6. Quantum Mechanics 2, 3

lecture 23, October 20, 2017

housekeeping

Exam 2

- Next Friday, October 27
- Thornton and Rex, Chapters 3,4,5

today

real quantum mechanics

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

THE TIME-DEPENDENT SCHROEDINGE EQUATION

DEFINE THE MOMENTUM OPERATOR $\hat{P}_x \equiv \frac{\hbar}{i}\frac{\partial}{\partial x}$

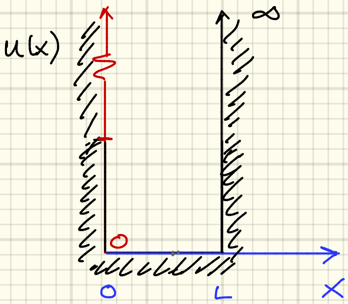
DEFINE THE ENERGY OPERATOR $\hat{E} \equiv -\frac{\hbar}{i}\frac{\partial}{\partial t}$

TAKE ANY CLASSICAL EQUATION AND MAKE SUBSTITUTIONS:

$$\left.\begin{array}{l} P_{x,y,z} \longrightarrow \hat{P}_{x,y,z} \\ E \longrightarrow \hat{E} \end{array}\right\} \text{ and "operate on" } \psi$$

CALLED "FIRST QUANTIZATION" this is "to quantize"

"Infinite square well"



$V(x) = \infty \qquad x < 0$

$V(x) = \infty \qquad x > L$

$V(x) = 0 \qquad 0 < x < L$

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

Impose boundary conditions:

$\psi(0) = 0 \Rightarrow B = 0$

$\psi(L) = 0 \Rightarrow \psi(L) = A \sin kL = 0$

so: $kL = n\pi$

$\Rightarrow \psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$ ✓

Impose normalization:

$$\int_{\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = 1 = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \longrightarrow 1 = A^2 \cdot \left(\frac{L}{2}\right) \Rightarrow A = \sqrt{\frac{2}{L}}$$

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

$n =$ "quantum number"

"the state"

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$$

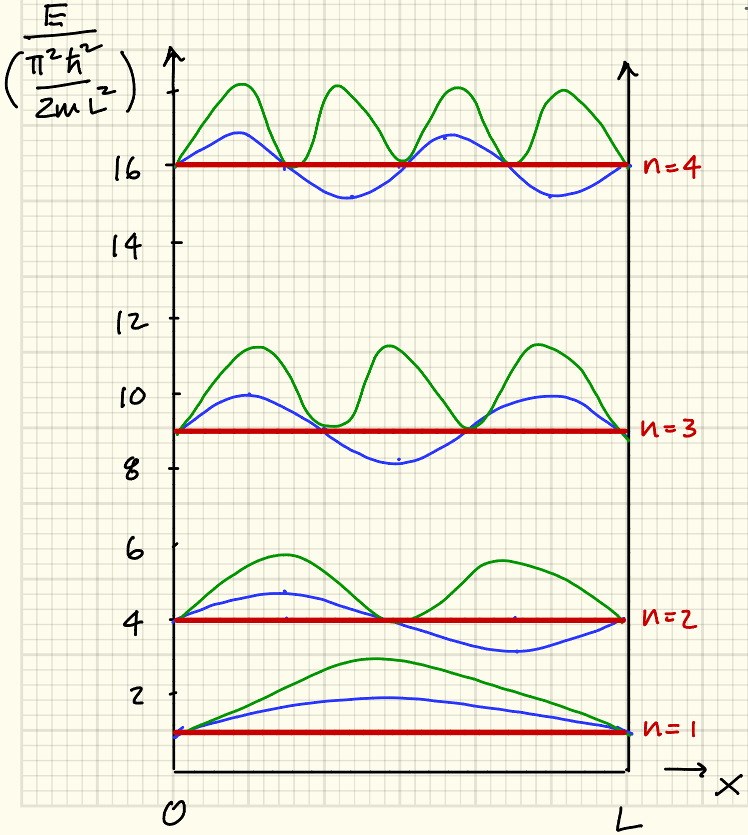
also, use wave number:

$$p = \frac{h}{\lambda} = \frac{2\pi}{2\pi} \frac{h}{\lambda}$$

$$k = \frac{2\pi}{\lambda} \Rightarrow p = \hbar k$$

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

— Energy — Wavefunction — Probability density



Think about this lowest energy:

zero-point energy

happens all the time in QM

Uncertainty demands it!

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

$$\frac{p^2}{2m} = E_1 \Rightarrow \quad \frac{p_1^2}{2m} = \frac{\pi^2\hbar^2}{2mL^2}$$

uncertainty in position $\Delta x \cong L/2$

uncertainty in mom: $\Delta p \sim p_1/2$

$$p_1 = \frac{\pi\hbar}{L}$$

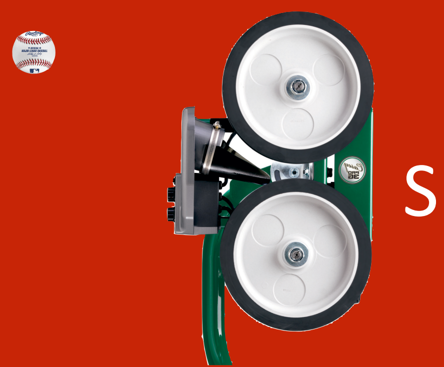
$$2\Delta p = \frac{\pi\hbar}{2\Delta x}$$

$$\Delta p \Delta x = \frac{\pi\hbar}{4} = \frac{\pi}{2}\,\frac{\hbar}{2} \geq \frac{\hbar}{2} \quad \checkmark$$

