SJP QM 3220 Formalism 1

The Formalism of Quantum Mechanics:

Our story so far …

- State of physical system: normalizable $\Psi(x, t)$
- Observables: operators $\hat{x}$, $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$, $\hat{\mathcal{H}}$
- Dynamics of Ψ: TDSE $i\hbar \frac{\partial \Psi}{\partial t} = \hat{\mathcal{H}}\Psi$

To solve, 1st solve TISE: $\hat{\mathcal{H}}\psi = E\psi$

Solutions are stationary states $\psi_n(x)$, E_n ═► special solutions of TDSE:

$$\Psi_n(x,t) = \psi_n(x) e^{-iE_n t/\hbar}$$

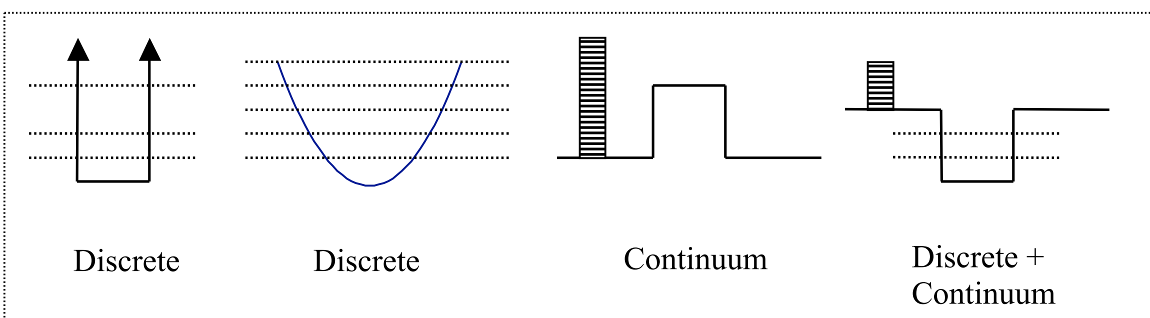
TDSE linear ═► any linear combo. of solutions is also a solution.

Discrete case: $\Psi(x,t) = \sum_n c_n e^{-iE_n t/\hbar}\psi_n(x) \quad (n = 1,2,3,\cdots)$

Continuum case:

$$\Psi(x,t) = \int dk\, \phi(k) e^{-i\omega(k)t} \underbrace{\psi_k(x)}_{e^{+ikx}/\sqrt{2\pi}}$$

(k any real number)



ψ_n's , ψ_k's form complete, orthonormal sets:

$$\int dx\, \psi_m^* \psi_n = \delta_{mn}$$

$$\int dx\, \psi_{k'}^* \psi_k = \frac{1}{2\pi}\int dx\, e^{i(k-k')x} = \delta(k-k')$$

SJP QM 3220 Formalism 1

Notice similarity of Ψ's to vectors;

- Vector $\vec{V}$ // complex function $\Psi(x, t)$
- Scalar real number a // complex number c
- Any linear combination of vectors is a vector
  $\vec{C} = a\vec{A} + b\vec{B}$ // $\Psi = \alpha\Psi_1 + \beta\Psi_2$
- Orthonormal basis vectors
  $\hat{x}\cdot\hat{x} = 1$, $\hat{x}\cdot\hat{y} = 0$ // $\int \psi_m^*\psi_n \, dx = \delta_{mn}$

  $\vec{V} = V_x\hat{x} + V_y\hat{y} + V_z\hat{z}$ // $\Psi = \sum_n c_n\psi_n$

  $V_x = \hat{x}\cdot\vec{V}$ // $c_n = \int dx \, \psi_n^*\Psi$
- Inner product
  $\vec{A}\cdot\vec{B} = \sum_{i=x,y,z} A_iB_i$ // $\int dx \, \Psi^*\Phi =$

$$\int dx \left(\sum_m d_m\psi_m\right)^* \left(\sum_n c_n\psi_n\right)$$

$$= \sum_{m,n} d_m^* c_n \underbrace{\int \psi_m^*\psi_n dx}_{\delta_{mn}} = \sum_n d_n^* c_n$$

The space of all complex, square-integrable functions $\Psi(x)$ is called Hilbert Space.

- Norm $\vec{V}\cdot\vec{V} = \left|\vec{V}\right|^2$ // $\int \Psi^*\Psi \, dx < \infty$

Hilbert Space is an infinite-dimensional vector space with complex scalars and normalizable vectors.

SJP QM 3220 Formalism 1

Postulate 1: Every possible physical state of a system corresponds to a normed vector in Hilbert Space. The correspondence is 1-to-1 except that vectors that differ by a phase factor (scalar of modulus 1) corresponds to the same state $\Psi(x, t) \Longleftrightarrow e^{i\theta}\,\Psi(x, t)$

Dirac Notation:

$$\int_{-\infty}^{+\infty} dx f^*(x)\; g(x) = \langle f|g\rangle = \text{ complex number}$$

$$\Rightarrow \quad \begin{array}{l} \langle f|g\rangle = \langle g|f\rangle^* \\ \langle f|f\rangle \text{ is real, non-negative} \end{array}$$

c any complex number:
$$\langle f|c\cdot g\rangle = c\langle f|g\rangle$$
$$\langle c\cdot f|g\rangle = c^*\langle f|g\rangle$$

Postulate 2: (to be stated shortly!) associates with every observable a linear, hermitean operator. But first, a little background:

Definition: An operator $\hat{Q}$ is hermitean (or hermitian, both spellings are common) if $\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle$ for all f, g in Hilbert space (H-space).
Which can be written (in position representation) as $\int dx f^*(\hat{Q}g) = \int dx(\hat{Q}f)^* g$

Question: Is the operator $\hat{Q} = \frac{d}{dx}(\ )$ Hermitian? (The answer will be no.)
Let's see why!

$$\underbrace{\int dx f^* \frac{dg}{dx}}_{parts} \overset{?}{=} \int dx\left(\frac{df}{dx}\right)^* \cdot g$$

$$\underbrace{f^*(x)g(x)\Big|_{-\infty}^{+\infty}}_{0} - \int \frac{d}{dx}(f^*)\cdot g(x)\; dx = -\int\left(\frac{df}{dx}\right)^* \cdot g(x)\; dx$$

So the answer is NO, there's an extra unwanted minus sign that cropped up. It is NOT the case that for this particular operator, that $\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle$. Instead, we found here $\langle f|\hat{Q}g\rangle = -\langle \hat{Q}f|g\rangle$ and that means Q is NOT hermitian.

