E.F. Deveney: BSC Physics PH402 Observables Expectations Variance Scherrer C3

Note Title 3/18/2006

So we've got

Schrö-Born interpretation of Q.M.

Solve: 0.) $\hat{H}\Psi(x,t) = i\hbar\frac{\partial\Psi}{\partial t}$

& w/ Ψ we have

1.) $\int N^2 \Psi^*\Psi\, dx = 1$ solve for N

Then $\Psi(x,t) \rightarrow \underbrace{N\Psi(x,t)}_{\text{= Normalized wavefunction}}$

2.) Then $\Psi^*\Psi = \frac{\text{prob}}{\text{length}}$

$\Psi^*\Psi\, dx = \text{probability.}$

$\boxed{\text{So what?}}$

To do more.... We'll need to revisit Probability Theory.

no Longer deterministic VIEW of particles!

Before doing that .... recall where we are at

Light = particle + wave ⇒ Wave Equat → Wave Funct

e^- = particle + wave ⇒ Wave Equat → Wave Funct

(everything!) = particle + wave ⇒ wave Equat → wave Funct

& Best we can do for either is Probability

& $|\psi^*\psi|\,dx = \text{prob} = |E|^2 dx$

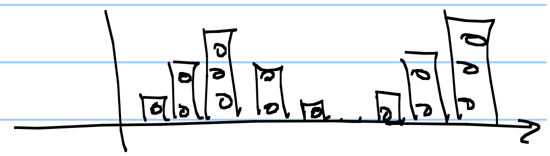
double slit

Ideas from Griffith Intro to Quantum Mechanics

So... probability PART II

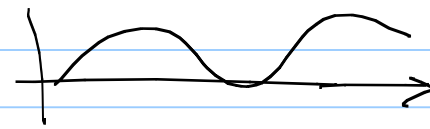
Keep in mind

1) discret prob =



discrete sized bin's Δx — P_i for each bin

2.) Continuous prob $\Rightarrow$



$\lim \Delta x \to dx$

$\&$ $\quad \text{prob} = \rho(x)dx$

$\rho(x) = \text{prob density} = \frac{\text{prob}}{\text{length}}$

So $p(x) = \rho(x)\,dx$

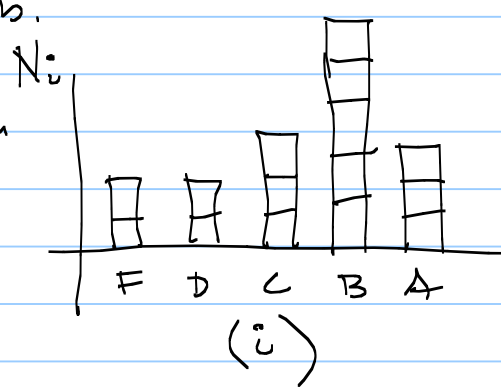
Start again w/ discrete prob.

TEST

Bin (i)	#, N_i	P_i
A	3	3/15
B	5	5/15
C	3	3/15
D	2	2/15
F	2	2/15

$N_{TOT} = 15$

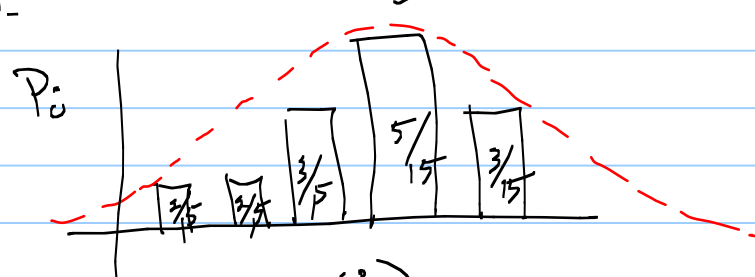
Histogram



Turn to Probability (ie Normalize)

Note $P_i = \frac{N_i}{N_{TO}}$

prob=



Note: $\sum_i P_i = \frac{N_A}{15} + \frac{N_B}{15} + \frac{N_C}{15} + \frac{N_D}{15} + \frac{N_F}{15} = \frac{15}{15} = 1 \Longleftarrow$ just as it should be! add up all prob = 1

Probability Histogram.

What can you do w/ your prob Histogram?