Nature's little joke

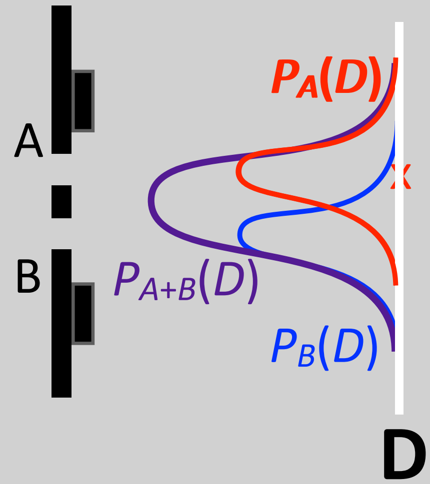
is encapsulated in a famous Feynman-description

a Gedankenexperiment...



two slit experiment

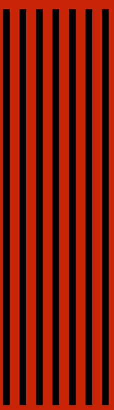
2 + 1 ways



Two slit experiment with classical baseballs

$$P_A(D) + P_B(D) = P_{A+B}(D)$$

Like the "classical" situation of asking what is the probability of getting heads or tails in a coin flip...you'd add 0.5 and 0.5.



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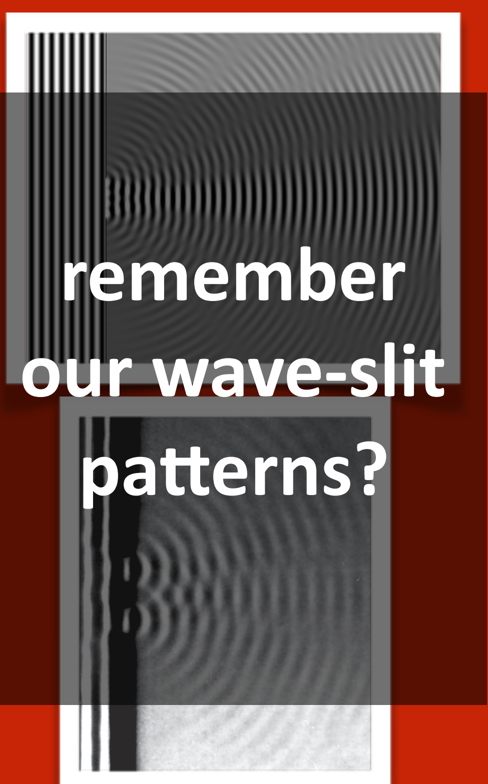
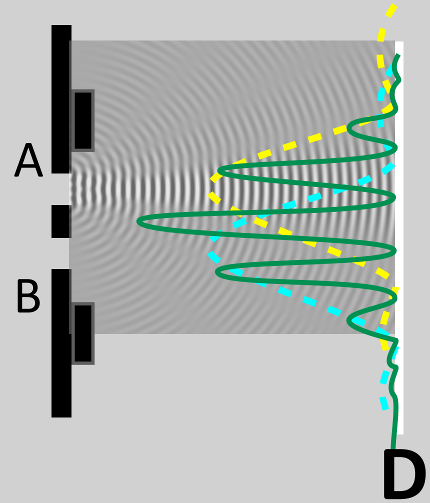


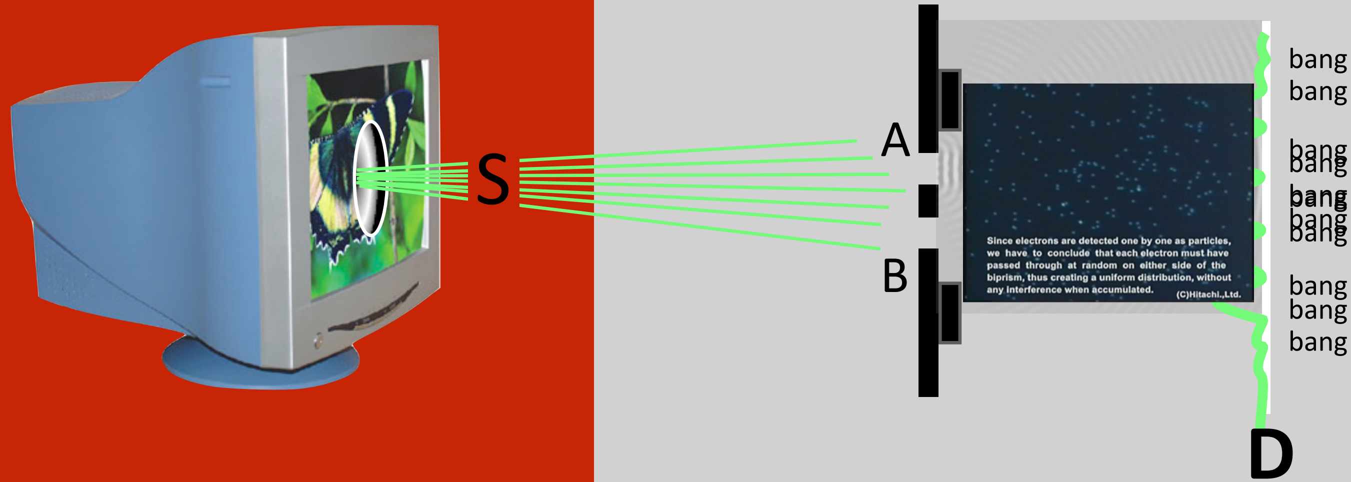
remember our wave-slit patterns?