By the way, the "surface turm" in our integration by parts gave me zero because f and g belong to Hilbert space, and thus should vanish off at infinity (so they're normalizable!)

Question: Is the operator $\hat{Q} = \frac{\hbar}{i}\frac{\partial}{\partial x}(\ )$ hermitian? Answer is Yes! Let's see why:

$$\int f^* \frac{\hbar}{i}\frac{\partial g}{\partial x}dx \underbrace{=}_{\text{int. by parts}} -\int \frac{\hbar}{i}\frac{\partial}{\partial x}(f^*)\cdot g = +\int\left(\frac{\hbar}{i}\frac{df}{dx}\right)^* g\, dx$$

=> $\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle$

Question: Is the operator $\hat{Q} = c\cdot(\ )$ hermitian (if c is some constant?)

$$\langle f|c\cdot g\rangle \overset{?}{=} \langle c\cdot f|g\rangle$$

$$c\langle f|g\rangle \overset{?}{=} c^*\langle f|g\rangle \Rightarrow$$

It depends! This operator is hermitian only <u>if</u> c is <u>real</u>.

Why are hermitean operators special? Why only hermitean operators associated with physical observables? Because hermitean operators produce <u>real</u> eigenvalues (and measurements of observables always produce <u>real</u> values).

Eigenvalue equation: $\hat{Q}\ \underbrace{f(x)}_{\text{eigenfunction}} = \underbrace{q}_{\text{eigenvalue}}\cdot f(x)$

Theorem: The eigenvalues of a hermitean operator $\hat{Q}$ are real.

Proof: Assume *f*(x) is an eigenfunction: $\hat{Q}f = qf$

$\langle Q\rangle \equiv \underbrace{\langle f|\hat{Q}f\rangle}\ =\ \underbrace{\langle \hat{Q}f|f\rangle}$ where $\hat{Q}$ is hermitean

$$q\langle f|f\rangle = \langle q\cdot f|f\rangle = q^*\langle f|f\rangle$$

$\Rightarrow (q-q^*)\langle f|f\rangle = 0 \Rightarrow q = q^*$ (since $\langle f|f\rangle \neq 0$)

SJP QM 3220 Formalism 1

Theorem: The eigenfunctions of a hermitean operator with distinct (different) eigenvalues are orthogonal.

Proof: Given $\hat{Q} f(x) = q \cdot f(x)$, $\hat{Q}\, g(x) = q' \cdot g(x)$ (with $q \neq q'$)

$$\underbrace{\langle f | \hat{Q} g \rangle} \quad = \quad \underbrace{\langle \hat{Q} f | g \rangle} \quad \text{(since } \hat{Q} \text{ hermitean)}$$

$$q' \langle f | g \rangle \quad = \quad q^* \langle f | g \rangle \quad = \quad q \langle f | g \rangle \quad \text{(q real)}$$

$\Rightarrow (q' - q)\langle f | g \rangle = 0 \Rightarrow \langle f | g \rangle = 0$ since (q' -q) $\neq$ 0 by assumption.

Postulate 2: (Operators + Observables) This is a long postulate with 3 parts, and many texts break this up into 2 or 3 postulates.

1) For every physical observable Q (x, p, E, etc.) there corresponds a linear hermitean operator $\hat{Q}$ in the Hilbert Space which possesses a complete, orthonormal set of eigenfunctions f_n (x) and the corresponding eigenvalues q_n

   $\hat{Q} f_n(x) = q_n \cdot f_n(x)$ (n could be discrete or continuous)

2) The only possible results of a measurement of Q are one of the eigenvalues $q_n = \{q_1, q_2, q_3, \ldots\}$

3) The momentum operator is $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}(\ )$
   The position operator is $\hat{x} = x \cdot (\ )$

   Any function Q(x, p) has operator $\hat{Q} = Q(\hat{x}, \hat{p})$

An example of $\hat{Q} = Q(\hat{x}, \hat{p})$ is the energy operator (or Hamiltonian),

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}(\ ) + V(x) \cdot (\ )$$

Solutions of $\hat{\mathcal{H}}\psi_n = E_n \psi_n$ form an orthonormal set (since $\hat{\mathcal{H}}$ is hermitian!)

That ψ_n's form a <u>complete</u> set can be proven in some special cases like the infinite square well or S.H.O., but in general, completeness is taken as a <u>postulate</u>.

If energy is measured, the *only possible result* is one of the E_n's.

*

SJP QM 3220 Formalism 1

The momentum eigenstates are solutions of: $\hat{p} f_p(x) = p \cdot f_p(x)$, where $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$.

Eigenfunctions: $f_p(x) = Ae^{ikx}$ (any constant A)

Eigenvalues: $p = \hbar k$ (k any real number)

Proof: $\frac{\hbar}{i}\frac{d}{dx}(Ae^{ikx}) = \hbar k(Ae^{ikx})$. (That's it!)

In this case, the eigenvalues of p form a continuum (<u>any</u> real value of $p = \hbar k$ is permitted) and this leads to some mathematical subtleties.

Are the f_p's orthonormal? (Ans: kind of … yes)

$$\int f_{p'}(x) \cdot f_p(x)\, dx = \delta(p - p')$$

"Delta function orthogonality"

$f_p(x) = Ae^{ipx/\hbar}$ ($p = \hbar k$, any real k (+) or (-))

Adjust A so that $< f_{p'} | f_p > = \delta (p - p')$

$$\left\langle f_{p'} \middle| f_p \right\rangle = |A|^2 \underbrace{\underbrace{\int dx\, e^{i(p-p')/\hbar}}_{2\pi\delta\left(\frac{p-p'}{\hbar}\right)}}_{\text{using } \delta(c\cdot x) = \frac{1}{|c|}\delta(x) \to 2\pi\hbar\delta(p-p')} = \underbrace{\underbrace{|A|^2 2\pi\hbar}_{\text{want this to be }=1}}_{\Rightarrow A = \frac{1}{\sqrt{2\pi\hbar}}} \delta(p - p')$$

Thus, $f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{+ip\cdot x/\hbar}$ <u>for</u> <u>any</u> real p, (+) or (-)

Question: are the f_p's a complete set?

