Notice that in 1D problems, like the 1D infinite well or the 1D SHO, we only needed one number (n) to uniquely specify an eigenstate. This state label is called a **quantum number** or q-number and it is always in a 1-to-1 correspondence with the eigenvalues of an observable operator.

But in 3D problems, we need 3 quantum numbers (n_x , n_y , n_z) to fully specify a state [or equivalently (n , n_y , n_z), (n , n_x , n_z), etc where $n = \sqrt{n_x^2 + n_y^2 + n_z^2}$]. Just specifying n (or just n_x) is insufficient, since the eigenstates of $\hat{H}$ (or $\hat{H}_x$) are degenerate. In cases with degeneracy, more than one quantum number is required to specify a state, and the other quantum numbers are associated with other operators that must commute with the first. If two operators commute (examples: $[\hat{H}, \hat{H}_x] = 0$, $[\hat{H}_x, \hat{H}_y] = 0$) then there exists a set of orthonormal simultaneous eigenstates of both operators. We proved this for the case of operators with non-degenerate states, but it is also true when there are degeneracies. (We will show below that when operators do not commute, it is impossible to find simultaneous eigenstates.)

Claim: If N quantum numbers [example: (n_x , n_y , n_z)] are required to uniquely specify a state, then there must exit N commuting operators [example: $(\hat{H}_x, \hat{H}_y, \hat{H}_z)$] whose simultaneous eigenstates are non-degenerate and whose N eigenvalues provide the quantum numbers that uniquely label the state. Such a set of operators is called a **complete set of commuting operators** (CSCO). We will give a proof later, when we talk about matrix formulation of QM.

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

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

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

Proof: $\frac{\partial}{\partial t}\langle Q\rangle = \frac{d}{dt}\langle\Psi|\hat{Q}\Psi\rangle = \langle\frac{\partial\Psi}{\partial t}|\hat{Q}\Psi\rangle + \langle\Psi|\frac{\partial}{\partial t}(\hat{Q}\Psi)\rangle$

Now, $\frac{\partial}{\partial t}(\hat{Q}\Psi) = \hat{Q}\frac{\partial\Psi}{\partial t}$ (since $\hat{Q}$ assumed t-independ.)

$\Rightarrow \frac{\partial}{\partial t}\langle Q\rangle = \langle\frac{\partial\Psi}{\partial t}|\hat{Q}\Psi\rangle + \langle\Psi|\hat{Q}\frac{\partial\Psi}{\partial t}\rangle$

$\frac{\partial\Psi}{\partial t} = -\frac{i}{\hbar}\hat{H}\Psi$ (TDSE) $\Rightarrow$

Note: (+) not (−)

$$\frac{\partial\langle Q\rangle}{\partial t} = +\frac{i}{\hbar}\underbrace{\langle\hat{H}\Psi|\hat{Q}\Psi\rangle}_{\langle\Psi|\hat{H}\hat{Q}\Psi\rangle \text{ since } \hat{H} \text{ hermitean}} - \frac{i}{\hbar}\langle\Psi|\hat{Q}\hat{H}\Psi\rangle$$

$$= \frac{i}{\hbar}\langle\Psi|(\hat{H}\hat{Q}-\hat{Q}\hat{H})\Psi\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle \checkmark$$

So any observable Q whose operator $\hat{Q}$ commutes w/ the hamiltonian $\hat{H}$ has $\langle Q\rangle = \langle\Psi|\hat{Q}\Psi\rangle$ = constant in time for <u>any</u> $\Psi(x,t)$

$[\hat{H},\hat{Q}] = 0 \Rightarrow \langle Q\rangle = \text{const} \Longleftrightarrow$ Q is <u>conserved</u>.

In classical mech, conservation of Q $\Rightarrow$ Q = const for isolated system

In QM, conservation of $Q \Rightarrow \langle Q \rangle = \text{const}$
Classically, measured conserved $Q \Rightarrow$ get same Q everytime. But in QM, measure conserved Q, get one of the q_n's ($\hat{Q} f_n = q_n f_n$). In QM, conservation of Q only evident if you make ~~repeated~~ many measurements on an ensemble of identical systems.

Examples: • $[\hat{H}, \hat{H}] = 0 \Rightarrow \frac{d}{dt}\langle E \rangle = 0$

$\Rightarrow \langle E \rangle = \text{const}$ (already knew this: $\langle E \rangle = \sum_n E_n |c_n|^2$)

• $[\hat{H}, \hat{x}] \neq 0 \Rightarrow \dfrac{d\langle x \rangle}{dt} \neq 0$

$\Rightarrow \langle x \rangle$ changes w/ time in general

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

$$= \frac{1}{2m}\Big(\hat{p}\underbrace{[\hat{p}, \hat{x}]}_{-i\hbar} + \underbrace{[\hat{p}, \hat{x}]}_{-i\hbar}\hat{p}\Big) = -\frac{i\hbar}{m}\hat{p}$$

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

~ example of Ehrenfest's Thm: Expectation values obey Classical Laws.