Two slit experiment with waves

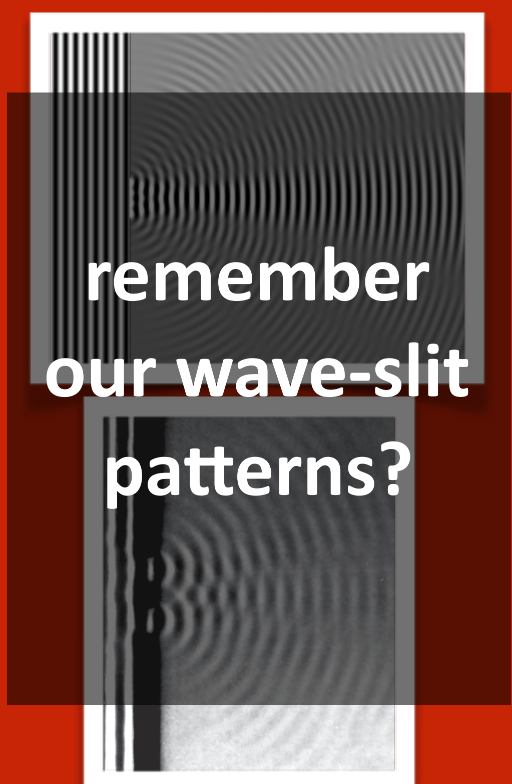
$$P_A(D) + P_B(D) \neq P_{A+B}(D)$$

Interference causes the characteristic diffraction pattern



Two slit experiment with electrons?

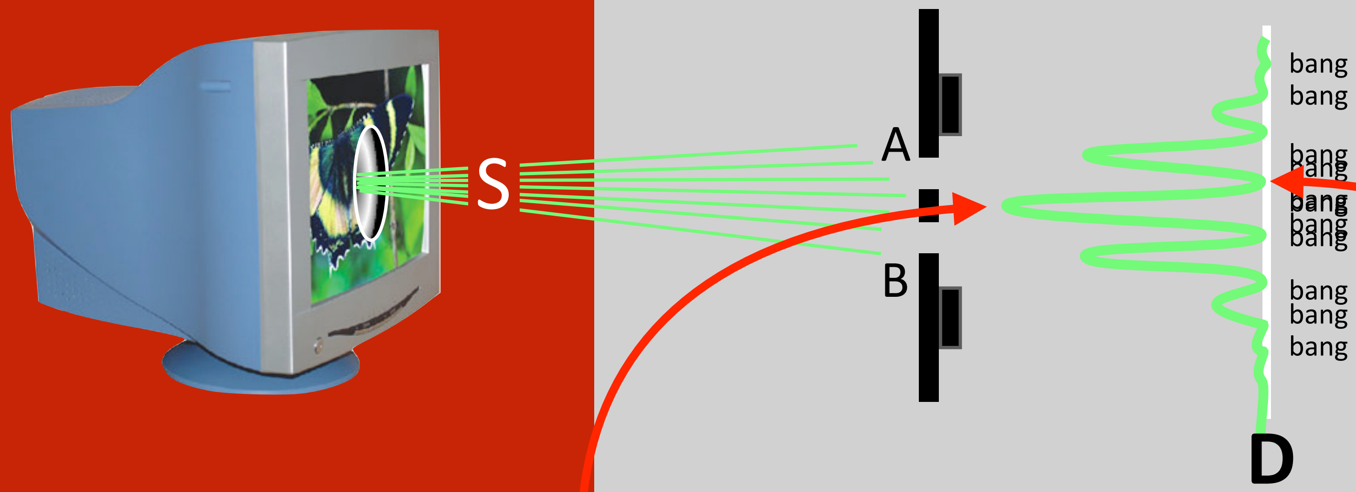
$$P_A(D) + P_B(D) \neq P_{A+B}(D)$$



Interference causes the characteristic diffraction pattern

Same result as for waves.

Maybe not a surprise given what's come before, eh?



probabilities don’t add

it’s the **quantum fields** that do the wavy-ness!