Fourier Analysis (Planchevel's Theorem) says that any f(x) can be written

$f(x) = \frac{1}{\sqrt{2\pi}} \int dk\, F(k)\, e^{+ikx}$, where

$$F(k) = \frac{1}{\sqrt{2\pi}} \int dx\, f(x)\, e^{-ikx}$$

SJP QM 3220 Formalism 1

Now, any Ψ (x, t) is a function of x (at arbitrary t), and thus (from the previous page)

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int dk\ \Phi_k(k,t)\ e^{+ikx} \quad \text{, where}$$

$$\Phi_k(k,t) = \frac{1}{\sqrt{2\pi}} \int dx\ \Psi(x,t)\ e^{-ikx}$$

A quick change of variables, $k \to p = \hbar k,\ dk = dp/\hbar$, leads us to *define*

$$\Phi(p,t) = \frac{\Phi_k(k,t)}{\sqrt{\hbar}} \quad \text{(where } p = \hbar k\text{)}$$

Putting it all together:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\ \Phi(p,t)\ e^{ipx/\hbar}$$

$$\Phi_k(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dx\ \Psi(x,t)\ e^{-ipx/\hbar}$$

$$\Psi(x,t) = \int dp\ \Phi(p,t)\, f_p(x) \quad \Rightarrow f_p \text{ is are complete}$$

Note! Previously we wrote similar relations when Ψ (x, t) was a free particle state (V= 0). But <u>any</u> function Ψ (x, t) can be Fourier analyzed. In the special case of free particle, then

$$\Phi_k(k,t) = \phi(k) e^{-i\omega t} \quad \text{, where } \omega = \frac{\hbar k^2}{2m}$$

but this particular (simple) time-dependence in Φ(k, t) is true <u>only</u> for the special case of a free particle.

Φ(p, t) is called the momentum-space wave function. It is the Fourier transform of Ψ(x,t)

and tells "how much $p = \hbar k = h/\lambda$" is in Ψ. Φ(p, t) contains all the same info as Ψ(x,t).

*

SJP QM 3220 Formalism 1

We're ready now to re-state Postulate 3. Previously, Postulate 3 was stated as

Prob (find position in x $\to$ x + dx) = $|\Psi|^2$ dx.

Our re-statement will look very different, but will be same.

Postulate 3: If a system is in state $\Psi(x,t)$, and a measurement of observable Q is made

on the system, where the corresponding operator $\hat{Q}$ has eigenfunctions $f_n(x)$ and eigenvalues q_n:
$\hat{Q} f_n(x) = q_n f_n(x)$, then the strongest predictive statement that can be made about the result of that measurement is:

Prob (measure q_n) = $|\langle f_n | \Psi \rangle|^2$ (discrete spectrum)

If spectrum is <u>continuous</u>, $\hat{Q} f_q(x) = q f_q(x)$ (with <u>any</u> real value of q) then

Prob (measure $q_n \to q + dq$) = $|\langle f_q | \Psi \rangle|^2$ dq

*

Example of Postulate 3:
Suppose a system has discrete energy eigenvalues:
$\hat{\mathcal{H}}\psi_n = E_n \psi_n \quad (n = 1, 2, 3, ...)$

and your system is in a state that is a <u>linear</u> combo

$$\Psi(x,t) = \sum_n c_n(t)\, \psi_n(x) = \sum_n c_n \cdot e^{-iE_n t/\hbar} \psi_n(x)$$

$(c_n(t) = c_n \cdot e^{-iE_n t/\hbar}$ where $c_n = \int dx\, \psi_n^* \Psi$),

then a measurement of energy will yield value E_n with probability =

$|\langle \psi_n | \Psi \rangle|^2 = |c_n|^2$

If the system is already in a particular (single, pure) eigenstate n_0:

$$\Psi(x,t) = \psi_{n_0}(x)\, e^{-iE_n t/\hbar} \Rightarrow$$

$$\Psi(x,t) = \sum_n c_n\, e^{-iE_n t/\hbar}\, \psi_n(x) \text{ where } c_{n_0} = 1 \text{ and all other } c_n\text{'s} = 0$$

then measurement of energy will yield E_{n0} with probability $|c_{n_0}|^2 = 1$

This *means* an eigenstate of energy is state of definite energy. (Look back, think about it, convince yourself! The formalism can look opaque, but if you have an eigenstate of H, there is only ONE TERM in our expansion, and there is thus only one possible result when you measure energy)

A similar argument applies to any observable: an eigenstate of $\hat{Q}$ is a state of definite Q (and the value of Q = the eigenvalue of the eigenstate)

*

Previously, we asserted that the expectation value of Q =
$\langle \hat{Q} \rangle = \int dx \Psi^* \hat{Q} \Psi = \langle \Psi | \hat{Q} \Psi \rangle$. (We've used this, in the "integral form", many times!)

We can now show this f*ollows* from Postulate3:

$$\langle \Psi | \hat{Q}\Psi \rangle \underbrace{=}_{Hermiticity} \langle \hat{Q}\Psi | \Psi \rangle \underbrace{=}_{\text{completeness}} \left\langle \hat{Q} \sum_n c_n f_n \middle| \Psi \right\rangle$$

$$\underbrace{=}_{\hat{Q} f_n = q_n f_n} \left\langle \sum_n c_n q_n f_n \middle| \Psi \right\rangle \underbrace{=}_{q_n^* = q_n} \sum_n c_n^* q_n \underbrace{\langle f_n | \Psi \rangle}_{c_n}$$

$$= \sum_n q_n |c_n|^2 = \sum_n q_n \cdot \text{ Prob } (q_n)$$

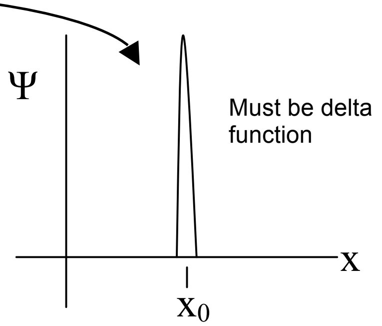
= weighted average of q_n's.
(This is what you would *mean* by "the expectation value" of measurements of Q.)

SJP QM 3220 Formalism 1

Eigenstates of $\hat{\mathcal{H}}$ = states of definite energy

Eigenstates of $\hat{p}$ = states of definite momentum

Eigenstates of $\hat{x}$ = states of definite position



Let's look at these position eigenstates $g_{x_0}(x)$

$$\hat{x} g_{x_0}(x) = x_0 g_{x_0}(x)$$

variable x particular x = x_0

$$\hat{x} = x \cdot (\ \ ) \Rightarrow x \cdot g(x) = x_0 g(x) \Rightarrow (x - x_0) g(x) = 0$$

=> g(x) is zero everywhere, except at x = x_0

$\Rightarrow g_{x_0}(x) = \delta(x - x_0)$

Notation: $g_{x0}(x)$

Postulate 3 says Prob ($x_0 \rightarrow x_0 + dx$) = $|\langle x_0 \mid \Psi(x,t)\rangle|^2\, dx$

$$= \left| \int dx\, \delta(x - x_0) \Psi(x,t) \right|^2 dx = |\Psi(x_0,t)|^2 dx$$

(agrees with our previous version of Postulate 3, what we've been using all along).

