notes about mixed states

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1 pure state and mixed state

A pure state of a quantum system is denoted by a vector ket with unit length.

We used to just call it a state. But now it is a state for a whole system. There is another kind of state that needs to be distinguished.

2 Definition of Trace operation

Trace operation is a map definded as:

$$\mathrm{Tr}(\hat{K}) = \sum_n \langle n| \hat{K} |n\rangle$$

So the definition of trace operation includes a set of basis $\{|n\rangle\}$. However the basis does not affect the value of trace.

3 Property of Trace operation

1. a basis change leaves it invariant

   proof: recall the representation transformation.

2. cyclical property

   $$\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A}) \quad \mathrm{Tr}(\hat{A}\hat{B}\hat{C}) = \mathrm{Tr}(\hat{B}\hat{C}\hat{A}) = \mathrm{Tr}(\hat{C}\hat{A}\hat{B})\cdots$$

   proof:

   Starting from $\hat{A}\hat{B}$

   $$\mathrm{Tr}(\hat{A}\hat{B}) = \sum_m \sum_k a_{mk} b_{km} = \sum_m \sum_k b_{km} a_{mk} = \mathrm{Tr}(\hat{B}\hat{A})$$

   for $\hat{A}\hat{B}\hat{C}$, set $\hat{C} = \hat{A}\hat{B}$

   In an infinite-dimensional hilbert space some care has to be taken.

3. express the expectation value

   For any operator $\hat{O}$, we want to know its expectation value under state $|\psi\rangle$.

$$\begin{aligned}\langle\hat{O}\rangle &= \langle\psi|\,\hat{O}\,|\psi\rangle \\ &= \mathrm{Tr}(\hat{O}\,|\psi\rangle\langle\psi|) \\ &= \mathrm{Tr}(|\psi\rangle\langle\psi|\,\hat{O})\end{aligned}$$

   proof:

$$\begin{aligned}\langle\hat{O}\rangle &= \langle\psi|\,\hat{O}\,|\psi\rangle \\ &= \langle\psi|\left(\sum_n |n\rangle\langle n|\right)\hat{O}\,|\psi\rangle = \langle\psi|\,\hat{O}\left(\sum_k |k\rangle\langle k|\right)|\psi\rangle \\ &= \mathrm{Tr}(\hat{O}\,|\psi\rangle\langle\psi|) = \sum_n \langle n|\,\hat{O}\,|\psi\rangle\langle\psi|\,|n\rangle \\ &= \mathrm{Tr}(|\psi\rangle\langle\psi|\,\hat{O}) = \sum_k \langle k|\,|\psi\rangle\langle\psi|\,\hat{O}\,|k\rangle\end{aligned}$$

4. express the overlaps of two state (ψ, ϕ)

$$|\langle\phi|\psi\rangle|^2 = \mathrm{Tr}(|\phi\rangle\langle\phi|\,|\psi\rangle\langle\psi|) = \mathrm{Tr}(|\psi\rangle\langle\psi|\,|\phi\rangle\langle\phi|)$$

$$\begin{aligned}|\langle\phi|\psi\rangle|^2 &= \langle\psi|\phi\rangle\langle\phi|\psi\rangle \\ &= \langle\psi|\left(\sum_n |n\rangle\langle n|\right)|\phi\rangle\langle\phi|\psi\rangle = \langle\psi|\phi\rangle\langle\phi|\left(\sum_k |k\rangle\langle k|\right)|\psi\rangle \\ &= \sum_n \langle n|\,|\phi\rangle\langle\phi|\,|\psi\rangle\langle\psi|\,|n\rangle = \mathrm{Tr}(|\phi\rangle\langle\phi|\,|\psi\rangle\langle\psi|) \\ &= \sum_k \langle k|\,|\psi\rangle\langle\psi|\,|\phi\rangle\langle\phi|\,|k\rangle = \mathrm{Tr}(|\psi\rangle\langle\psi|\,|\phi\rangle\langle\phi|)\end{aligned}$$

4 definition of density operator

In the property of trace operation, we have aquitanted $|\psi\rangle\langle\psi|$ many times. Now we name it as density operator(this is the density operator for a pure state)

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

And we define a more general type of states. by introducing the mixture of pure states:

$$\hat{\rho} = \sum_{k=1}^{N} p_k \left|\psi_k\right\rangle\left\langle\psi_k\right|$$

where $\{\left|\psi\right\rangle_k\}$ is just a set of some random pure states, $0 < p_k \leq 1$, $\sum_k p_k = 1$

A state is called a mixed state when $\hat{\rho}$ can not be written as a density operator for a pure state(for which $N = 1$, and $p_1 = 1$).