$$\psi$$

$$P_A(D) + P_B(D) \neq P_{A+B}(D)$$

$$P_D = |\psi_A + \psi_B|^2$$

$$P_D = \psi_A^2 + \psi_A^2 + \psi_A \psi_A^*$$

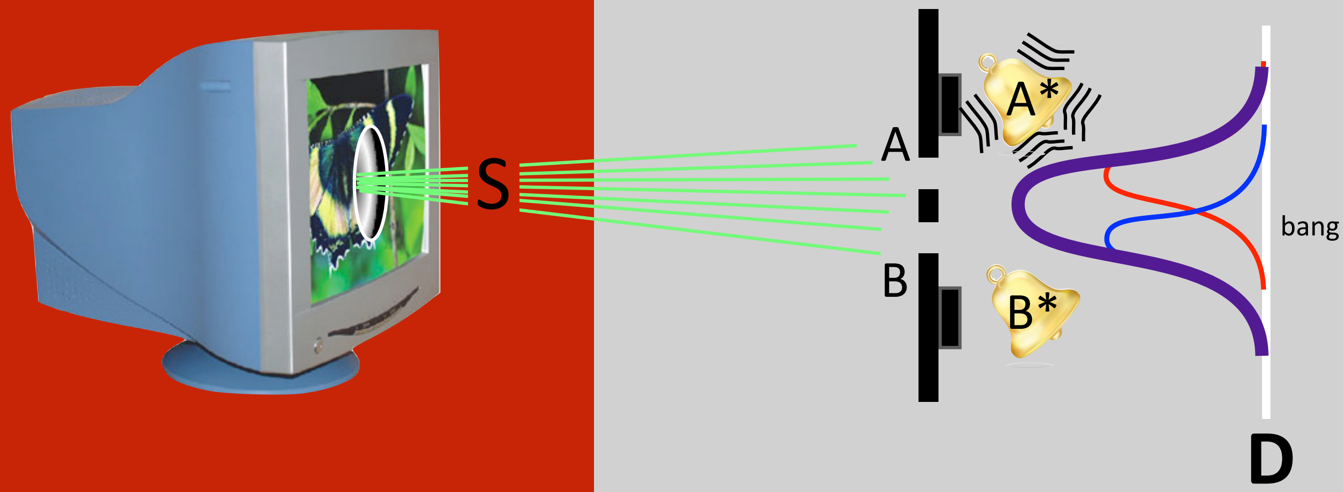
at some points this can be negative, sometimes positive

which gap did any electron come through?

okay…let’s trick it

rig an alarm that sounds when an electron goes through a slit.

Hah!



Two slit experiment with **electrons** and an alarm?

So the sequence “S-A-A*-D occurred.

Every time A* rings - red curve. B* rings, blue curve.

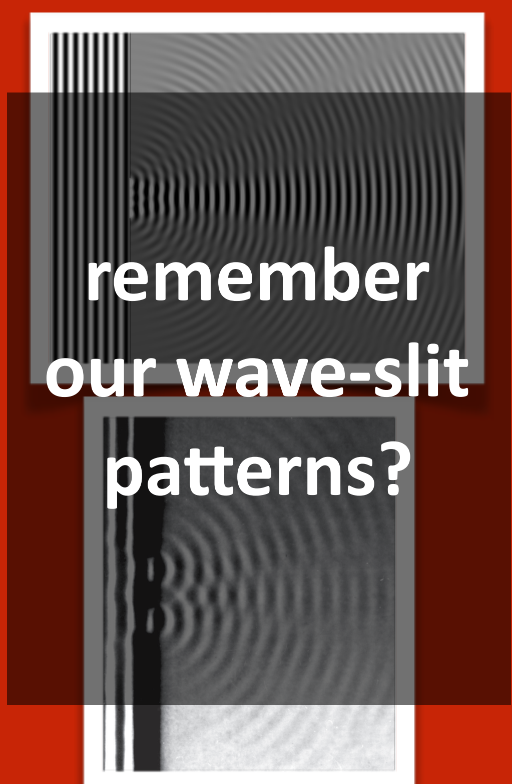
Same result as for baseballs.

Interference has gone away!!

Now: A* is a DISTINGUISHABLE event from B*

We specified the path...

and that changed the reality.



remember our wave-slit patterns?

summarize

the classical situations

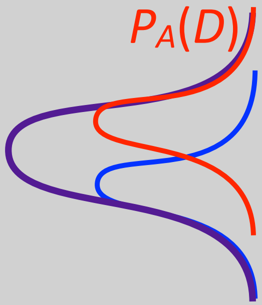
For **macroscopic objects**: outcomes add "normally":

The result of

whatgoesthroughA and whatgoesthroughB is

the sum of whatgoesthrough(A **or** B)

one or the other



For **waves**: outcomes interfere:

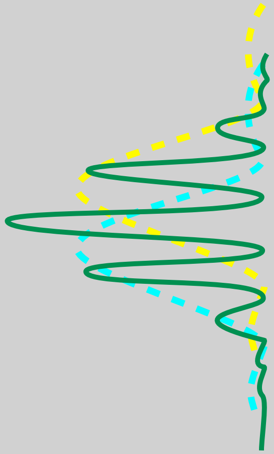
the result of

whatgoesthroughA and whatgoesthroughB is

the interference of whatgoesthrough(A **and** B)

both at the same time

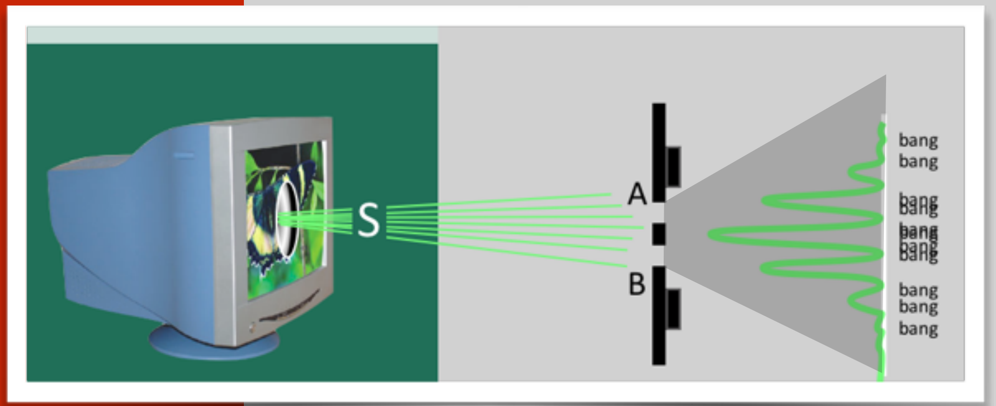
the waves interfere

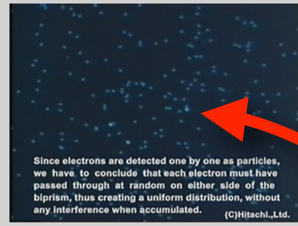


where is the electron

it’s real only when you make a measurement

and your measurement can determine how it’s real





The electron is real at the screen.
it’s unambiguously...there.
the “bang” is a measurement

what about here?