Postulate 4: (Wave function collapse)
If a measurement of observable Q gives result q_n, then the wavefunction instantly collapses into the corresponding eigenfunction of Q, $f_n(x)$.

Discrete spectrum example:

$$\Psi(x,t) = \sum_n c_n(t)\, \psi_n(x) = \sum_n c_n \cdot e^{-iE_n t/\hbar} \psi_n(x) \quad \text{(where } \psi_n(x) \text{ is an eigenstate of } \hat{\mathcal{H}}$$

If measure energy, and if find $E = E_{n_0} \Rightarrow$

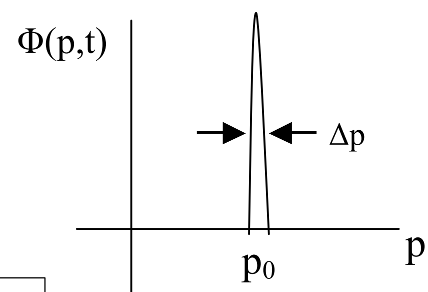
$$\Psi \underbrace{\Rightarrow}_{\text{collapse}} \psi_n(x) \qquad \text{, and the new } \Psi(x,t) = e^{-iE_{n0} t/\hbar} \psi_{n_0}(x)$$

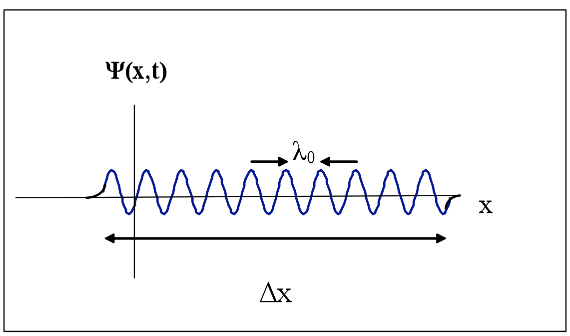
Continuous spectrum example:

$$\Psi(x,t) = \int dp\, \Phi(p,t) \underbrace{\frac{e^{ipx/\hbar}}{\sqrt{2\pi}}}_{\substack{f_p(x),\\ \text{momentum e-states}}} = \int dp\, \Phi(p,t) f_p(x)$$

$|\Phi(p_0)|^2$ is the probability density, telling you the probability if you measure momentum, that you will get p within $p_0 \to p_0 + \Delta p$.
No measurement of continuous variable has infinite precision. Precision Δp depends on measurement. This means that in practice, collapse is to a normalizable Ψ that is *almost* an eigenstate $f_{p_0}(x)$

After collapse:





$p_0 = h/\lambda$

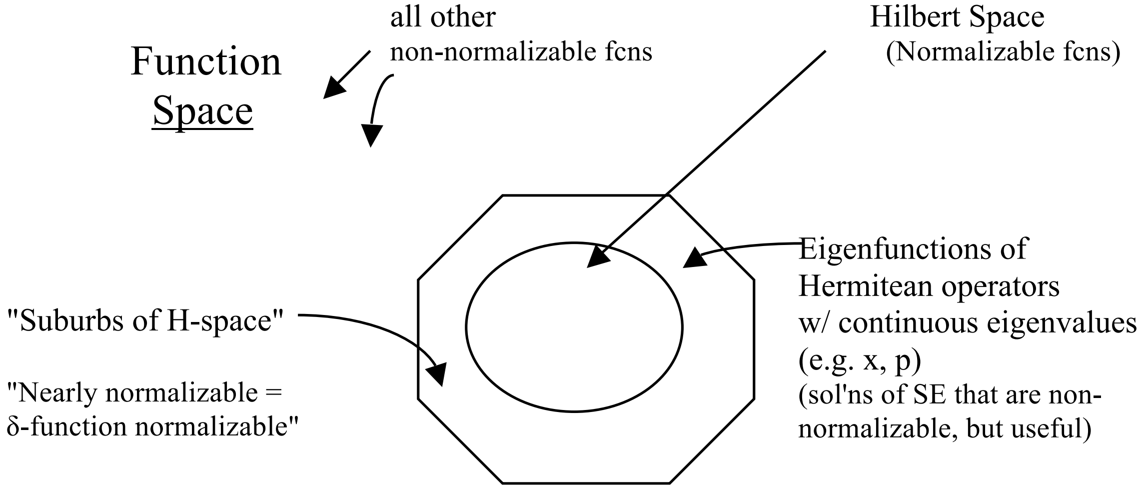
$\Delta x \cdot \Delta p \approx \hbar$

(uncertainty principle)

$$\text{Prob}\,(p_0 \to p_0 + dp) = \left|\left\langle f_{p_0}(x) \middle| \Psi(x,t) \right\rangle\right|^2 dp$$
$$= \left|\Phi(p_0,t)\right|^2 dp$$

*

SJP QM 3220 Formalism 1



To make our list of postulates complete:

Postulate 4: (Schrödinger Equation): The time evolution of the wavefunction $\Psi(x,t)$ is determined by the TDSE:

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

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

To solve TDSE: Separation of variables =>
special solutions $\Psi_n(x,t) = e^{-iE_n t/\hbar}\cdot\Psi_n(x)$

E_n's, ψ_n(x)'s are from TISE : $\hat{\mathcal{H}}\Psi_n(x) = E_n\Psi(x)$

General solution to TDSE:

$$\Psi_n(x,t) = \sum_n c_n\psi_n(x) = \sum_n c_n e^{-iE_n t/\hbar}\cdot\psi_n(x)$$

$$c_n = c_n(t=0) = \int \psi_n^*\Psi(x,0)dx = \langle\psi_n|\Psi(x,0)\rangle$$

(ψ_n's form complete orthonormal set, since $\hat{\mathcal{H}}$ is hermitean!)

<u>Any</u> hermitean operator associated with an observable has a complete orthonormal set of eigenfunctions, but the energy eigenfunctions are <u>special</u> in that they provide the time-dependence of Ψ (x,t).

