08. Quantum Mechanics: Density Operators

1. States as Density Operators

- *Motivation*: Suppose a quantum system is associated with an *ensemble* $\{|\psi_i\rangle, p_i\}$ of vector states $|\psi_i\rangle$, each with a probability p_i.

  Suppose we don't know what state our quantum system is in; suppose all we know are its possible states.

- *Recall*: In Gibbs' approach to classical statistical mechanics, we considered an ensemble of *classical* states to be a *classical* phase space Γ with a probability distribution $\rho(x, t)$ defined on it.

  - *In QM, we use a vector space $\mathcal{H}$ instead of a classical phase space Γ.*
  - *What should we use instead of the function $\rho(x, t)$?*

    Answer: An operator...

Def. 1 (*Density operator*). The **density operator** ρ for a system in an ensemble $\{|\psi_i\rangle, p_i\}$ of m vector states $|\psi_i\rangle \in \mathcal{H}$ each with probablity p_i, is defined by

$$\rho = \sum_{i=1}^{m} p_i |\psi_i\rangle\langle\psi_i|, \quad \text{where } \sum_{i=1}^{m} p_i = 1.$$

Warning! Same notation but different mathematical objects:
ρ in QM is an operator.
$\rho(x,t)$ in classical Stat Mech is a function.

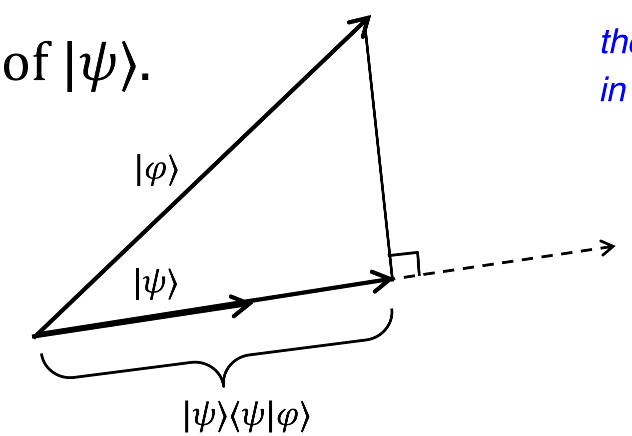
- Note 1: $|\psi\rangle\langle\psi|$ is an *operator*.
  - It acts on a vector $|\varphi\rangle$ and gives you another vector $|\psi\rangle\langle\psi|\varphi\rangle$.

vector $|\psi\rangle$

inner product (number) $\langle\psi|\varphi\rangle$

the magnitude of $|\varphi\rangle$ in the direction of $|\psi\rangle$!

- Note 2: $|\psi\rangle\langle\psi|$ is a "*projection*" operator.
  - It projects a vector $|\varphi\rangle$ in the direction of $|\psi\rangle$.



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- *Note 3*: The vector states $\{|\psi_i\rangle\}$ are not necessarily orthogonal to each other, and m is not necessarily the dimension n of $\mathcal{H}$.

But: ρ can always be expressed in terms of a basis $\{|\phi_i\rangle\}$ of $\mathcal{H}$ as

$$\rho = \sum_{i=1}^{n} \lambda_i |\phi_i\rangle\langle\phi_i|$$

where $|\phi_i\rangle$ are eigenvectors of ρ with eigenvalues $\lambda_i \geq 0$.

← *Because ρ is Hermitian!*

- *And*: Since ρ is supposed to represent an ensemble of vector states, in this case $\{|\phi_i\rangle, \lambda_i\}$, we require $\sum_{i=1}^{n} \lambda_i = 1$.

← *The sum of the eigenvalues of a density operator is 1!*

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- *Note 4*: A density operator can describe more than one ensemble of vector states.

Example:

Suppose: $|a\rangle = \sqrt{3/4}|0\rangle + \sqrt{1/4}|1\rangle$

$|b\rangle = \sqrt{3/4}|0\rangle - \sqrt{1/4}|1\rangle$

Then: $|0\rangle = \sqrt{1/3}|a\rangle + \sqrt{1/3}|b\rangle$

$|1\rangle = |a\rangle - |b\rangle$

So: $\rho = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b|$ *corresponds to* → $\{|a\rangle, |b\rangle; \frac{1}{2}, \frac{1}{2}\}$

$= \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$ *corresponds to* → $\{|0\rangle, |1\rangle; \frac{3}{4}, \frac{1}{4}\}$

distinct ensembles, same density operator

2. Pure States and Mixed States

Why use density operators to represent states?

> **Def. 2** (*Pure/mixed density operator state*). If a density operator can be expressed as $\rho = |\psi\rangle\langle\psi|$, then it is called a **pure density operator state**. Otherwise, it is called a **mixed density operator state**.

- Note 1: An "ignorance" interpretation of mixed density operator states is not always appropriate!

$$\rho = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2| + \cdots$$

Ignorance as to what vector state the system is in?

- Concern 1: ρ can describe more than one ensemble of vector states.

Recall:

Let: $|a\rangle = \sqrt{3/4}|0\rangle + \sqrt{1/4}|1\rangle$

$|b\rangle = \sqrt{3/4}|0\rangle - \sqrt{1/4}|1\rangle$

If the system is in the density operator state ρ, should it be associated with the ensemble $\{|a\rangle, |b\rangle; 1/2, 1/2\}$ or the ensemble $\{|0\rangle, |1\rangle; 3/4, 1/4\}$?