5 understanding of density operator

It is an operator. It is an abstract elements. It can be related to matrix with bases, but it does not equal to one matrix.

For example, if we consider a particle moving in 1-D, and define $\psi(x) = \langle x|\psi\rangle$.

The corresponding density matrix in the basis $\{\left|x\right\rangle\}_{x\in(-\infty,+\infty)}$ is

$$\begin{aligned}\hat{\rho} &= \left|\psi\right\rangle\left\langle\psi\right| \quad \text{insert two identities}\\ &= \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}x' \left|x'\right\rangle\left\langle x'\right| \left|\psi\right\rangle\left\langle\psi\right| \left|x\right\rangle\left\langle x\right| \\ &= \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}x' \psi^*(x)\psi(x') \left|x'\right\rangle\left\langle x\right| \end{aligned} \tag{1}$$

This is how the matrix looks like, if we want it more specific, that is knowing the elements of the matrix.

The elements of the matrix is :

$$\left\langle x'\right| \hat{\rho} \left|x\right\rangle = \psi(x')\psi^*(x)$$

6 property of density operator

1. for pure state, if $\langle\psi|\psi\rangle = 1$, $\hat{\rho}^2 = \hat{\rho}$; for mixed states, $\hat{\rho}^2 \neq \hat{\rho}$.

   proof:

$$\hat{\rho}^2 = \left|\psi\right\rangle\left\langle\psi\right| \left|\psi\right\rangle\left\langle\psi\right| = \left|\psi\right\rangle\left\langle\psi\right|$$

$$\begin{aligned}\hat{\rho}^2 &= \left(\sum_{k=1}^{N} p_k \left|\psi_k\right\rangle\left\langle\psi_k\right|\right)\left(\sum_{k'=1}^{N} p_{k'} \left|\psi_{k'}\right\rangle\left\langle\psi_{k'}\right|\right) \\ &= \sum_{k=1}^{N}\sum_{k'=1}^{N} p_k p_{k'} \langle\psi_k|\psi_{k'}\rangle \left|\psi_k\right\rangle\left\langle\psi_{k'}\right| \\ &= \sum_{k=1}^{N} p_k^2 \left|\psi_k\right\rangle\left\langle\psi_k\right| + \cdots\end{aligned}$$

Actually, I don't know how exactly this does not equal to $\hat{\rho}$. I need more explanation.

2. for pure state, $\mathrm{Tr}(\hat{\rho}^2) = 1$; for mixed state, $\mathrm{Tr}(\hat{\rho}^2) < 1$.

   The value of $P = \mathrm{Tr}(\hat{\rho}^2)$ is called the purity of a state.

3. for pure states, $\mathrm{Tr}(\hat{\rho}) = 1$; for mixed states, $\mathrm{Tr}(\hat{\rho}) = 1$.

   proof:

$$\begin{aligned}\mathrm{Tr}(\hat{\rho}) &= \sum_n \langle n|\, \hat{\rho}\, |n\rangle \\ &= \sum_n \langle n|\psi\rangle\langle\psi|n\rangle \\ &= \sum_n |\langle\psi|n\rangle|^2 \\ &= 1\end{aligned}$$

$$\begin{aligned}\mathrm{Tr}(\hat{\rho}) &= \sum_n \langle n| \left(\sum_{k=1}^{N} p_k\, |\psi_k\rangle\langle\psi_k|\right) |n\rangle \\ &= \sum_k p_k \left(\sum_n \langle n|\psi_k\rangle\langle\psi_k|n\rangle\right) \\ &= \sum_k p_k \\ &= 1\end{aligned}$$

4. has an advantage compared to a ket:

   a given physical state can be described by any ket of the form $e^{i\theta}\,|\psi\rangle$, but by only one density operator $\hat{\rho}$

5. express the expectation value

   for pure state, the expectation value for $\hat{O}$, $\langle\hat{O}\rangle = \mathrm{Tr}(\hat{O}\hat{\rho}) = \mathrm{Tr}(\hat{\rho}\hat{O})$.

   for mixed state, we would expect an average value of $O_k = \mathrm{Tr}(|\psi_k\rangle\langle\psi_k|\,\hat{O})$ for each pure state, and then the expectaion value for the mixed state is that $\langle\hat{O}\rangle = \sum\limits_k p_k O_k$.

   proof:

$$\begin{aligned}\langle\hat{O}\rangle &= \langle\psi|\,\hat{O}\,|\psi\rangle \\ &= \mathrm{Tr}(\hat{O}\,|\psi\rangle\langle\psi|) = \mathrm{Tr}(\hat{O}\hat{\rho}) \\ &= \mathrm{Tr}(|\psi\rangle\langle\psi|\,\hat{O}) = \mathrm{Tr}(\hat{\rho}\hat{O})\end{aligned}$$

6. for pure state, $\hat{\rho}$ is Hermitian, it can be dioganalized

   for mixed state, $\hat{\rho}$ is also Hermitian, and it can also be dioganalized.