We have to say that an electron:

- goes through both slits
- and is in a “superposition” state,
  *here of **both** the state* ψ_A *and the state* ψ_B

As soon as measurement is made...the superposition goes away and the potentiality becomes the actuality...according to the probabilistic prediction of the Schroedinger Equation.

what we can say is real

is now very tricky

and not understood.

We know that quantum fields contain all of their potentialities

and a measurement "collapses" them into just one outcome

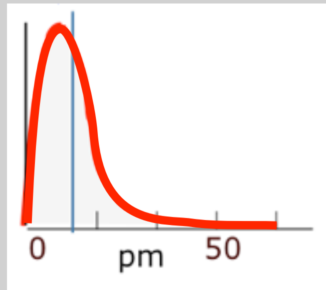
the concept of a "measurement" is totally not understood.

the wavefunctions are everywhere

spread out and overlapping

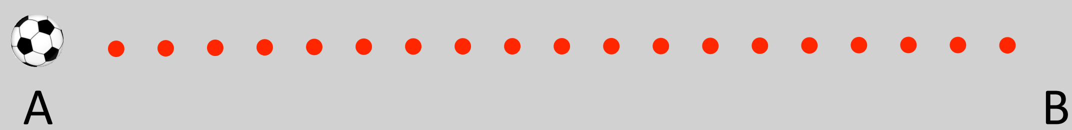
that's how molecules stay together

but…jeez. everywhere.



doesn't go to zero.

There's a probability that the electron in one of your water molecules might spend a brief time at the Louvre



Something big…seems to have a definite trajectory

Something tiny…doesn't.

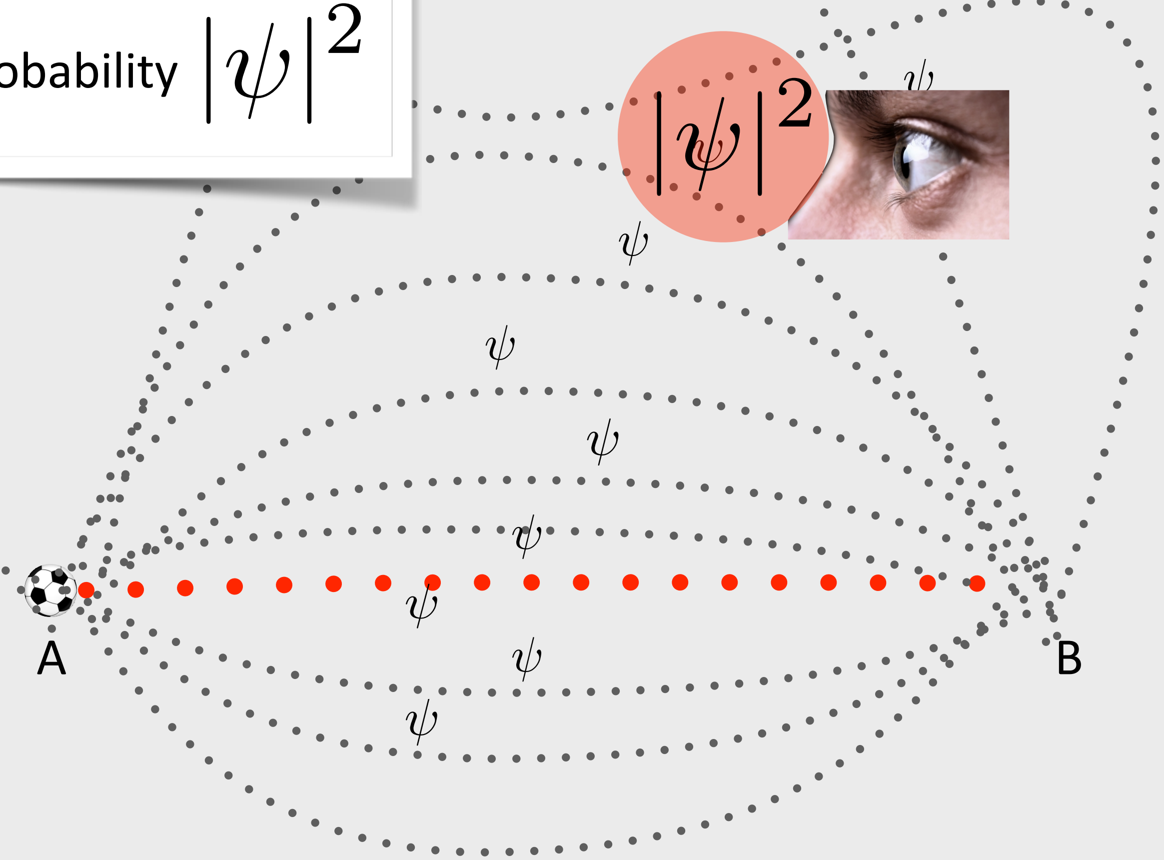
the wavefunctions are everywhere

They're waves, after all.

make a measurement....there

Only then is it real.

the electron is there with probability $|\psi|^2$



Feynman's picture was one of particles: which take all possible paths

We can calculate the wavefunction at any point, very precisely...it's completely deterministic

The trajectory of a big object?

