SN	total homework	homework %	total exam	exam %	not quite course %
A35744732	80	80.8%	25	50.0%	70%
A36590609	84	84.8%	32	64.0%	78%
A35348617	4	4.0%	14	28.0%	12%
A35762223	95	96.0%	31	62.0%	85%
A39010642	69	69.7%	22	44.0%	61%
A37546634	89	89.9%	47	94.0%	91%
A35697830	86	86.9%	21	42.0%	72%
A36311847	93	93.9%	46	92.0%	93%
A28812827	61	61.6%	31	62.0%	62%
A35369914	80	80.8%	22	44.0%	68%
A35955440	73	73.7%	39	78.0%	75%
A35057767	95	96.0%	41	82.0%	91%
A36747844	86	86.9%	25	50.0%	74%
A36631057	67	67.7%	16	32.0%	56%
A36889380	88	88.9%	27	54.0%	77%
A36636038	0	0.0%	0	0.0%	0%
A36220020	16	16.2%	0	0.0%	11%
A37112790	24	24.2%	27	54.0%	34%
A37062131	93	93.9%	36	72.0%	87%
A38447802	89	89.9%	39	78.0%	86%
A28619424	51	51.5%	9	18.0%	40%
A35520786	65	65.7%	23	46.0%	59%
A37048340	74	74.7%	32	64.0%	71%
A37050885	62	62.6%	31	62.0%	62%
A36185194	56	56.6%	25	50.0%	54%
A38869178	64	64.6%	24	48.0%	59%
A34056444	81	81.8%	31	62.0%	75%
A30678782	73	73.7%	22	44.0%	64%
A36931722	87	87.9%	41	82.0%	86%
A35268153	90	90.9%	45	90.0%	91%
A36245097	80	80.8%	30	60.0%	74%
	99	100.0%	50	100.0%	100%

Remember: the final grade has the following fractions:

homework: 25%
exams: 45%
final: 30%

not reflected in "not quite course %" column.

WHEN WE LAST LEFT OUR HERO...

Let me say at the outset that in this discourse, I am opposing not a few special statements of quantum mechanics held today (1950's), I am opposing as it were the whole of it, I am opposing its basic views that have been shaped 25 years ago when Max Born put forward his probability interpretation, which was accepted by almost everybody.

I don't like it, and I'm sorry I ever had anything to do with it.

Schrodinger

The STATE of a quantum mechanical system

electron, proton, neutron, nucleus, etc...

(photons are harder and more complicated)

is represented by the WAVE FUNCTION, $\Psi(\vec{x},t)$.

It is complex and not directly observable.

what is observable is the probability that something may happen...

$$\Psi^*(\vec{x},t)\,\Psi(\vec{x},t)\,d^3\vec{x}$$

is the probability that the particle will be found in the region inside $\vec{x}$ to $\vec{x} + d^3\vec{x}$

$$\frac{\int_a^b \Psi^*(x,t)\,\Psi(x,t)\,dx}{\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Psi(x,t)\,dx}$$

is the probability to find the particle between $x=a$ & $x=b$

Ψ is often called the "probability amplitude" or just "amplitude".

For non-relativistic circumstances, Ψ satisfies the Schrödinger Equation. In 1 dimension:

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

Observables are related to quantum mechanics through "operators", eg. $\hat{A}$

$$\langle A \rangle = \frac{\int \Psi^*(x,t)\,\hat{A}\,\Psi(x,t)\,dx}{\int \Psi^*(x,t)\,\Psi(x,t)\,dx}$$

"expectation value" for A

We have discussed a few:

position	$\hat{x}$	x
momentum	$\hat{p}_x$	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
energy	$\hat{E}$	$i\hbar\frac{\partial}{\partial t}$

and there can be others:

kinetic energy	$\hat{K}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
potential energy	$\hat{V}$	$V(x)$

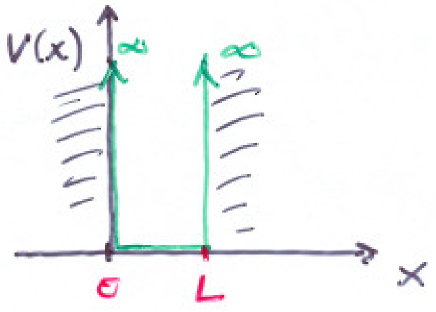
When $V = V(x)$ only, the wavefunction can be factorized

$$\Psi(x,t) = \psi(x)\, e^{-i\omega t}$$

and the Time-Independent Schrödinger Equation can be used for a variety of circumstances:

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

"Infinite Well" Quantum Mechanically.