• Showed in HW, $[\hat{H}, \hat{p}_x] = i\hbar \frac{\partial V}{\partial x}$

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

~ Ehrenfest again

(Classical: $dp/dt = F_{net} = -\partial V/\partial x$)

The Heisenberg Uncertainty Principle

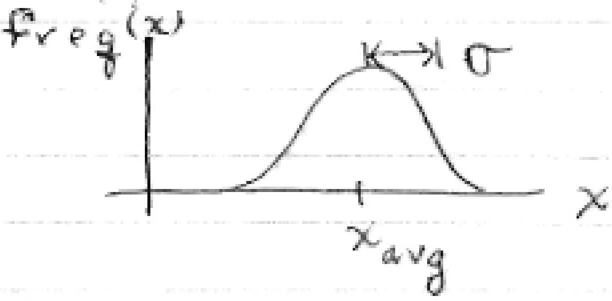
Recall standard deviation $\sigma_Q = \sqrt{\sigma_Q^2} = \sqrt{\langle(\hat{Q} - \langle Q\rangle)^2\rangle}$

Classically, for any random variable x:

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

$x - \langle x\rangle$ = deviation

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



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

$\sqrt{\langle(x - \langle x\rangle)^2\rangle} \cong$ rms deviation $\simeq$ |spread| about avg

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

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

~ "Generalized Uncertainty Principle"

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

$[\hat{x}, \hat{p}_x] = i\hbar \Rightarrow \sigma_x \, \sigma_p \geqq \hbar/2$

~ the original Heisenberg Uncertainty Principle

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

$\Rightarrow$ if x known precisely ($\Delta x \cong 0$), Δp very large

if p known precisely ($\Delta p \simeq 0$), Δx very large

Note: large $\Delta p \Rightarrow$ large p (since, if p known small $\Rightarrow \Delta p$ small)

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

$$KE = \frac{p^2}{2m} \gtrsim \frac{(\Delta p)^2}{2m} \simeq \frac{\hbar^2}{2m(\Delta x)^2}$$

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

$\Rightarrow$ 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 of the observer. The uncertainty is in Nature. If the particle has a well-defined momentum, then it does not (can not) have a well-defined position.

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

$(\hat{A}-\langle A\rangle)$ hermitean

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

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

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

Schwartz Inequality: $|\vec{A}|^2|\vec{B}|^2 \geq \underbrace{|\vec{A}\cdot\vec{B}|^2}_{A^2B^2\underbrace{\cos^2\theta}_{<1}}$

Now $\langle f|g\rangle$ is some complex nbr z, and

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

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

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

$$= \langle \hat{A}\hat{B} \rangle - \langle A\rangle\langle \hat{B}\rangle - \langle \hat{A}\rangle\langle B\rangle + \langle A\rangle\langle B\rangle$$

(since ~~...~~ $\langle \langle A\rangle \Psi | \hat{B}\Psi\rangle = \langle A\rangle \langle \Psi|\hat{B}\Psi\rangle = \langle A\rangle\langle \hat{B}\rangle$ etc.) real!

$$\langle f|g\rangle = \langle \hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle - \langle A\rangle\langle B\rangle + \langle A\rangle\langle B\rangle$$

$$= \langle \hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle$$

Notation: $\langle A\rangle \equiv \langle \Psi|\hat{A}\Psi\rangle = \langle \hat{A}\rangle$

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

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

$$\Rightarrow \sigma_A^2 \sigma_B^2 = \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}]\rangle \right)^2$$ Done.

In addition to the position-momentum U.P.:

$$\Delta x \cdot \Delta p \geq \hbar/2$$

there is the time-energy U.P.:

$$\Delta t \cdot \Delta E \geq \hbar/2$$ (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.

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

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

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

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

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

$$= (\hbar/2)^2\left(d\langle Q\rangle/dt\right)^2$$

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

Define $\Delta E = \sigma_H$ = (1 sigma) uncertainty in energy

Define $\Delta t = \frac{\sigma_Q}{|d\langle Q\rangle/dt|} \Rightarrow \sigma_Q = \left|\frac{d\langle Q\rangle}{dt}\right|\cdot\Delta t$

Δt is time required for $\langle Q\rangle$ to change by 1 std. dev. σ

Examples • If Ψ is energy eigenstate, E known exactly $\Rightarrow \Delta E = 0 \Rightarrow \Delta t = \infty$.

It takes forever for a stationary state to change.

• If Ψ is superposition of E-eigenstates, E_1 + E_2 say, then $\Delta E \simeq |E_2 - E_1|$ and $\Delta t \simeq \hbar/|E_2 - E_1|$. Consistent with

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

(Homework Set 3)