Overwhelmingly probable quantum likelihood: the classical path

so where is a quantum

before it’s measured?

anywhere? everywhere?

yeah.

to take it to an absurd conclusion:
the dreaded Schroedinger's Cat

proposed by Schroedinger as an absurdity

because he too had become disgusted with this own creation - he switched to biology!

Schroedinger must have been a dog person

Imagine:

a radioactive source,

Geiger counter, and

a glass bottle of a deadly poison

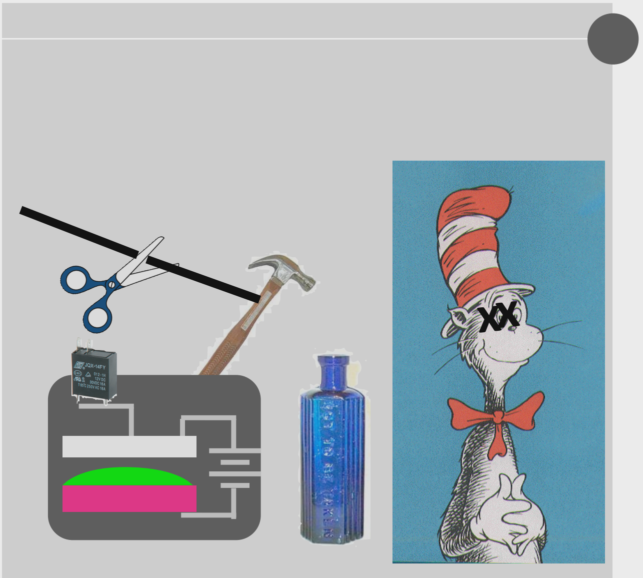
with a cat

in a box,

a weight drops on the glass, breaking it

after the first radioactive decay?

...dead cat.



Schroedinger must have been a dog person

Now imagine that the radioactive nucleus as a **half life of 10 sec**.

so, after 10 s,

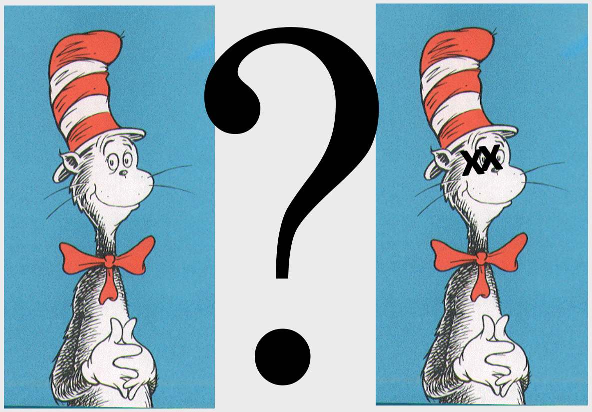
50-50 chance that it has decayed

Set it all up...wait for 10 seconds.

what is the state of the cat?

alive or dead?

or both?



‘‘Copenhagen Interpretation’’

It is meaningless

to speak of reality without a measurement

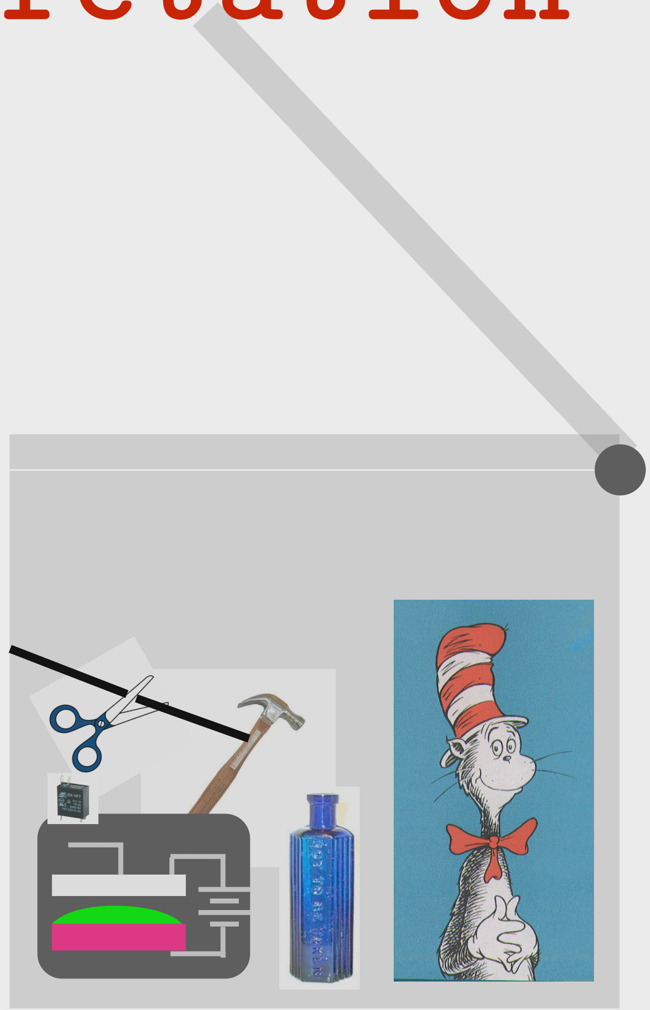
Entities have no definite reality

the cat is neither alive nor dead

or it is both

To know you must open the box

make a measurement



this is how we have to think about it:

before measurement: alive-dead state - **superposition state of both**

after measurement: is **either** alive **or** dead

here's our house

just before painting
last year

need to pick a color:

my wife says "red"

I say "blue"

SHERWIN-WILLIAMS
quantum paint

I expect it to be:

purple

mixing red and blue

but the quantum mechanical paint

that I paid extra for?

can’t “exist” in a superposition, mixed state.