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

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

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

In S.E. ... if $V = \infty$, then $\psi(x) = 0$ so,

$$\langle x \rangle_{\text{to right of } L} = \int_L^{\infty} \psi^*(x) \frac{d}{dx} \psi(x)\, dx = 0 \quad \text{since } \psi = 0$$

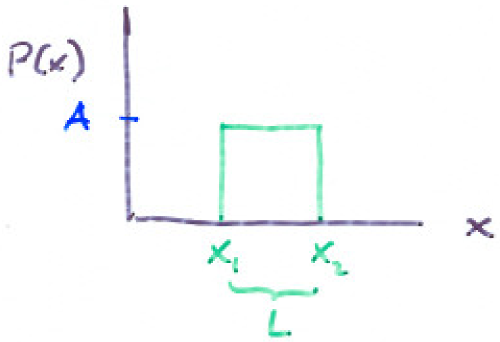
How about inside the well?

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + 0 = E\psi(x)$$

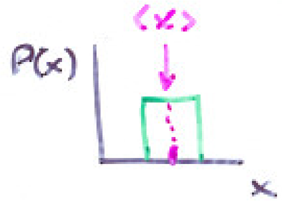
$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} E\psi = -\frac{2m}{\hbar^2} \frac{p^2}{2m} \psi$$

$$\frac{d^2\psi}{dk^2} = -\frac{p^2}{\hbar^2}\psi = -k^2\psi$$

Probabilities & Averages



What's the average value of x?



$$\langle x\rangle = \frac{\int_{-\infty}^{\infty} x\, P(x)\, dx}{\int_{-\infty}^{\infty} P(x)\, dx}$$

$$P(x) = 0 \qquad x < x_1 \,,\; x > x_2$$

$$\quad = A \qquad x_1 < x < x_2$$

$$= \frac{\int_{x_1}^{x_2} x\, A\, dx}{\int_{x_1}^{x_2} A\, dx}$$

$$= \frac{A \left.\frac{x^2}{2}\right|_{x_1}^{x_2}}{A x \Big|_{x_1}^{x_2}} = \frac{\frac{1}{2}\left(x_2^2 - x_1^2\right)}{x_2 - x_1} = \frac{\frac{1}{2}(x_2 - x_1)(x_2 + x_1)}{x_2 - x_1}$$

$$\langle x\rangle = \tfrac{1}{2}(x_2 + x_1) \qquad x_2 = x_1 + L$$

$$\langle x\rangle = \tfrac{1}{2}(x_1 + L + x_1) = \tfrac{1}{2}(2x_1 + L)$$

$$\langle x\rangle = x_1 + \tfrac{1}{2}L \quad ✓$$

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

general solution:

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

Boundary conditions require

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

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

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

Normalization requires

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

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

& we can determine A:

$$\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2} \quad \text{so,}$$

$$A^2\left(\frac{L}{2}\right) = 1$$

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

$n = 1, 2 \ldots$

wave functions are standing waves

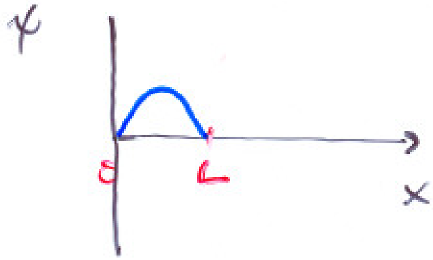
since $\frac{2mE}{\hbar^2} = k^2 = \left(\frac{n\pi}{L}\right)^2$

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

If an object is subject to such a potential "well" — where is it?

