6. Quantum Mechanics 2, 2

lecture 22, October 18, 2017

housekeeping

I got nothin’

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:

$$\left.\begin{aligned} P_{x,y,z} &\longrightarrow \hat{P}_{x,y,z} \\ E &\longrightarrow \hat{E} \end{aligned}\right\}$$ and "operate on" ψ

CALLED "FIRST QUANTIZATION" this is "to quantize"

PROPERTIES OF $\psi(x,t)$

boundary conditions in solving the S.E.

1) ψ must be finite everywhere

2) ψ must be single-valued

3) ψ and $\frac{\partial \psi}{\partial x}$ must be continuous at any potential (U) boundary

4) $\psi \to 0$ as $x \to \pm\infty$

5) OBTW... ψ is complex

uh oh... not like E of optics

... cannot be an actual thing

→ we can't touch, smell, measure, feel, watch, interact with, or detect the wave function

Is it real? Join the argument... surely not

This bothered Schroedinger. We all know how to

make an imaginary variable A into a real variable

$$A^* A$$

so he first tried to say:

$$\psi^*(x,t)\,\psi(x,t)\,dx = |\psi(x,t)|^2 dx = C(x)\,dx$$

electron charge density

NOPE

The answer is strange.

Sandy: Oh Danny, is this the end?
Danny: No Sandy. It's only the beginning.

"I am now convinced that theoretical physics is actually philosophy."

Olivia Newton John's grandpa Max Born

figured it out

$$|\psi(x,t)|^2 dx = P(x)\,dx$$

the probability density of finding the quantum particle represented by $\psi(x,t)$ between x & $x+dx$

ψ sometimes called the probability amplitude

The probability that the partice ... IS ... = 1.0   It has to be someplace

so a condition on ψ : $\int_{-\infty}^{\infty} \psi^*(x,t)\,\psi(x,t)\,dx = 1 = P = \int_{-\infty}^{\infty} P(x)\,dx$

probability... so, cannot be > 1

we "normalize" wavefunctions in order to insure this

Certainly, the particle need not be everywhere

wonder about x_A to x_B? Calculate: $\int_{x_A}^{x_B} \psi^*(x,t)\,\psi(x,t)\,dx$

No potential? No problem.. $U = 0$ means free.

Then $E = \frac{p^2}{2m}$ BUT

$$\psi(x,t) = e^{i(p_x x - Et)/\hbar}$$

can't be the wavefunction since

$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = \infty$$

But not unexpected

implies a particular p_x and particular x

Uncertainty forbids that.

U often determines the form of ψ

$U = U(x,t)$ or $U(x)$

time dependent

time independent

TIME INDEPENDENT $U(x)$

then ψ factorizes and solutions to the S.E. can be explored

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

upper case

lower case

NOW!

$$\hat{E}\,\Psi(x,t) = i\hbar \frac{\partial}{\partial t} \Psi(x,t)$$

$$= i\hbar\, \psi(x) \frac{d}{dt} e^{-iEt/\hbar}$$

$$= i\hbar \left(-\frac{iE}{\hbar}\right) \psi(x)\, e^{-iEt/\hbar}$$

$$= E\,\Psi(x,t)$$

So,

$$\frac{p^2}{2m} + U(x) = E \xrightarrow{\text{1st quantization}}$$

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

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)\underline{e^{-iEt/\hbar}} + U(x)\psi(x)\underline{e^{-iEt/\hbar}} = E\psi(x)\underline{e^{-iEt/\hbar}}$$

multiply $e^{+iEt/\hbar} \longrightarrow$

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

TIME INDEPENDENT SCHROENDINGER EQUATION

Probabilities:

$$\int \Psi^*(x,t)\Psi(x,t)\,dx = \int \psi^*(x)\psi(x)\,e^{+iEt/\hbar}\,e^{-iEt/\hbar}\,dx$$

$$= \int \psi^*(x)\psi(x)\,dx \neq f(t)$$

Think about weighted averages

How do you calculate your gpa?

$$\langle grade \rangle = \frac{N_{4.0}\,(4.0) + N_{3.5}\,(3.5) + \cdots}{N_{4.0} + N_{3.5} + \cdots}$$

$$\langle x \rangle = \frac{N_1 x_1 + N_2 x_2 + \cdots}{N_1 + N_2 \cdots} = \frac{\sum_i N_i x_i}{\sum_i N_i}$$

A continuous quantity?