Once you have P_i's (ie prob distribution funct)

1.) Most Likely Grade ---- 1 time measurement

$$= P_i \text{ max} \quad (B = 5/15) = \text{Grade}_{M.L.}$$

2.) Median $\equiv$ i such that $\frac{N_{TOT}}{2}$ are > & <

here $C^+/B^- = \text{Grade}_{med}$

$\Downarrow$ new name

3.) AVERAGE = MEAN = $\langle$EXPECTATION Value$\rangle$

note $\langle\ \rangle$ bracket

which IS NOT

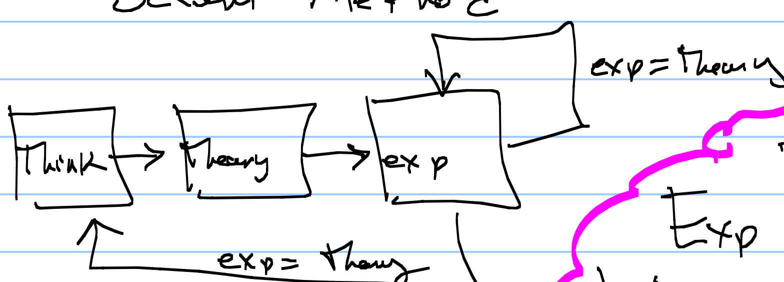
$$= \overline{\text{grade}} = \text{grade}_{ave} = \langle \text{grade} \rangle = \langle g \rangle$$

4.) What is standard deviation (ie average distance from the Ave = mean = $\langle exp \rangle$

$$\equiv \sqrt{\sum_i \frac{(\text{grade}_i - \overline{\text{grade}})^2}{N_{TOT}}}$$

We'll have to Understand all $\underline{\underline{4}}$

$\boxed{\text{Why?}}$ Scient Method



We need to know --

Exp $\overset{?}{=}$ theory

& Account for Errors that can't be beat

1.) most likely -- easy, P_i max $= 5/15 = B = 3$

2.) median ... 1/2 above, 1/2 below $\Rightarrow$ C+/B- = 2.9-3.1

OK now work...

3.) $\overline{\text{average}}$ = mean = ⟨expectation⟩

GPA G

$g_i: g_A = 4$
$g_B = 3$
$g_C = 2$
$g_D = 1$
$g_F = 0$

we know

$$\overline{\text{average}} = \frac{\sum (N_i) g_i}{N_{TOT}}$$

$$= \frac{(N_A) g_A + (N_B) g_B + (N_C) g_C + (N_D) g_D + (N_F) g_F}{N_{TOT}}$$

$$= g_A \left(\frac{N_A}{N_T}\right) + g_B \left(\frac{N_B}{N_T}\right) + g_C \left(\frac{N_C}{N_T}\right) + g_D \left(\frac{N_D}{N_B}\right) + g_F \left(\frac{N_F}{N_F}\right)$$

recognize

$$\frac{N_i}{N_T} = P_i$$

$$= g_A P_A + g_B P_B + g_C P_C + g_D P_D + g_F P_F$$

$$\langle ave \rangle = \sum_i g_i P_i$$

= sum over all gpa ((grade$_i$) (prob of grade$_i$))

Actually a Big result.

In general say you want the average GPA

$$\langle g \rangle = \sum_i g_i P_i$$

But then say you want aver GPA^2; $\langle g^2 \rangle = \sum_i g_i^2 P_i$

So it is generally true — BIG result

$$\underbrace{\langle f(i)\rangle}_{\substack{\text{ave}, \langle\text{exp}\rangle \\ \text{mean} \\ \text{of } f(i)}} = \sum_i f(i) P_i$$

= ALL expectations this way!

That's it!

Now recall most likely ≠ average!

H.W. Compute for our simple examples

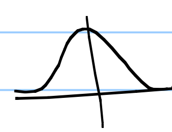
For our grade stats ...→ most likely & $\langle gpa\rangle$ based on gpa

$g_A = 4$, $g_B = 3$, $g_C = 2$, $g_D = 1$, $g_F = 0$

$$\langle g\rangle = \sum_i g_i P_i = g_A P_A + g_B P_B + g_C P_C + g_D P_D + g_F P_F$$

Now Bit of measurement Theory .....

Errors ⇒ ① part of nature — can't be completely eliminated

② Random  equal high, equal low } about true

tailing off for from true

= Gaussian or normal

system + random

≠ Accurate (true)

= precise (repeatable)

③ Systematic ⇒ part of technique of equipment that is always wrong every time.