Comment about probabilities and normalization: consider normalized basis states $\psi_n(x)$ and <u>un</u>-normalized $\Psi = c_1\psi_1 + c_2\,\psi_2$. Note that $\langle\Psi\,|\,\Psi\rangle = |\,c_1\,|^2 + |\,c_2\,|^2 \neq 1$.
In this case, postulate 3 should read:

$$\text{Prob (find } q_1 \text{)} = \frac{|c_1|^2}{|c_1|^2 + |c_2|^2} = \frac{|\langle\psi_1|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle}$$

(You must divide by $\langle\Psi\,|\,\Psi\rangle$ for probabilities to add up to 1)

$$\sum_n \text{Prob (find } q_n \text{)} = \frac{\sum_n |\langle\psi_n|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle} = \frac{\sum_n |c_n|^2}{\sum_n |c_n|^2} = 1$$

Review to this point:

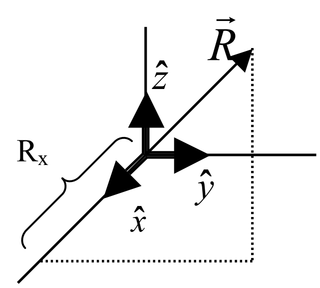
System Ψ (x,t). Measure Q. $\hat{Q} f_n(x) = q_n f_n(x)$

Post3: Find q_n with Prob $= |\langle f_n(x)|\Psi\rangle|^2$

Post4: Ψ (x,t) $\underset{\text{collapse!}}{\rightarrow}$ f_n (x)

$\langle f_n(x)|\Psi\rangle$ is "projection of Ψ onto f_n (x)"

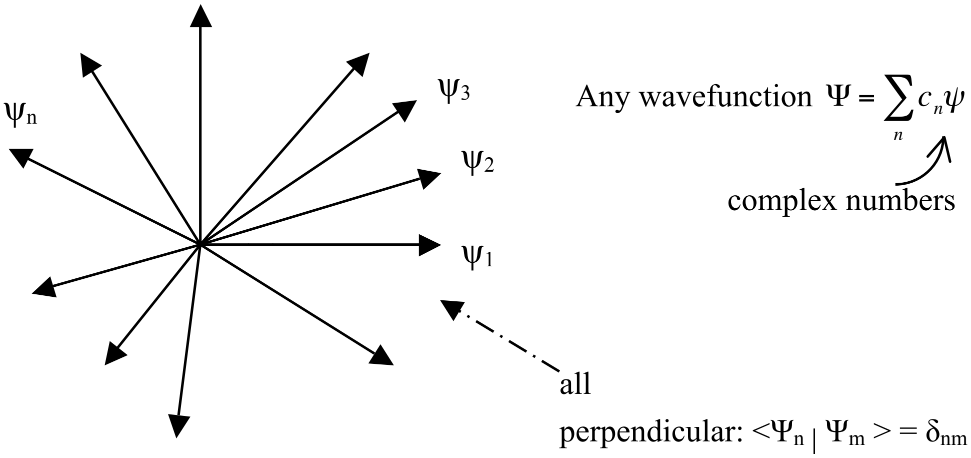
Euclidean space $R_x = \hat{x}\cdot\vec{R} =$ projection of $\vec{R}$ along $\hat{x}$



SJP QM 3220 Formalism 1

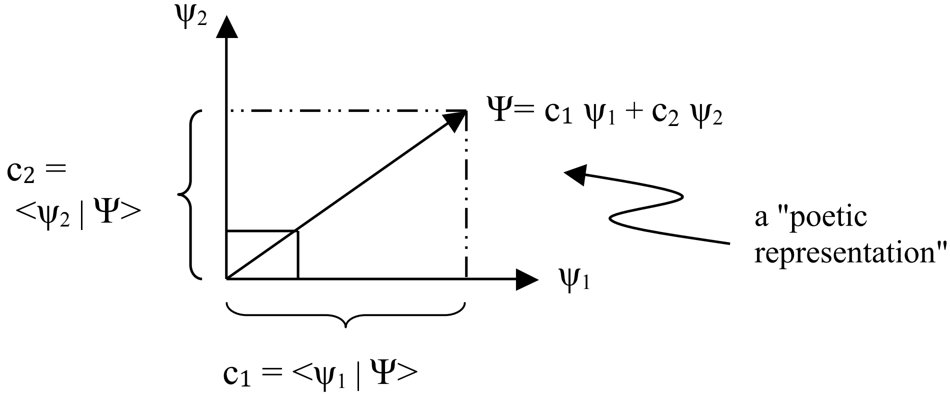
Hilbert Space is a complex, infinite-dimensional vector space.

Basis states: ψ_n from $\hat{\mathcal{H}}\psi_n = E_n\psi_n$



Any wavefunction $\Psi = \sum_n c_n \psi$

complex numbers



$$\Psi = \sum_n c_n \psi_n(x)$$: c_n tells how much of Ψ is along ψ_n axis in H-space

$$= \sum_n \langle \psi_n | \Psi \rangle\, \psi_n(x)$$

SJP QM 3220 Formalism 1

We have now seen 3 different equivalent ways to represent the wavefunctions:

$\Psi(x,t)$, $\Phi(p,t)$, $\{c_n\}$

$\Psi(x,t) = \langle x|\Psi\rangle$

$\Phi(p,t) = \langle p|\Psi\rangle$

$\{\ c_n\ \} = \{\ \langle\psi_n|\Psi\rangle\ \}$

$\{\ c_n\ \}$ looks different than functions Ψ and Φ, but not really: $\{\ c_n\ \}$ is an infinite set of numbers that associate a number (c_n) with a "coordinate" n.
Likewise Ψ(x,t) is ∞ set of numbers that associate a number Ψ(x) with a coordinate x.

Multiple ways to represent the "state" of the system, like multiple ways to represent an ordinary vector: $\vec{V} = (V_x,V_y,V_z) = (V_{x'},V_{y'},V_{z'}) = (V_r,V_\theta,V_\varphi)$
There is a vector $\vec{V}$ which exists independent of its representation in any particular basis.

Likewise, there is a "state vector" | S > or | Ψ > which exists "out there" in an abstract Hilbert space, independent of any representation.

Dirac's Notation: abstract state vector = | Ψ > (or | S > to avoid confusion with Ψ(x)).
| Ψ > is called a "ket" because it is the right hand side of a "brac·ket" < ψ_n | Ψ >.

When can two different operators have simultaneous eigenfunctions? Answer (to be shown): When they <u>commute</u>.

(Recall Definition): Commutator of operators $\hat{A}$ and $\hat{B} = [\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} =$ an operator
So, 2 operators commute if their commutator is zero: $\hat{A}\hat{B} - \hat{B}\hat{A} \Leftrightarrow \; = [\hat{A},\hat{B}] = 0$
Why would we care if there are states that are simultaneously eigenfunctions of 2 operators $\hat{A}$ and $\hat{B}$?
Recall: eigenfunction of $\hat{A}$ is a state of definite A, so eigenfunction of both $\hat{A}$ and $\hat{B}$ = state of definite A and B.