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

In Quantum Mechanics averages are called Expectation Values

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

works for functions:

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

order matters

Many expectation values are operators, so must appear

operating to the RIGHT $\longrightarrow$

OBSERVABLES:

represented by OPERATORS THIS WAY

$$\langle A \rangle = \frac{\int_{-\infty}^{\infty} \Psi(x,t)\, \hat{A}\, \Psi(x,t)\, dx}{\int_{-\infty}^{\infty} \Psi(x,t)\, \Psi(x,t)\, dx}$$

We're seen 2 so far p and E $\longrightarrow$ $\hat{p}$ and $\hat{E}$

we can certainly measure (**observables**) a system's

average position and/or average momentum and/or average energy

$\langle x \rangle$ $\qquad$ $\langle p \rangle$ $\qquad$ $\langle E \rangle$

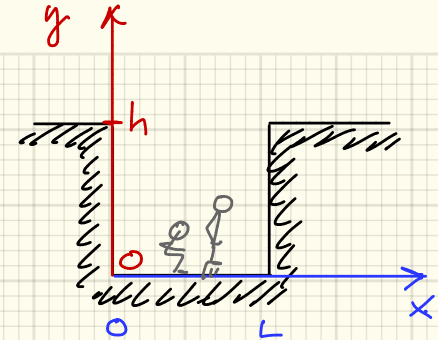
$$\langle p_x \rangle = \frac{\int_{-\infty}^{\infty} \Psi^*(x,t)\, \hat{p}_x \Psi(x,t)\, dx}{\int_{-\infty}^{\infty} \Psi(x,t)\, \Psi(x,t)\, dx}$$

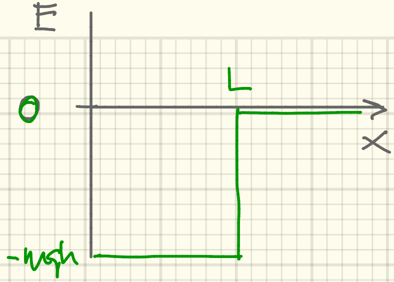
$$\langle p_x \rangle = \frac{-i\hbar \int_{-\infty}^{\infty} \Psi^*(x,t)\, \frac{\partial}{\partial x} \Psi(x,t)\, dx}{\int_{-\infty}^{\infty} \Psi^*(x,t)\, \Psi(x,t)\, dx}$$

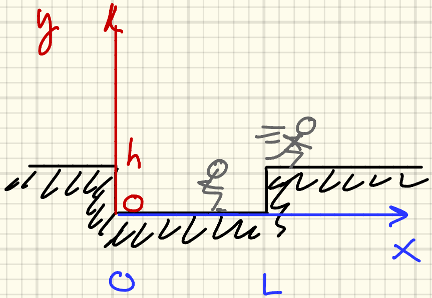
$$\langle E \rangle = \frac{i\hbar \int_{-\infty}^{\infty} \Psi^*(x,t)\, \frac{\partial}{\partial t} \Psi(x,t)\, dx}{\int_{-\infty}^{\infty} \Psi^*(x,t)\, \Psi(x,t)\, dx}$$

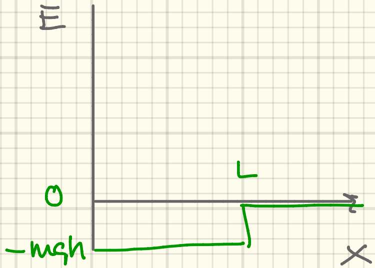
The circumstances determine the functional form of $\Psi(x,t)$

$U(x,t)$









$V(x)$ characterizes your state & motion and possibilities

Operators :

position	$\hat{x}$	x
momentum	$\hat{p}_x$	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
energy	$\hat{E}$	$i\hbar\frac{\partial}{\partial t}$
kinetic E	$\hat{K}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
potential E	$\hat{V}$	$V(x)$

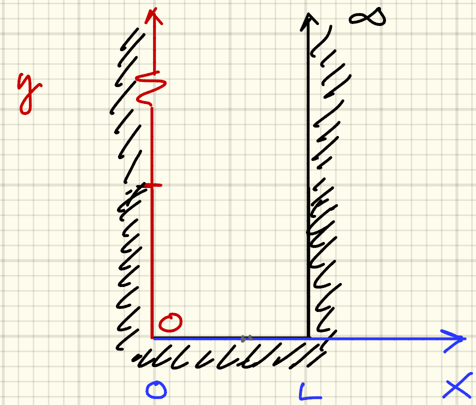
"PARTICLE IN A BOX"   "INFINITE SQUARE WELL"

Eigenvalue equations: give me the potential

I'll tell you ψ and E

... basically

"Infinite square well"



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

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

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

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

So:

$$\langle A \rangle_{x>L} = \int_L^\infty \psi^*(x)\, \hat{A}\, \psi(x)\, dx = 0 \quad \text{since } \psi = 0$$

inside the well? $V(x) = 0$ $0 < x < L$

S.E.