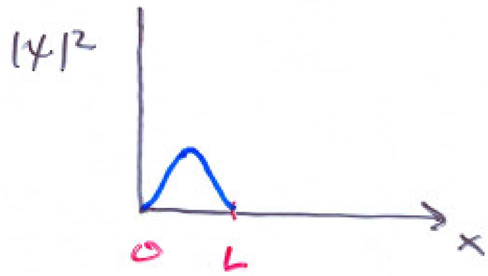
lowest energy state:

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



with $E = \frac{\pi^2\hbar^2}{2mL^2} \neq 0$!

But that's not "where" $\longrightarrow$ probability $\propto |\psi|^2$



and THAT'S all you can know.

where:

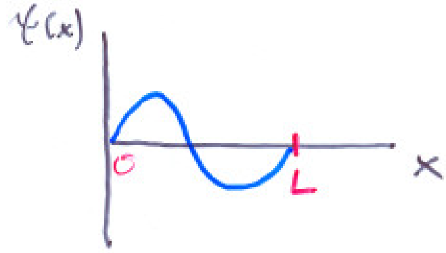
"MEANINGLESS" $\equiv$ not measurable.

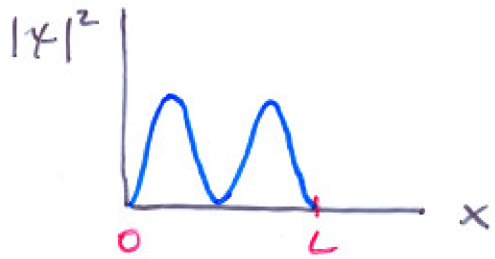
I'm pushing a philosophy here...

next level $(n=2)$

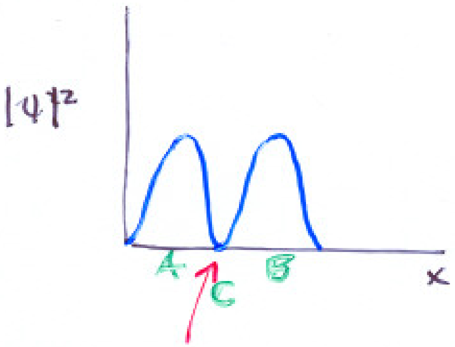
$$\psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$$

$$E_2 = 4E_1 = 4\,\frac{\pi^2\hbar^2}{2mL^2}$$





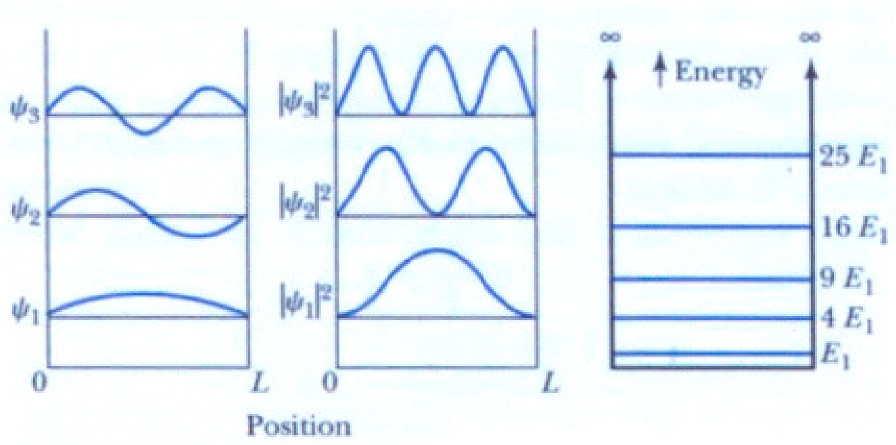
now THIS is weird.



electron has ZERO probability of being at the center!