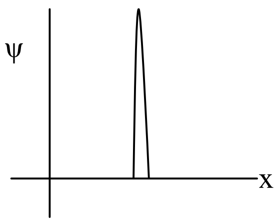
Example: $[\hat{x},\hat{p}_x] = ?$

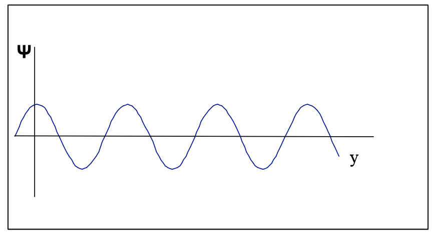
$$[\hat{x},\hat{p}_x]f = \frac{\hbar}{i}\underbrace{\left[x\frac{\partial f}{\partial x} - \frac{\partial}{\partial x}(x\cdot f)\right]}_{x\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial x} - \underbrace{\left(\frac{\partial x}{\partial x}\right)}_{1}\cdot f} = \frac{-\hbar}{i}\cdot f$$

Operate on arbitrary state f(x): $= -\frac{\hbar}{i}$. This is true for any f, so $[\hat{x},\hat{p}_x] = i\hbar$

But, $\left[\hat{x}, \hat{y}\right] = 0$, $\left[\hat{x}, \hat{p}_y\right] = 0$, $\left[\hat{p}_x, \hat{p}_y\right] = 0$

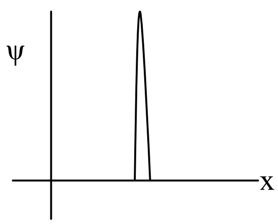
So, it is possible to have a state that is simultaneously a state of definite x and definite p_y.

=> 

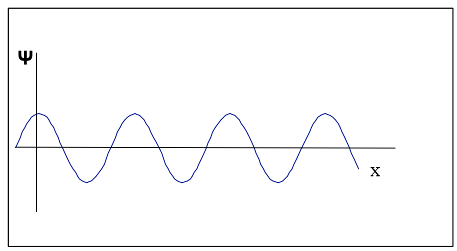
AND 

both allowed simultaneously (subject to usual caveat about non-renormalizable states.)

But, it is NOT possible to have simultaneous eigenstates of $\hat{x}$ and $\hat{p}_x$

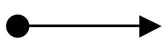


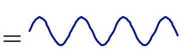
Can't have both!

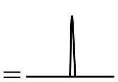


This is <u>very</u> different from the classical situation:

x, $p_x = m\, v_x$ ← can have well-defined, precise values of x AND p_x



In QM, if we start with a state of definite p_x (ψ = ) and we measure x, then

ψ collapses to a state of definite x (ψ = ) and the momentum information is destroyed.

SJP QM 3220 Formalism 1

Theorem: If $\left[\hat{A}, \hat{B}\right] = 0$,then there exist simultaneous eigenfunctions of $\hat{A}$ and $\hat{B}$:

Proof: Given ψ such that $\hat{A}\psi = a\psi$, $\hat{B}\psi = b\psi$ (same ψ), assume that Â ψ = a ψ, assume that ψ is a non-degenerate eigenfunction of Â. (We'll relax this condition later.) ψ = non-degenerate eigenfunciton of Â means that only ψ and multiples of ψ (=c ψ) are eigenfunctions. No other <u>linearly</u> <u>independent</u> eigenstates exist.

Now, operate with $\hat{B}$ on both sides of Â ψ = a ψ:

$\underbrace{\hat{B}\,\hat{A}\,\psi} = \hat{B}\,a\,\psi = a\,\hat{B}\,\psi$ (since $\hat{B}$ is linear op)

$\hat{A}\left(\hat{B}\psi\right) = a\left(\hat{B}\,\psi\right) \Rightarrow \hat{B}\,\psi$ is also eigenstate of $\hat{A}$

$\hat{A}$

But assumed eigenstate of Â non-degenerate =>

$\hat{B}\psi$ is a multiple of $\psi \Rightarrow \hat{B}\psi = b\psi$ for some b (Done).

So ψ is a state of definite A (value =a) and a state of definite B (value = b).

It can be shown that $\left[\hat{\mathcal{H}}, \hat{p}_x\right] = i\hbar\dfrac{\partial V}{\partial x}$

(this would be a straightforward HW problem)

- ⇨ if V = 0 = constant (free particle), then ∂ V / ∂ x = 0, and in this case [$\hat{\mathcal{H}}$, p_x] = 0 => it IS possible to have states of definite energy and definite momentum.

Easy, we've seen this: $\psi(x) = Ae^{i(kx-\omega t)}$

$\hat{p}\psi = \hbar k\psi$, $\hat{\mathcal{H}}\,\psi = \left(\dfrac{\hbar^2k^2}{2m}\right)\psi$

(But only true for <u>free</u> particle. If any V(x) ≠ const. present, then eigenstates of $\hat{\mathcal{H}}$ are <u>not</u> p eigenstates.)

SJP QM 3220 Formalism 1

Now that we have some familiarity with commutation relations, we can show how expectation values change with time:

Theorem: For any (linear hermitean) operator $\hat{Q}$ (that does not depend on time)

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\left\langle\ \left[\hat{\mathcal{H}}, \hat{Q}\right]\ \right\rangle$$

Proof:

$$\frac{d}{dt}\langle Q\rangle = \frac{d}{dt}\langle\Psi|\hat{Q}\Psi\rangle = \left\langle\frac{\partial\Psi}{\partial t}\middle|\hat{Q}\Psi\right\rangle + \left\langle\Psi\middle|\frac{\partial}{\partial t}\left(\hat{Q}\Psi\right)\right\rangle$$

Now, $\frac{\partial}{\partial t}\left(\hat{Q}\Psi\right) = \hat{Q}\frac{\partial\Psi}{\partial t}$ (since $\hat{Q}$ assumed t - independent)

$$\Rightarrow \qquad \frac{d}{dt}\langle Q\rangle = \left\langle\frac{\partial\Psi}{\partial t}\middle|\hat{Q}\Psi\right\rangle + \left\langle\Psi\middle|\hat{Q}\frac{\partial\Psi}{\partial t}\right\rangle$$

On the other hand, we know $\frac{\partial\Psi}{\partial t} = \frac{-i}{\hbar}\hat{\mathcal{H}}\,\Psi$ (this is the TDSE) $\Rightarrow$

Note: (+) not (-), do you see why?