Because we need to compare

$$\text{Theory} \stackrel{?}{=} \text{Experiment}$$

we need to know

$$\text{Theory} \pm \text{Theoretical error} \stackrel{?}{=} \text{Experiment} \pm \text{Experiment Error}$$

If you do not give idea you are not telling the truth & you are not doing Science!

Theory ± Theory Error | Exp ± Exp Error

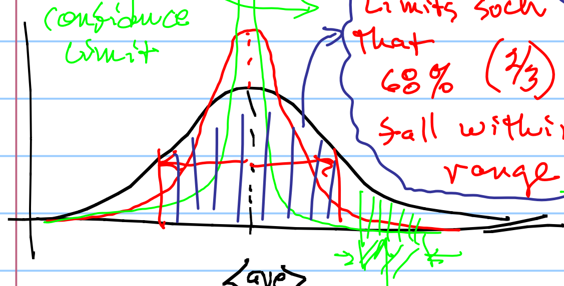
take PH414

$\langle ave \rangle \pm \underbrace{\text{Stand deviation}}_{\text{measure of average distance from } \langle ave \rangle}$

1 std = 68 confidence limit

2 std = 95% confidence limit

Limits such that 68% (2/3) fall within range



1) $\langle ave \rangle \pm \dfrac{\text{Stand deviat}}{\sqrt{N}}$

N = # of measurement

measurement experiments

2) $\text{Counts} \pm \sqrt{\text{counts}}$

counting experiments

∴ 1/3 = correct theory but out of this range

1) Normal distributions Gaussians

2) Binomial distributions

3 Theories but 3 different probability distributions but same ⟨ave⟩

what distinguishes the 3 Theories are the standard Deviations!

NOTE is Experiment falls here ... rules out green theory!

So.... can't say enough about computing standard deviation ($\rightarrow$ not in Scherrer --- see Griffiths)

Lets try it... For N_{TOT} measurements of position x_i

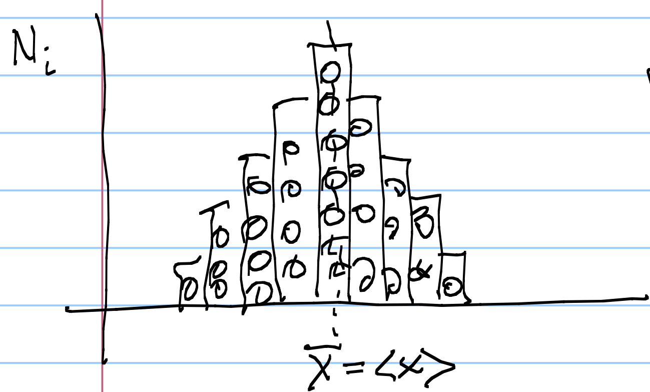
$$std = \sqrt{\frac{\sum (x_i - \bar{x})^2}{N_{TOT}}} \qquad \text{where } \Delta = \langle j \rangle - \langle i \rangle$$

measure from $\bar{x}$

def σ = variance = std^2

$$\sigma = \frac{\sum (x_i - \bar{x})^2}{N_{TOT}} =$$

Keep in mind orig Histogram



#'s of x_i = # in each Bin!

so

$$\sigma = \sum \frac{N_i (x_i - \bar{x})^2}{N_{TOT}}$$

$$= \sum \left[\frac{N_i}{N_T} \left(x_i^2 - 2x_i\bar{x} + \bar{x}^2 \right) \right]$$

$$= \sum P_i \left(x_i^2 - 2x_i\bar{x} + \bar{x}^2 \right)$$

$$=$$

$$\sigma = \sum x_i^2 P_i - 2\bar{x} \sum x_i P_i + \bar{x}^2 \sum P_i$$

Hey just def of $\langle i \rangle = \sum i P_i$

$$\sigma = \langle x^2 \rangle - 2\bar{x}\bar{x} + \bar{x}^2 = \langle x^2 \rangle - \langle x \rangle^2$$

This is BIG!

This is BIG result!

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

(expectation of x^2) − (expectation of x)^2

= variance!

& std $= \sqrt{\sigma}$ = error in theory!

1 stand deviation = 68%, 2/3 of chance answer is in this range!

Note; still 1/3 chance the answer is Good & not in this Range!