Only one state.

sometimes it’s red

but the quantum mechanical paint

that I paid extra for?

sometimes it's blue

it's never the mixture

that it potentially might be

one or the other

More red paint?

not redder...just red more often

the cat is either alive or dead, not both.

I think I can safely say that nobody understands quantum mechanics.

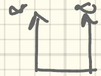
Richard Feynman

But we can calculate with Quantum Mechanics very, very well.

We’re all highly skilled Quantum *Mechanics*

Physics Here?

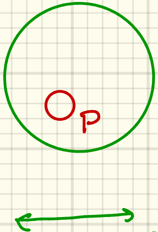
Glad you asked.

$\exists$ many physical systems that can be approximated by 

A proton trapped inside of a nucleus

E & M repulsion? Doesn't matter... strong force is way stronger

nucleus



$D_N \sim 4\,\text{fm}$

$4\times10^{-15}\,\text{m} = 4\times10^{-9}\times10^{-6}\,\text{m}$

$= 4\times10^{-6}\,\text{nm}$

what's E_1?

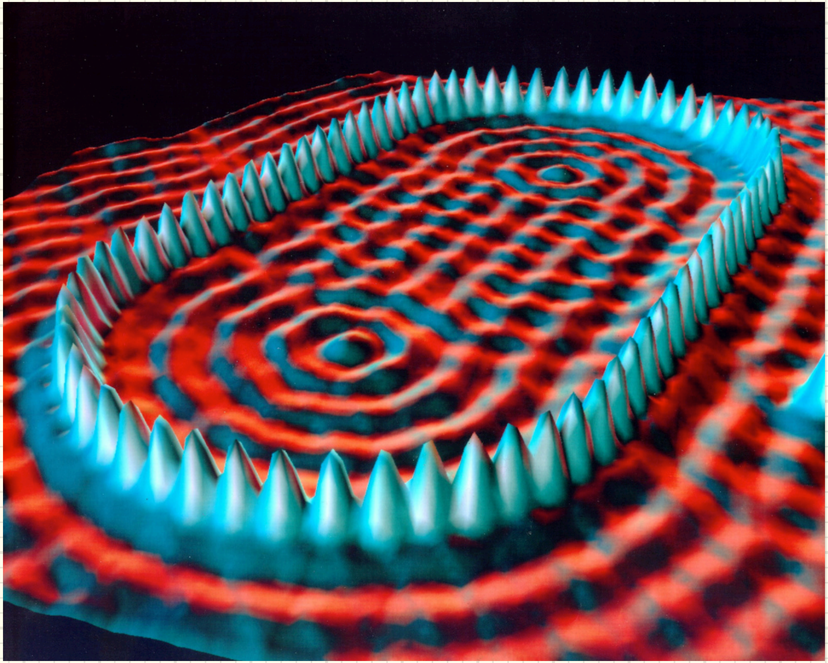
$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

$$= \frac{\pi^2(\hbar c)^2}{2mc^2 D_N^2}$$

$$= \frac{\pi^2(200\,\text{eV}\cdot\text{nm})^2}{2(938\times10^6\,\text{eV})(4\times10^{-6}\,\text{nm})^2}$$

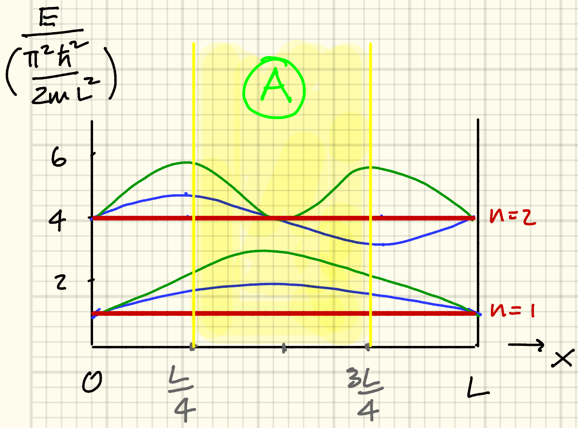
$$= 1.3\times10^7\,\text{eV}$$

$E_1 = 13\,\text{MeV}$ not bad



the quantum corral

LIMITED REGION ?



$$P(A)_n = \int_{L/4}^{3L/4} \psi^*(x)\psi(x)\,dx$$

$$= \frac{2}{L}\int_{L/4}^{3L/4} \sin^2\left(\frac{n\pi x}{L}\right)dx$$

$$\vdots$$

$$= \frac{2}{L}\left[\frac{L}{4} - \frac{L}{4\pi n}\left(\sin\frac{6\pi n}{4} - \sin\frac{2\pi n}{4}\right)\right]$$

$$P(A)_n = \frac{1}{2} - \frac{1}{\pi n}\left(\sin\underbrace{\frac{6\pi n}{4}}_{3n\pi/4} - \sin\frac{2\pi n}{4}\right)\Bigg]$$