$$\frac{d\langle Q\rangle}{dt} = +\frac{i}{\hbar}\underbrace{\left\langle\hat{\mathcal{H}}\Psi\middle|\hat{Q}\,\Psi\right\rangle}_{\left\langle\Psi\middle|\hat{\mathcal{H}}\hat{Q}\Psi\right\rangle} - \frac{i}{\hbar}\left\langle\Psi\middle|\hat{Q}\hat{\mathcal{H}}\Psi\right\rangle$$

since $\mathcal{H}$ is hermitean

$$= \frac{i}{\hbar}\left\langle\Psi\middle|(\hat{\mathcal{H}}\hat{Q} - \hat{Q}\,\hat{\mathcal{H}})\Psi\right\rangle = \frac{i}{\hbar}\left\langle\left[\hat{\mathcal{H}},\hat{Q}\right]\right\rangle \quad \text{(As we claimed!)}$$

So any observable Q whose operator $\hat{Q}$ commutes with the Hamiltonian $\mathcal{H}$ has $\langle Q\rangle = \left\langle\Psi\middle|\hat{Q}\Psi\right\rangle =$ constant in time for <u>any</u> time $\Psi(x,t)$.

$$\left[\hat{\mathcal{H}},\hat{Q}\right] = 0 \Rightarrow \langle Q\rangle = \text{const} \Leftrightarrow \text{Q is } \underline{\text{conserved}}.$$

In classical mechanics, conservation of Q means Q = constant for isolated system.

In QM, conservation of Q means $\langle Q \rangle$ = constant.
Classically, measured conserved Q => get same Q every time. But in QM, if you measure a conserved Q, get one of the q_n's ($\hat{Q}\,f_n = q_n f_n$). In QM, conservation of Q is only evident if you make many measurements on an ensemble of identical systems.

SJP QM 3220 Formalism 1

Examples:

- $\left[\hat{\mathcal{H}},\hat{\mathcal{H}}\right] = 0 \Rightarrow \frac{d}{dt}\langle \mathrm{E}\rangle = 0$ => < E > = constant.

We really already know this: $\langle \mathrm{E}\rangle = \sum_n E_{\mathrm{n}}|c_n|^2$ is time independent.

- $\left[\hat{\mathcal{H}},\hat{x}\right] \neq 0 \Rightarrow \frac{d\langle x\rangle}{dt} \neq 0$ => < x > changes with time in general.

In fact, we can work out the commutator on the left:

$$\left[\hat{\mathcal{H}},\hat{x}\right] = \left[\frac{\hat{\mathrm{p}}^2}{2\mathrm{m}} + V(\hat{x}),\hat{x}\right] = \frac{1}{2\mathrm{m}}\left[\hat{p}^2,\hat{x}\right]$$

$$= \frac{1}{2m}\left(\hat{p}\ \underbrace{\left[\hat{p}\ ,\ \hat{x}\right]}_{-i\hbar} + \underbrace{\left[\hat{p}\ ,\ \hat{x}\right]}_{-i\hbar}\ \hat{p}\right) = -\frac{i\hbar}{m}\hat{p},\ \text{which means}$$

$$\frac{d\langle x\rangle}{dt} = \frac{\langle \hat{p}\rangle}{m}$$

We've seen this many times before, but now it's formally derived. It's "Ehrenfest's theorem", and tells us that expectation values obey Classical Laws.

- You showed in a HW, $\left[\hat{\mathcal{H}},\hat{p}_x\right] = i\hbar\frac{\partial \mathrm{V}}{\partial \mathrm{x}}$

=> $$\frac{d\langle p_x\rangle}{dt} = \left\langle -\frac{\partial V}{\partial x}\right\rangle$$

Ehrenfest again: It's Newton's 2^{nd} law!!

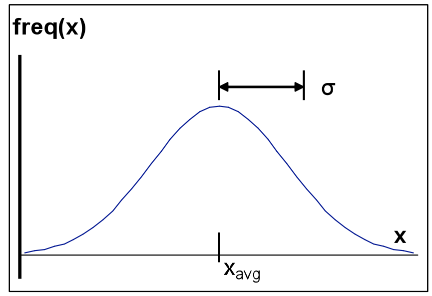
Classically: $dp/dt = F_{net} = -\partial V/\partial x$

SJP QM 3220 Formalism 1

The Heisenberg Uncertainty Principle

Recall standard deviation $\sigma_Q = \sqrt{\sigma_Q^2} = \sqrt{\left\langle \left(\hat{Q} - \langle Q \rangle \right)^2 \right\rangle}$

Classically, for any random variable x:



$\langle x \rangle = x_{\text{avg}}$

$x - \langle x \rangle$ = deviation

$\langle x - \langle x \rangle \rangle$ = avg deviation = 0

$\left\langle \left(x - \langle x \rangle \right)^2 \right\rangle$ = avg (deviation)$^2 \neq 0$

$\sqrt{\left\langle \left(x - \langle x \rangle \right)^2 \right\rangle}$ = rms deviation ≅ |spread| about avg

Theorem: (proof later) For any two (linear, hermitean) operators $\hat{A}, \hat{B}$:

$$\boxed{\sigma_A \ \sigma_B \geq \frac{1}{2i} \left\langle \left[\hat{A}, \hat{B} \right] \right\rangle}$$

This is called a "Generalized Uncertainty Principle"

Example: $\hat{A} = x, \hat{B} = \hat{p}_x$

$[\hat{x}, \hat{p}_x] = i\hbar \quad \Rightarrow \quad \sigma_A \ \sigma_B \geq \hbar/2$

That's the original Heisenberg Uncertainty Principle, *derived* now!

Often written (sloppily) $\Delta x \cdot \Delta p \approx \hbar$

=> if x known precisely ($\Delta x \approx 0$), Δp very large
if p known precisely ($\Delta p \approx 0$), Δx very large

Note: large Δp implies large p (since, if p <u>known</u> small => Δp small)

But if p large, then KE = $p^2/2m$ large. So, if Δx small (particle confined to small space) then $\Delta p \cong \hbar/\Delta x \approx p$ is large => energy is large:

$$\text{KE} = \frac{p^2}{2m} \geq \frac{(\Delta p)^2}{2m} \cong \frac{\hbar^2}{2m(\Delta x)^2}$$

We saw this in ground state of particle in infinite square well: $E_{grd} = \hbar^2\pi^2 / 2ma^2$

=> it always takes a big energy to confine particle to a small space.

Note: The Uncertainty Principle does not refer to uncertainty in the mind or even (just) the apparatus of the observer. The uncertainty is in Nature itself. If the particle has well-defined momentum, then is does not (can not) have a well-defined position.