So Theory Best answer is

$$\langle x \rangle \pm \sqrt{\sigma_x}$$

1 std = 68% confidence range

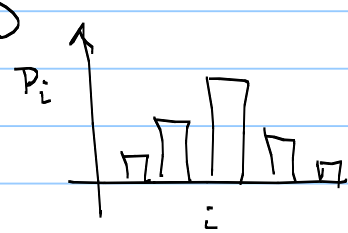
2 std = 95% confidence range

↳ note 5% chance Theory still good w/ #'s outside of $\langle x \rangle \pm 2\sqrt{\sigma}$

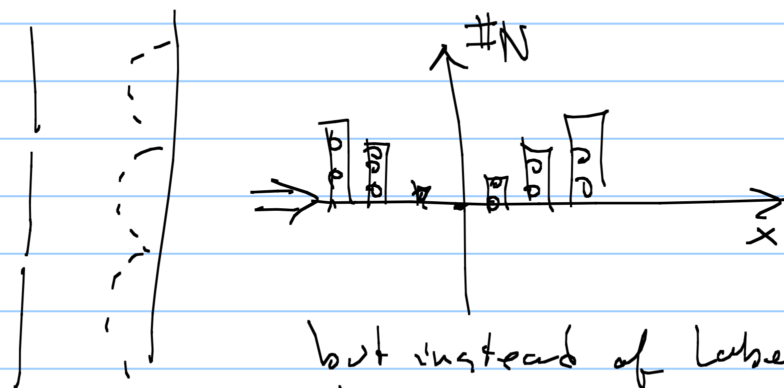
H.W. compute $\langle g \rangle \pm \sqrt{\sigma_g}$

Ok:

So we've got $\left.\begin{array}{l}\text{most likely}\\ \text{median}\\ \langle \exp \rangle\\ \sigma\end{array}\right\}$ for discrete prob.



We've agreed that w/



Histogram of #'s & bins $= \Delta x$

but instead of labeling finite bins ith

we let $\Delta x \to dx$

Then as $dx \to 0$, bin width $\to 0$

& $\text{prob}(x) \propto dx$ ← bin size

so

$$\underbrace{\text{prob}(x) = \rho(x)\, dx}$$

ρ ← prob density $= \dfrac{\text{prob}}{\text{length}}$.

So... important connection is

	discrete	$\Longrightarrow$ contin
most Likely	P_i max	$\rho(x)\,dx = \max$
$\langle$average$\rangle$ $= \langle f(i) \rangle$	$\sum f(i) P_i$	$\langle f(x) \rangle = \int f(x)\,\rho(x)\,dx$
std	$\langle f(i)^2 \rangle - \langle f(i) \rangle^2$	$\langle f(x)^2 \rangle - \left(\langle f(x) \rangle\right)^2 = \sqrt{\sigma_{f(x)}}$
$\sqrt{\sigma_{f(i)}}$	$\sum_i f(i)^2 P_i - \left(\sum f(i) P_i\right)^2$	$\int f(x)^2 \rho(x)\,dx - \left(\int f(x)\,\rho(x)\,dx\right)^2 = \nearrow$

where simply

$$\rho(x) = \psi^* \psi = \text{prob density}$$

from Schrö

i is what you want to measure!

So: Theoretical

$$\langle \exp \rangle = \text{average} = \int \underbrace{(\text{thing you want to measure})}_{\text{compute}} \Psi^* \Psi \, dx$$

Now how to we compute from Ψ ?

well recall $\hat{p} = -i\hbar \frac{\partial}{\partial x} \Psi = \hbar k \Psi$

p

So (idea)

$$\langle \exp \rangle = \int \Psi^* \hat{O} \Psi \, dx$$

operator of thing you want to compute

such that

$$\langle exp \rangle = \int \Psi^* \underset{(x)}{(\text{quantity})} \Psi \, dx$$

$$= \int \text{quantity}(x) \, \Psi^*(x) \, \Psi'(x) \, dx$$

note

if eigen problem

$\hat{O}\Psi = o\Psi$

But is not

$\hat{O}\Psi = o\Psi'$

still ok

$\Psi^* \Psi'$ still $= \frac{\text{prob}}{\text{Length}}$

so

$$= \int \text{quantity}(x) \, \frac{\text{prob}}{\cancel{\text{long}}} \, d\cancel{\text{length}}$$

continuous sum over continuous values & continuous probabilities!