$n=1$?

$$P(A)_1 = \frac{1}{2} - \frac{1}{\pi}\left(\sin\frac{6\pi}{4} - \sin\frac{2\pi}{4}\right)$$

$$= \frac{1}{2} - \frac{1}{\pi}(-1 - 1)$$

$$= \frac{1}{2} + \frac{2}{\pi}$$

```
(2 / L) * Integrate[Sin[Pi * x / L] ^ 2, {x, (L / 4), (3 L / 4)}]
```

In[1]:= $\frac{2+\pi}{2\pi}$

```
Simplify[%]
```

$\frac{2+\pi}{2\pi}$

In[5]:= `Evaluate[%]`

Out[5]= $\frac{1}{2} + \frac{1}{\pi}$

In[6]:= $N\left[\frac{1}{2} + \frac{1}{\pi}\right]$

Out[6]= 0.81831

How about very large n? $P(A)_n \to 0.5$, the classical result.

Bohr's Correspondence Principle again.

Uncertainty, Grown Up

Remember the "Standard Deviation"?

set of N measurements, x_i

with mean, $\langle x \rangle$

a measure of uncertainty is the S.D.

$$\sigma \equiv \sqrt{\frac{\sum_i (x_i - \langle x \rangle)^2}{N}}$$

$$\sqrt{\underbrace{\frac{\sum_i (x_i)^2}{N}}_{\langle x^2 \rangle} - 2\langle x \rangle \underbrace{\frac{\sum_i x_i}{N}}_{\langle x \rangle} + \langle x \rangle^2 \underbrace{\sum_i \frac{1}{N}}_{1}} = \sqrt{\langle x^2 \rangle - 2\langle x \rangle^2 + \langle x \rangle^2}$$

so $\sigma = \langle x^2 \rangle - \langle x \rangle^2$

we'll call this $(\Delta x)^2$

now: QM.

$$\langle x\rangle = \int \psi^* \hat{x} \psi \; dx$$

for the infinite square well.

$$\langle x\rangle = \int_0^L x \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) dx$$

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

$$\langle x\rangle = \frac{2}{L}\cdot\frac{L^2}{4} = \frac{L}{2} \quad \checkmark$$

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

$$\vdots$$

$$\langle x^2\rangle = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2} \quad \Rightarrow \quad (\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{L}{3} - \frac{L^2}{2n^2\pi^2} - \frac{L^2}{4}$$

$$\Delta x = \sqrt{\frac{L^2}{12} - \frac{L^2}{2n^2\pi^2}}$$

Momentum: $(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2$

$$\langle p \rangle = \int_0^L \psi^* \hat{p} \psi \, dx$$

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

$$= \frac{2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \left(\frac{n\pi}{L}\right) \left(\frac{\hbar}{i}\right) \cos\left(\frac{n\pi x}{L}\right) dx$$

odd · even $= 0$

$$\langle p \rangle = 0$$

$$\langle p^2 \rangle = \int \psi^* \hat{p}^2 \psi \, dx = \int \psi^* - \hbar^2 \left[\frac{\partial^2}{\partial x^2} \psi\right] dx$$

$$\langle p^2 \rangle = \frac{n^2 \pi^2 \hbar^2}{L^2}$$

$$\Delta p = \sqrt{\frac{n^2 \pi^2 \hbar^2}{L^2} - 0} = \sqrt{\frac{n^2 \pi^2 \hbar^2}{L^2}}$$

$$\Delta x \, \Delta p = \sqrt{\frac{L^2}{12} - \frac{L^2}{2n^2\pi^2}} \cdot \sqrt{\frac{n^2\pi^2\hbar^2}{L^2}}$$

$$\vdots$$

$$= \frac{\hbar}{2}\sqrt{\frac{n^2\pi^2}{3} - 2} = \frac{\hbar}{2}\sqrt{\underbrace{3.28\,n^2 - 2}_{>1}}$$

SO:

$\Delta x \, \Delta p \geq \frac{\hbar}{2}$ as expected from the Uncertainty Principle

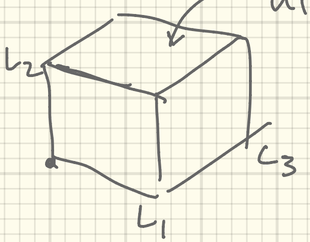
MULTIDIMENSIONAL BOX

S.E. : $$-\frac{\hbar^2}{2m}\underbrace{\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)}+U(x,y,z)\psi = E\psi$$

$\psi = \psi(x,y,z)$

Laplacian Operator: $\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z)+U(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$$



$U(x,y,z)$ inside $= 0$
outside $= \infty$

same boundary conditions as 1 D

general solutions: $\psi = A \sin k_1 x \sin k_2 y \sin k_3 z$

$$k_i = \frac{n_i \pi}{L_i}$$

now 3 quantum numbers $n_1 n_2 n_3$.

when the total wavefunction is a product, the energies (eigenvalues) are sums:

(cube): $$E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2mL^2}\left(n_1^2 + n_2^2 + n_3^2\right)$$

with ground state: $$E_{111} = \frac{3\pi^2 \hbar^2}{2mL^2}$$