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

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

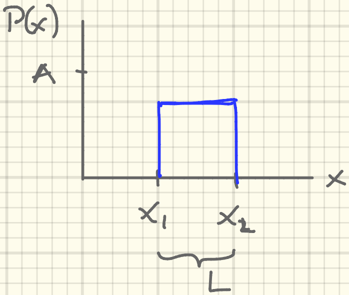
often work w/ wave number

$k = \frac{p}{\hbar} = \frac{\sqrt{2mE}}{\hbar}$

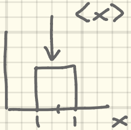
$k^2 = \frac{2mE}{\hbar^2}$

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

Lots of average quantities coming...



What's the average value?

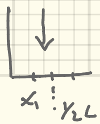


$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x\, P(x)\, dx}{\int_{-\infty}^{\infty} P(x)\, dx}$$

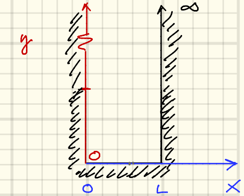
$$P(x) = 0 \qquad x < x_1 \qquad x > x_2$$
$$= A \qquad x_1 < x < x_2$$

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

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



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



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

Impose boundary conditions:

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

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

so: $kL = n\pi$

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

Normalization:

$$\int_{-\infty}^{\infty}\psi^*(x)\,\psi(x)\,dx = 1 = A^2\int_0^L \sin^2\left(\frac{n\pi x}{L}\right)dx \longrightarrow \text{gives us } A.$$

$$\int \sin^2 x\,dx = \frac{1}{2}x - \frac{1}{4}\sin 2x$$

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

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

$dy = \frac{n\pi\,dx}{L}$

$dx = \frac{L}{n\pi}dy$ $\qquad = \frac{L}{n\pi}\left[\frac{1}{2}y\Big|_0^{n\pi} - \frac{1}{4}\sin 2y\Big|_0^{n\pi}\right] = \frac{L}{n\pi}\left[\frac{1}{2}\cdot n\pi - 0\right] = \frac{L}{2}$

So the properly normalized wavefunctions are:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad n = 1, 2 \ldots \qquad \text{STANDING WAVES}$$

Energies:

$$k^2 = \frac{2mE}{\hbar^2} \longrightarrow k_n = \frac{n\pi}{L}$$

$$\text{\&} \quad \left(\frac{n\pi}{L}\right)^2 = \frac{2mE_n}{\hbar^2}$$

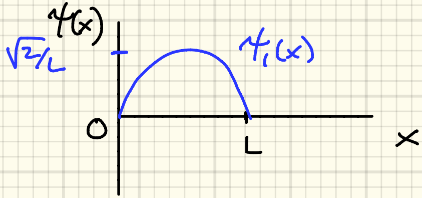
$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad n = 1, 2, 3 \ldots$$

Recap!

1) started with potential
2) solved Schroedinger Equation generally $\rightarrow \psi_1$
3) imposed boundary conditions to simplify $\rightarrow \psi_2$
4) normalized $\psi \rightarrow \psi_{FINAL, n}$
5) evaluated E_n

Look at lowest state $\quad n=1 \quad \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$

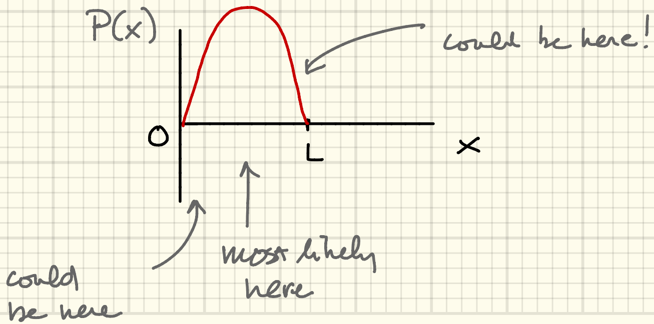
$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right)$$



with $E_1 = \frac{\pi^2\hbar^2}{2mL^2} \neq 0$!

lowest state has finite energy.

Where is the electron? ⟶ all we can calculate is a probability. $\quad P \propto |\psi|^2$

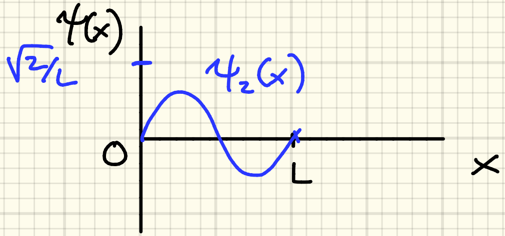


"where is it"? not a valid question.