Then: $\rho = \tfrac{1}{2}|a\rangle\langle a| + \tfrac{1}{2}|b\rangle\langle b|$ *corresponds to* $\{|a\rangle, |b\rangle; 1/2, 1/2\}$

$= \tfrac{3}{4}|0\rangle\langle 0| + \tfrac{1}{4}|1\rangle\langle 1|$ *corresponds to* $\{|0\rangle, |1\rangle; 3/4, 1/4\}$

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← *Ignorance as to what vector state the system is in?*

- <u>*Concern*</u> <u>2</u>: An ignorance interpretation cannot be applied to a mixed density operator state of a subsystem of a composite system in a pure *entangled* density operator state.

← *To be demonstrated later...*

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- *Note 2*: A mixed density operator state is not the same thing as a superposed vector state!

Example:

- The mixed density operator state $\rho = ½|a\rangle\langle a| + ½|b\rangle\langle b|$ corresponds to an *ensemble* of vector states $\{|a\rangle, |b\rangle; ½, ½\}$.
- The pure density operator state $\rho = ½\{|a\rangle + |b\rangle\}\{\langle a| + \langle b|\}$ corresponds to a *single* vector state $\frac{1}{\sqrt{2}}\{|a\rangle + |b\rangle\}$.

3. A Test for Mixedness

Def. 3 (*Trace*). Let O be an operator on a vector space $\mathcal{H}$ with basis $\{|v_i\rangle\}$. The **trace** $\mathrm{Tr}(O)$ of O is defined by

$$\mathrm{Tr}(O) \equiv \sum_i \langle v_i|O|v_i\rangle$$

The sum of the diagonal elements of a matrix representation of O

- *Note 1*: If O is a Hermitian operator on $\mathcal{H}$, then its eigenvectors $\{|\lambda_i\rangle\}$ form a basis for $\mathcal{H}$, and

$$\mathrm{Tr}\,O = \sum_i \langle \lambda_i|O|\lambda_i\rangle = \sum_i \lambda_i \langle \lambda_i|\lambda_i\rangle = \sum_i \lambda_i$$

The trace of a Hermitian operator is the sum of its eigenvalues!

- *Note 2*: Recall that the sum of the eigenvalues of a density operator state ρ is 1.
    - *So*: $\mathrm{Tr}\,\rho = 1$ for both pure and mixed density operator states.

Claim (*Test for mixedness*).

(a) ρ is a pure density operator state *if and only if* $\mathrm{Tr}\,\rho^2 = 1$.

(b) ρ is a mixed density operator state *if and only if* $\mathrm{Tr}\,\rho^2 < 1$.

- *First note*:

$$\rho^2 = \sum_{i=1}^{n} \lambda_i |\phi_i\rangle\langle\phi_i| \sum_{j=1}^{n} \lambda_j |\phi_j\rangle\langle\phi_j|$$

$|\phi_i\rangle$ are eigenvectors of ρ with eigenvalues λ_i

$$= \sum_{i,j} \lambda_i \lambda_j |\phi_i\rangle\langle\phi_i|\phi_j\rangle\langle\phi_j|$$

$\langle\phi_i|\phi_j\rangle = 0$ unless $j = i$

$$= \sum_i \lambda_i{}^2 |\phi_i\rangle\langle\phi_i|$$

$|\phi_i\rangle$ are eigenvectors of ρ^2 with eigenvalues $\lambda_i{}^2$

$$\mathrm{Tr}\,\rho^2 = \sum_i \lambda_i{}^2$$

Proof of (a):

- *Suppose*: ρ is a pure density operator state.
  - *Then*: $\rho^2 = \rho$, and hence $\mathrm{Tr}\,\rho^2 = \mathrm{Tr}\,\rho = 1$.
- *Now suppose*: ρ is a density operator state and $\mathrm{Tr}\,\rho^2 = 1$.
  - *Then*: $\sum_i \lambda_i{}^2 = 1 = \sum_i \lambda_i$.
  - *And*: This holds if and only if one of the λ_i is 1 and the rest are 0.
  - *Thus*: ρ is pure.

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$|\phi_i\rangle$ *are eigenvectors of* ρ *with eigenvalues* λ_i

$$= \sum_{i,j} \lambda_i \lambda_j |\phi_i\rangle\langle\phi_i|\phi_j\rangle\langle\phi_j|$$

$\langle\phi_i|\phi_j\rangle = 0$ *unless* $j = i$

$$= \sum_i {\lambda_i}^2 |\phi_i\rangle\langle\phi_i|$$

$|\phi_i\rangle$ *are eigenvectors of* ρ^2 *with eigenvalues* ${\lambda_i}^2$

$$\mathrm{Tr}\,\rho^2 = \sum_i {\lambda_i}^2$$

Proof of (b):

- *Suppose*: ρ is a mixed density operator state.
  - *Then*: $\mathrm{Tr}\,\rho^2 = \sum_i {\lambda_i}^2 \leq \sum_i \lambda_i = 1$, with equality if and only if ρ is pure.
- *Now suppose*: ρ is a density operator state and $\mathrm{Tr}\rho^2 < 1$.
  - *Then*: $\mathrm{Tr}\,\rho^2 = \sum_i {\lambda_i}^2 < 1$, and $\sum_i \lambda_i = 1$.
  - *And*: This excludes the case of one of the λ_i being 1 and the rest 0.
  - *Thus*: ρ must be mixed.

Why get bogged down with all these linear algebra definitions of mixed density operator states and tests of mixedness?

- *Because*:
  - *Ultimately*: We're going to focus on a notion of entropy associated with density operator states (think of the analogy with the Gibbs entropy for classical ensembles).
  - *And*: That notion of entropy (called the "von Neumann" entropy) is first and foremost a measure of the degree to which a density operator state is mixed!
  - *Moreover*: As we'll see, it can also be interpreted (under certain conditions) as a measure of *entanglement*.

Next up…