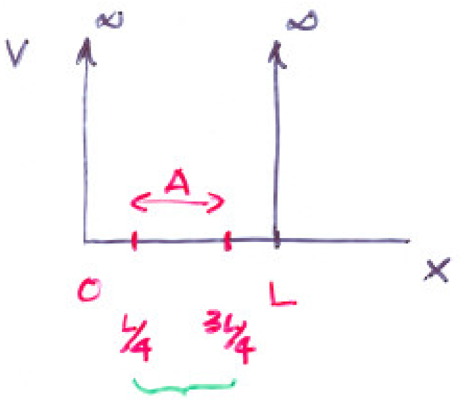
How can it "get" from A to B if it can't "pass" through C?

"PARTICLE" concept of moving from A to B without passing through points in-between is MEANINGLESS



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

energy levels are "quantized" according to the quantum number, n



what's the probability to be in this half of the well?

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

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

$$\vdots$$

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

$$P(A) = \frac{1}{2} - \frac{1}{2\pi n}\left(\sin \quad - \sin \quad\right)$$

suppose n is very... very large?

remember Correspondence Principle...

$$\lim_{n\to\infty} P(A) = 0.5$$ ... the classical result.

Remember the Standard Deviation ?

For a set of measurements x_i which have a mean $\langle x \rangle$ ... a measure of the "error" or uncertainty (!) is the standard deviation

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

under the radical:

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

$$= \langle x^2 \rangle - 2\langle x \rangle^2 + \langle x \rangle^2$$

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

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

now.. think quantum mechanically..

$$\langle x \rangle = \int \psi^* x \psi \, dx$$ find ~~$\langle x \rangle$~~ $\underline{\Delta x}$

for ∞ square well:

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

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

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

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

$$\vdots$$

$$\langle x^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}$$

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

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

now.. momentum..

$$\Delta p^2 = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$$ also

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

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

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

odd - even = 0

$\langle p\rangle = 0$ ✓

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

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

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

$$\Delta x \Delta p = \sqrt{\left(\frac{L^2}{12} - \frac{L^2}{2n^2\pi^2}\right)\left(\frac{n^2\pi^2\hbar^2}{L^2}\right)}$$

$$\stackrel{\vdots}{=} \frac{\hbar}{2}\sqrt{\frac{n^2\pi^2}{3} - 2} = \frac{\hbar}{2}\underbrace{\sqrt{3.28n^2 - 2}}_{\text{always} > 1}$$

$n=1 \quad \sqrt{} = 1.1$

So

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

as expected from

Uncertainty Principle ✓

3 DIMENSIONAL "WELL" → A BOX

The Schrödinger Equation is

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

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

↓

the Laplacian Operator "∇^2"

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

Think hard: a 3 spatial dimension box with ∞ potential

Sides: L_1, L_2, L_3

A general wave function of:

$$\psi = A\sin k_1 x\,\sin k_2 x\,\sin k_3 x$$

where

$$k_i = \frac{n_i\pi}{L_i} \qquad i = 1,2,3$$

same boundary conditions as 1-d well...

Energies depend on 3 quantum numbers

$n_1 \; n_2 \; n_3$

$$E = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right)$$

eg: a cube

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

The ground state

$$n_1 = n_2 = n_3 = 1$$

$$E_g = \frac{3\pi^2 \hbar^2}{2mL^2}$$

1st excited state ?

$n_1 = 2$	$n_2 = 1$	$n_3 = 1$
$= 1$	$= 2$	$= 1$
$= 1$	$= 1$	$= 2$

3 ways to do it...

each state has the same energy

$$E_1 = \frac{6\pi^2 \hbar^2}{2mL^2}$$

This is called a DEGENERACY:

states with same energies

BUT

different quantum numbers

One speaks of "lifting the degeneracy" by inducing some asymmetry ... often an electric or magnetic field

Here, one could make the box have different side-lengths

... suppose we have $L_1 = L$

$L_2 = 2L$

$L_3 = 3L$

$$E_n = \frac{\pi^2 \hbar^2}{2mL^2} \left(n_1^2 + \frac{n_2^2}{4} + \frac{n_3^2}{9} \right)$$

now ... each set of n_1, n_2, n_3 gives different E.