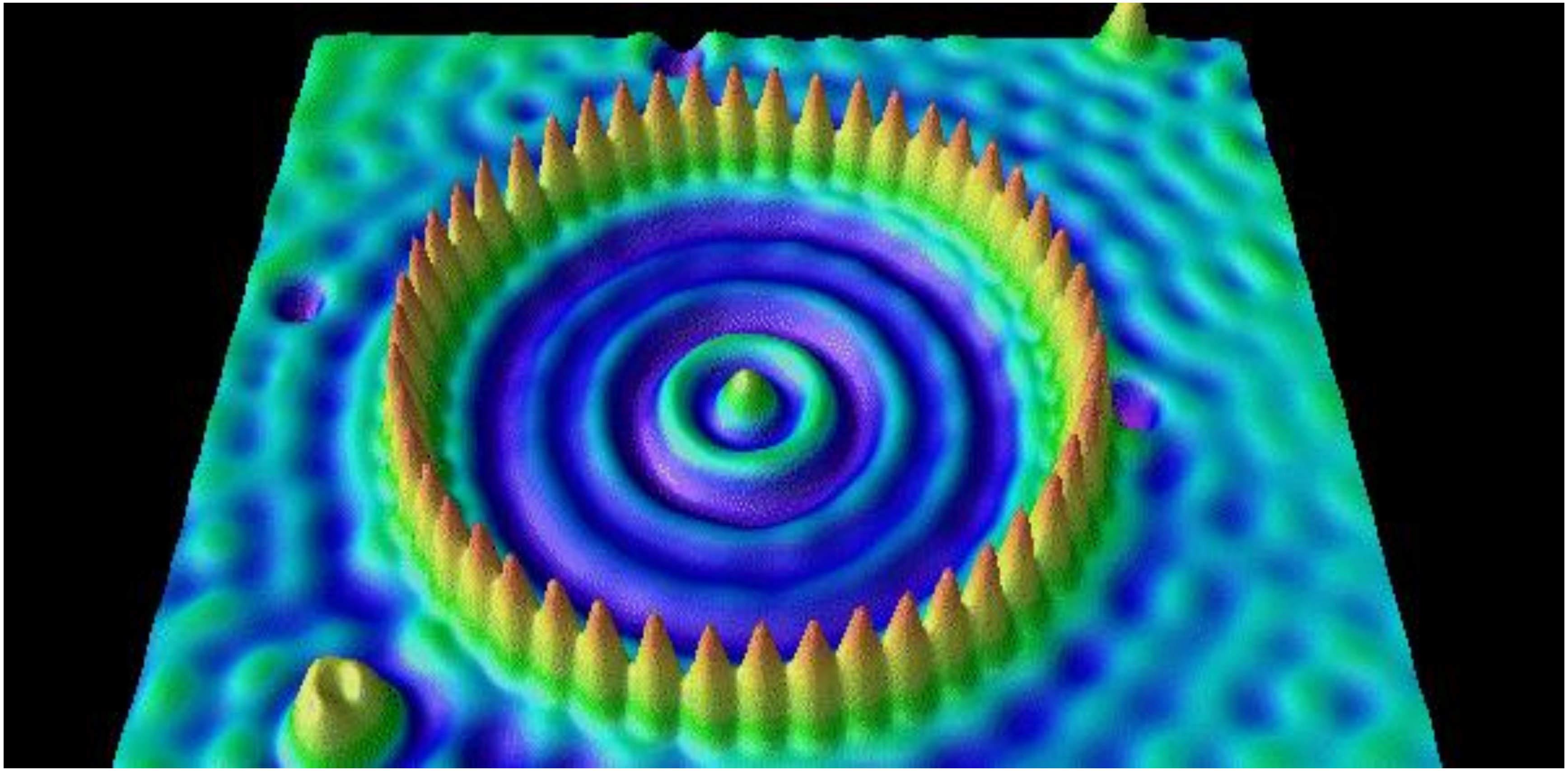




- Imaging of single iron atoms at the surface of copper.



Quantum “Corral”



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