Proof of Generalized Uncertainty Principle (same as in text):

(Â - <A>) hermitean defines f

$$\sigma_A^2 = \left\langle \Psi \middle| \left(\hat{A} - \langle A \rangle\right)^2 \Psi \right\rangle \overset{(\hat{A} - \langle A\rangle)\ \text{hermitean}}{=} \left\langle \left(\hat{A} - \langle A \rangle\right) \Psi \middle| \left(\hat{A} - \langle A \rangle\right) \Psi \right\rangle \overset{\text{defines } f}{=} \langle f | f \rangle$$

Similarly, $\sigma_B^2 = \langle g | g \rangle$ where $g = (\hat{B} - \langle B \rangle)\Psi$

$$\sigma_A^2 \sigma_B^2 = \langle f | f \rangle \langle g | g \rangle \geq \left| \langle f | g \rangle \right|^2$$

This is called the Schwartz Inequality (proven in homework) Translating into more conventional "vector" notation, it's equivalent to

$\left|\vec{A}\right|^2 \left|\vec{B}\right|^2 \geq \left|\vec{A} \cdot \vec{B}\right|^2$ which is just $A^2 B^2 \underbrace{\cos^2\theta}_{<1}$

Now $< f \mid g >$ is some complex number z, and

$$|z|^2 = (\operatorname{Re} z)^2 + (\operatorname{Im} z)^2 \geq (\operatorname{Im} z)^2 = \left(\frac{z - z^*}{2i}\right)^2$$

$$\Rightarrow \quad \sigma_A^2 \ \sigma_B^2 \ \geq \ \left(\frac{1}{2\,i}\left[\ \langle f | g \rangle \ - \ \langle g | f \rangle\ \right]\right)^2$$

Now $\langle f | g \rangle = \left\langle \ \left(\hat{A} - \langle A \rangle\right) \ \Psi \middle| \ \left(\hat{B} - \langle B \rangle\right) \ \Psi \right\rangle =$

$= \left\langle \hat{A}\hat{B} \right\rangle - \langle A \rangle \left\langle \hat{B} \right\rangle - \left\langle \hat{A} \right\rangle \langle B \rangle + \langle A \rangle \langle B \rangle$ (My notation here is that $\langle A \rangle = \left\langle \Psi \middle| \hat{A}\Psi \right\rangle = \left\langle \hat{A} \right\rangle$

since $\left\langle \langle \mathrm{A} \rangle \Psi \middle| \hat{B}\Psi \right\rangle = \langle A \rangle \left\langle \Psi \middle| \hat{B}\Psi \right\rangle = \langle A \rangle \langle B \rangle$ etc. I know that <A> is real, so it comes out of the ket

Thus, $\langle f | g \rangle = \left\langle \hat{A}\hat{B} \right\rangle - \langle A \rangle \langle B \rangle - \langle A \rangle \langle B \rangle + \langle A \rangle \langle B \rangle$

$= \left\langle \hat{A}\hat{B} \right\rangle - \langle A \rangle \langle B \rangle$ Likewise $\langle g | f \rangle = \left\langle \hat{B}\hat{A} \right\rangle - \langle B \rangle \langle A \rangle$

$$\Rightarrow \langle f | g \rangle - \langle g | f \rangle = \left\langle \hat{A}\hat{B} \right\rangle - \left\langle \hat{B}\hat{A} \right\rangle = \left\langle \hat{A}\hat{B} - \hat{B}\hat{A} \right\rangle \ = \ \left\langle \ \left[\hat{A}, \hat{B}\right] \ \right\rangle$$

Putting it all together, then,

$\Rightarrow \quad \sigma_A^2 \ \sigma_B^2 \ = \ \left(\frac{1}{2\,i}\left[\ \hat{A}, \hat{B}\ \right]\right)^2$ Which is the "generalized uncertainty principle", done.

*

SJP QM 3220 Formalism 1

In addition to the position-momentum U.P. : $\Delta x \cdot \Delta p \geq \hbar/2$

there is the time-energy U.P. : $\Delta t \cdot \Delta E \geq \hbar/2$. This looks similar, but is quite different.

In QM, time t is a parameter, not an observable. You don't measure "the time of a particle". There is no observable corresponding to time in (non-relativistic) QM.

Δt $\neq$ uncertainty in time measurement (there is no "expectation value of time")

Δt = time interval for system "to change significantly" (made precise below)

Recall $\frac{d\langle Q\rangle}{dt} = \frac{i}{\hbar}\left\langle \left[\hat{\mathcal{H}},\hat{Q}\right] \right\rangle$ and $\sigma_A^2\sigma_B^2 \geq \left(\frac{\left\langle \left[\hat{A},\hat{B}\right]\right\rangle}{2i}\right)$

Take $\hat{A} = \hat{\mathcal{H}},\ \hat{B} = \hat{Q} \Rightarrow \sigma_H^2\sigma_Q^2 \geq \left(\frac{1}{2i}\left\langle \left[\hat{\mathcal{H}},\hat{Q}\right]\right\rangle\right)^2$

$$= \left(\frac{1}{2i}\frac{\hbar}{i}\frac{d\langle Q\rangle}{dt}\right)^2$$

$$= \left(\frac{\hbar}{2}\right)^2\left(\frac{d\langle Q\rangle}{dt}\right)^2$$

$$\Rightarrow \sigma_H\sigma_Q \geq \frac{\hbar}{2}\frac{d\langle Q\rangle}{dt}$$

Define Δ E = σ_H = (1 sigma) uncertainty in energy.

Define $\Delta t = \frac{\sigma_Q}{\left|d\langle Q\rangle/dt\right|}$ $\Rightarrow$ $\sigma_Q = \left|\frac{d\langle Q\rangle}{dt}\right| \cdot \Delta t$, and we have our Energy-time U.P.

Δt is time required for < Q > to change by 1 standard deviation σ.

Examples:

- If Ψ is energy eigenstate, E known exactly => ΔE = 0 => Δt = ∞.

It takes forever for a stationary state to change.

- If Ψ is superposition of E-eigenstates, E_1 & E_2 say, then $\Delta E \approx |E_2 - E_1|$ and $\Delta t \cong \hbar/\left|E_2 - E_1\right|$. This is consistent with what we've seen before on homeworks:

$$|\Psi|^2 = \frac{|\psi_1|^2}{2} + \frac{|\psi_2|^2}{2} + 2\mathrm{Re}\left(\psi_1^*\psi_2\right)\cos\left(\frac{E_2 - E_1}{\hbar}\right)t\,.$$