One student asked for review of "pure" and "mixed" states. This is indeed a bit confusing.

A pure state is a system which is described by a single vector $|\psi\rangle$ in Hilbert space. But this deserves some comment because a single vector is often expressed as a linear combination of other vectors, eg basis vectors

We talked about system comprised of 2 spin ½ objects with $H = J\,\vec{S}_1 \cdot \vec{S}_2$ and found ground state

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)$$

This is a pure state even though it can be written as a linear combination of basis vectors

$|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$!

Note also that even though this is a pure state prob of measuring $S_1^z = +\hbar/2 = 1/2$ and prob of measuring $S_1^z = -\hbar/2 = 1/2$

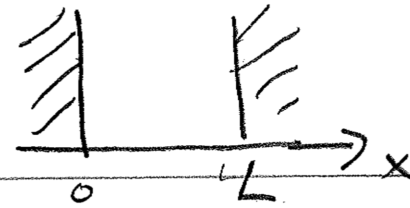
so a pure state doesn't imply measurements yield unique outcomes!

In fact, if you think about it, it would never make sense to try to define a pure state as implying a unique outcome for an observable because the nonzero comm relns of QM tell you this is not possible for all observables.

Q: why?

DMREV 3

Consider ∞ square well



$|\psi\rangle = |\phi_0\rangle \leftarrow$ ground state of $\hat{H}$

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

$p(n=1) = 1$

$p(n=2,3,\dots) = 0$

But we know $\psi(x) = \langle x|\psi\rangle = \langle x|\phi_0\rangle = \sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}$

so $|\psi\rangle = \int dx\, \psi(x)\, |x\rangle$

linear combination!

prob x is between x and $x+dx$ is $\frac{2}{L}\sin^2\frac{\pi x}{L}$

$\hat{x}$ doesn't commute with $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$

PURE STATE $\not\Rightarrow$ unique values for measurements.

DMREV-4

Ensemble / Mixed State

collection of QM systems with population w_i in $|\psi_i\rangle$

Funny/confusing thing probabilities + probabilities

ie. probability w_i you select $|\psi_i\rangle$ out of ensemble

but even given $|\psi_i\rangle$ there are probabilities of

measuring different values of observables!

Natural definition:

$$\langle \hat{A} \rangle = \sum_i \underbrace{w_i}_{\text{probability in } |\psi_i\rangle} \underbrace{\langle \psi_i | \hat{A} | \psi_i \rangle}_{\text{expectation value if in } |\psi_i\rangle}$$

Density matrix $\hat{\rho} = \sum_i w_i |\psi_i\rangle\langle\psi_i|$

$$\langle \hat{A} \rangle = \mathrm{Tr}\,\hat{\rho}\hat{A} = \mathrm{Tr} \sum_i w_i |\psi_i\rangle\langle\psi_i|\hat{A}$$

$|e_n\rangle$ any basis

$$= \sum_n \sum_i w_i \langle e_n|\psi_i\rangle\langle\psi_i|\hat{A}|e_n\rangle$$

$$= \sum_n \sum_i w_i \langle\psi_i|\hat{A}|e_n\rangle\langle e_n|\psi_i\rangle$$

$$= \sum_i w_i \langle\psi_i|\hat{A}|\psi_i\rangle \quad \text{as expected!}$$

DMREV-5

Pure and mixed states are distinguished by their value of $\mathrm{Tr}\,\hat{\rho}^2$.

First note $\mathrm{Tr}\,\hat{\rho} = \mathrm{Tr} \sum_i w_i |\psi_i\rangle\langle\psi_i|$

$$= \sum_n \sum_i w_i \langle e_n|\psi_i\rangle\langle\psi_i|e_n\rangle$$

$$= \sum_i w_i \underbrace{\sum_n \langle\psi_i|e_n\rangle\langle e_n|\psi_i\rangle}_{\langle\psi_i|\psi_i\rangle = 1}$$

$$= \sum w_i = 1. \quad \blacksquare$$

$$\mathrm{Tr}\,\hat{\rho}^2 = \mathrm{Tr} \sum_{ij} w_i w_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j|$$

$$= \sum_{ij} w_i w_j \sum_n \langle e_n|\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j|e_n\rangle$$

$$= \sum_{ij} w_i w_j \sum_n \langle\psi_i|\psi_j\rangle\underbrace{\langle\psi_j|e_n\rangle\langle e_n|\psi_i\rangle}_{\langle\psi_j|\psi_i\rangle}$$

$$= \sum_{ij} w_i w_j |\langle\psi_j|\psi_i\rangle|^2$$

$$\leq \sum_{ij} w_i w_j = 1$$

Equality iff $w_i = 1$ for <u>single</u> i.