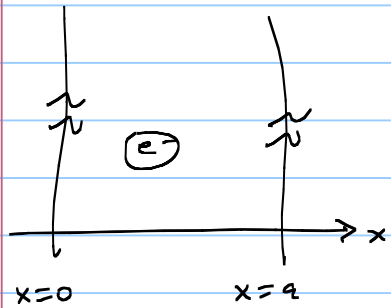
$$\langle exp \rangle = \int (\text{quantity}(x)) \, \text{prob}(x)$$

which looks just like discrete prob again

$$= \sum_i S(i) P_i$$

discrete sum over discrete values & probabilities

Let's make this legit... $\boxed{\text{Momentum}}$ = Prototype for 1) observables



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

Solve $\Psi(x,t) = \begin{cases} A\sin\left(\frac{\pi x}{a}\right)e^{\frac{-i\hbar\pi^2 t}{2ma}} & 0 \le x \le a \\ 0 & \text{otherwise} \end{cases}$

Now ask

what is average, <exp> of momentum?

Well

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

$$= \int \Psi^* \left(-i\hbar\frac{\partial}{\partial x}\right)\Psi \, dx$$

$$= \int \Psi^* (\hbar k)\Psi \, dx$$

$$= \int \hbar k\, \Psi^* \Psi \, dx$$

$$= \hbar k \underbrace{\int \Psi^* \Psi \, dx}_{=1} = \hbar k$$

$\hat{p} = -i\hbar\frac{\partial}{\partial x} \equiv$ operator for linear momentum

***Note:** 1) Here, Ψ was eigenfunction of $\hat{p}$. But we will postulate (just as we did in Schrö when added $\left(\frac{\hat{p}^2}{2m} + \hat{V}(x)\right)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$) that solving for Ψ will still work

* we only justified soln for E_k not $E_k + E_p$

2.) notice $\hat{p}$ = Linear! operator

recall definition of Linear

$$\hat{O}\left[f(x)+g(x)\right]=\hat{O}f(x)+\hat{O}g(x)$$

$$\hat{O}\left[c\,f(x)\right]=c\,\hat{O}f(x)$$

3.) notice that because Ψ is an eigen funct of $\hat{p}$

you get nice definite result---

$$\langle p\rangle=\hbar k$$

This is true in general

Ψ eigenfunction of $\hat{O}$'s

represent states in which the "particle" has definite or "fixed" value for that observable!

→ HUGE Q.M. Discussion Follows next!

So when Ψ = eigenfunct of $\hat{O}$, you Theoretical observable is Fixed exact $\Longrightarrow$

$\therefore$ $\langle p \rangle = \hbar k$ & $\langle p^2 \rangle - \langle p \rangle^2 = 0$ so Theory has $p \pm 0$, $\hbar k \pm 0$

Experiment, however will of course have error!

when $\Psi \neq$ eigenfunct of $\hat{O}$ Everything holds only will get $\langle\rangle \pm$ error!

$\Longrightarrow$ when $\Psi \neq$ eigenfunct of $\hat{O}$ will get

$$\langle \text{expect of observable} \rangle \pm \langle \text{Error} \rangle$$

> This is HUGE

Departure from Classical physics: Classically you always have well defined (at least in theory)

In Q.M., unless you have eigenfunctions, you will not have definite attributes observables!

Why? ..... a Bit Later!

Hint ... (Heisenburg uncertainty princ.)

OK: BIG Result in Q.M. & Terminology from $\hat{p} \Rightarrow$ prototype

1.) Measurable quantities $\equiv$ OBSERVABLES!
ex: momentum = an "observable"

2.) as w/ $\hat{p}$, all observables will have a
Linear $\hat{O}$
ex: 1) $\hat{p} = -i\hbar \frac{\partial}{\partial x}$

others 2) position
3) Energy
4) angular momentum } we will build these 1-2, & 3

why Linear? $\hat{L}\Psi \to c\Psi'$

Ψ' will Live in same function or vector (Hilbert) space as Ψ

and $\therefore$ Probability is preserved!

$\boxed{3.}$ ALL observables can be built from these (3) observable $\hat{O}$'s

so really only need to know these
ex: #4; $\vec{L} = \vec{r} \times \vec{p}$ = posit × momentum

So to build 2 & 3

Results on observables:

observable		$\hat{O}$
1) momentum :	$\vec{p}$ $\longleftrightarrow$	$-i\hbar \frac{\partial}{\partial x}$ ($-i\hbar\vec{\nabla}$ = 3D)
2) position:	$\vec{x}$	x
3) energy:	E_{TOT}	$i\hbar \frac{\partial}{\partial t}$

* remember all other observables can be built from these 3

observable (Experimentally measurable)

Let's do Energy next

.... we already know it!