2nd level $n=2$

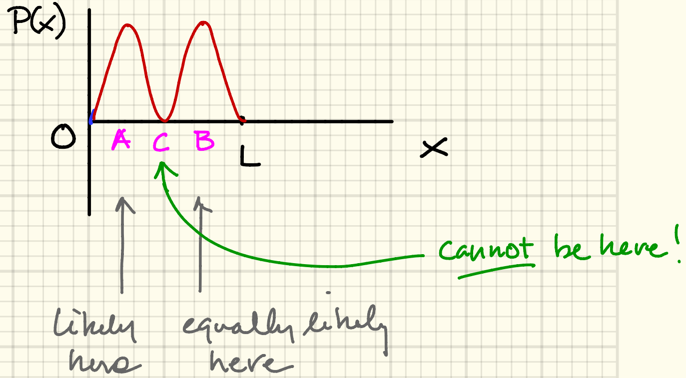
$$\psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$$

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



um.

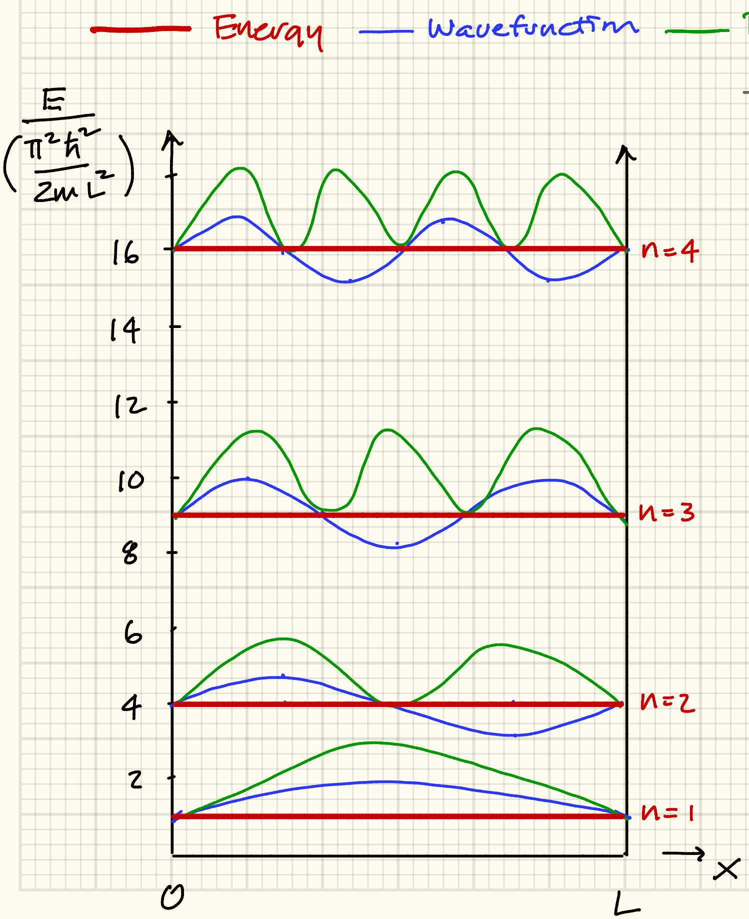
probability?



more ouch.

How does it "get" from A to B without passing through C?

another meaningless question.



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 $\Delta x \simeq L/2$

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

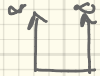
$$p_1 = \frac{\pi\hbar}{L}$$

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

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

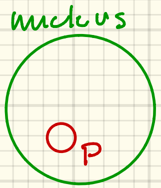
Physics Here?

Glad you asked.

∃ 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



what's E_1?

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} = \frac{\pi^2 (\hbar c)^2}{2mc^2 D_N^2} = \frac{\pi^2 (200\,\text{eV}\cdot\text{nm})^2}{2(938 \times 10^6\,\text{eV})(4\times 10^{-6}\,\text{nm})^2} = 1.3 \times 10^7\ \text{eV}$$

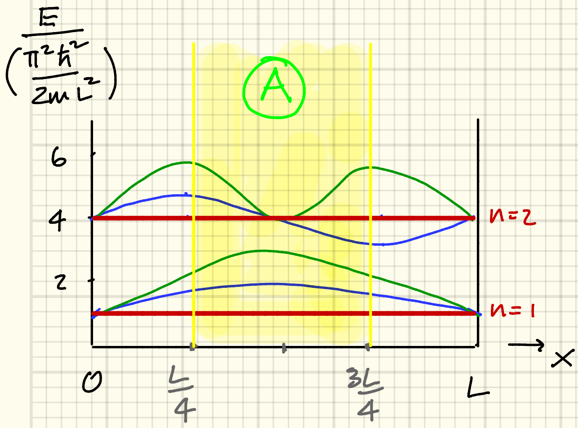
$E_1 = 13$ MeV not bad

$\longleftrightarrow$

$D_N \sim 4$ fm

$$4 \times 10^{-15}\,\text{m} = 4\times 10^{-9} \times 10^{-6}\,\text{m} = 4 \times 10^{-6}\,\text{nm}$$

LIMITED REGION ?



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

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

$$\vdots$$

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

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

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), (3L/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? $P(A)_n \rightarrow 0.5$, the classical result.

Bohr's Correspondance 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