~~for~~ $\Psi \propto e^{i(kx-\omega t)}$

we knew E_{TOT} (wave-like) $= hf = \frac{h}{2\pi} 2\pi f = \hbar\omega$

so $\hat{E} = i\hbar\frac{\partial}{\partial t}$ does the trick!

ex: $\langle E_{TOT} \rangle = \int \Psi^* \left(i\hbar \frac{\partial}{\partial t}\right)\Psi \, dx$

is Ψ = eigen funct of $\hat{E}$ Then

$\langle E_{TOT} \rangle$ = fixed value

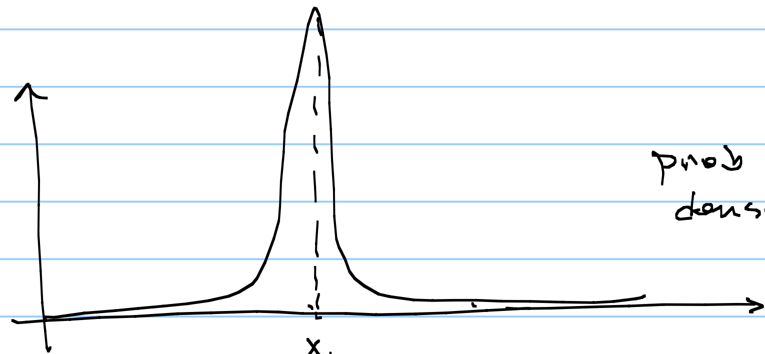
$= \int \Psi^* \hbar\omega \Psi \, dx = \hbar\omega \int \Psi^* \Psi \, dx$

$\langle E_{TOT} \rangle = \hbar\omega$

Again, not all Ψ = eigen functions of $\hat{E}$ so in general will get $\langle E_{TOT} \rangle \pm$ Error and finally position (1-D) $\hat{O}$.

well if

$|\Psi(x)|^2 =$



$|\Psi(x)|^2 dx = \text{prob} = \max @ x_1$

so how to pull out x_1 = position?

well

$$\int \Psi^*(x) \; x \; \Psi(x) \, dx$$

doesn't do anything to Ψ as an $\hat{O}$

$$= \int x \; \Psi^*(x) \Psi(x) \, dx$$

= prob ⇒ only big near x_1

$$= x_1$$

So

$$\langle x \rangle = \int \Psi^* \; x \; \Psi(x) \, dx$$

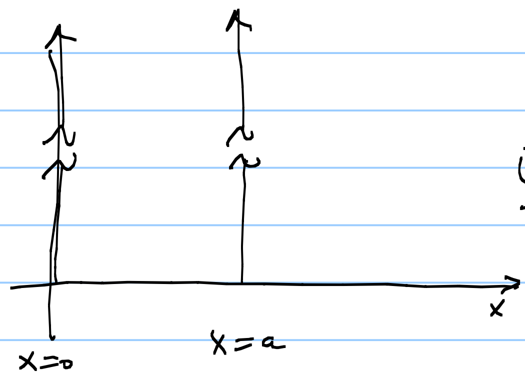
identify

$\langle x \rangle$ position $\hat{O} = x$

So we've got

$$\begin{array}{ccc} \text{observ} & & \hat{O} \\ x & \rightarrow & \hat{x} \\ \vec{p} & \rightarrow & -i\hbar\frac{\partial}{\partial x} \\ E_{TOT} & \rightarrow & i\hbar\frac{\partial}{\partial t} \end{array}$$

H.W. For our 1-D particle in ∞ well



$$\hat{H}\Psi = i\hbar\frac{\partial \Psi}{\partial t} = \text{Schrö}$$

$$\Psi(x,t) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)e^{-\frac{i\hbar\pi^2 t}{2ma}} & 0 \le x \le a \\ 0 & \text{otherwise} \end{cases}$$

Compute

$$\langle x\rangle \pm \Delta x$$
$$\langle p\rangle \pm \Delta p$$
$$\langle E\rangle \pm \Delta E$$

while noting, in particular, Ψ = eigenfunct of which $\hat{O}$? So expecting which Fixed observables!