   No matter it is a pure state or a mixed state, $\hat{\rho}$ can be rewritten as

   $$\hat{\rho} = \sum_k \lambda_k \left|\phi_k\right\rangle\left\langle\phi_k\right|$$

   where $\{\left|\phi_k\right\rangle\}$ need to be the basis of the Hilbert space.

   Looking back to the expression of a mixed state, where $\{\left|\psi_k\right\rangle\}$ do not have to be a basis. This is the best I can do. We need to understand this more carefully.

7. express the entropy of a state

   $$S(\hat{\rho}) = -\mathrm{Tr}(\hat{\rho}\log_2[\hat{\rho}])$$

   if you diagonalize $\hat{\rho}$ first, then

   $$S(\hat{\rho}) = -\sum_{k=1}^{d} \lambda_k \log_2 \lambda_k$$

   note that $\lim_{x\to 0} x\log_2 x = 0$, so a zero eigenvalue contributes zero to this entropy

8. express the evoluation

   A unitary operation acts on kets as $\left|\psi\right\rangle \to \hat{U}\left|\psi\right\rangle$.

   While a unitary operation acts on density operator as $\hat{\rho} \to \hat{U}\hat{\rho}\hat{U}^{\dagger}$.

7 maximally mixed state

1. definition:

   In a Hilbert space of dimension d the entropy can be at most $\log_2 d$. It is when the $\lambda_k = \frac{1}{d}$. This state is called the maximanlly mixed state(mm state), whose density operator is $\hat{\rho}_{\mathrm{mm}} = \frac{\hat{I}}{d}$.

2. property:

   invariant under rotations and any unitary transformation. It will always be $\hat{\rho}_{\mathrm{mm}} = \frac{\hat{I}}{d}$.

   A zero-angular momentum pure state

8 partial trace and reduced density operator

Consider a pure state for two qunatum systems A and B. In general, we can write the such a state as a superposition

$$|\Psi\rangle_{AB} = \sum_{n,m} a_{nm} |n\rangle_A |m\rangle_B \quad \text{where} \sum_{n,m} |a_{nm}|^2 = 1$$

Its density operator is $\hat{\rho}_{AB} = |\Psi\rangle_{AB}\langle\Psi|_{AB} = |\Psi\rangle_{AB}\langle\Psi|$. Usually, we don't give bras subscript, because the kets have shown the subscript.

Now consider a measurement just on system A, say an observable $\hat{O}_A$.

The expectation value of observable $\hat{O}_A$ should be

$$\langle\hat{O}_A\rangle = \mathrm{Tr}\left(\hat{\rho}_{AB}\left(\hat{O}_A \otimes \hat{I}_B\right)\right)$$

Details:

$$\begin{aligned}
\langle\hat{O}_A\rangle &= \mathrm{Tr}\left(\hat{\rho}_{AB}\left(\hat{O}_A\hat{I}_B\right)\right) = \mathrm{Tr}(\hat{\rho}_{AB}\hat{O}_A) \quad \otimes \text{ is neglected} \\
&= \sum_n \sum_m \langle n| \langle m| \left(\hat{\rho}_{AB}\left(\hat{O}_A\hat{I}_B\right)\right) |m\rangle_B |n\rangle_A \quad \text{move } \hat{O}_A \text{ to the left} \\
&= \sum_n \sum_m \langle n| \langle m| \hat{\rho}_{AB} |m\rangle_B \hat{O}_A |n\rangle_A \\
&= \sum_n \langle n| \left(\sum_m \langle m| \hat{\rho}_{AB} |m\rangle_B\right) \hat{O}_A |n\rangle_A
\end{aligned}$$

Here we define two important concepts: partial trace and reduced density operator. They are both based on a multi-system situation.

$$\mathrm{Tr}_B(\hat{O}) = \sum_m \langle m| \hat{O} |m\rangle_B$$

$$\hat{\rho}_A = \sum_m \langle m| \hat{\rho}_{AB} |m\rangle_B = \mathrm{Tr}_B(\hat{\rho}_{AB})$$

Clearly, partial trace does not take the whole basis but 'part of part of' the whole basis.
And reduced density operator describes the state of system A by itself.

If we use the partial trace and reduced density operator. The expectation value

$$\langle\hat{O}_A\rangle = \mathrm{Tr}\left(\hat{\rho}_{AB}\left(\hat{O}_A \otimes \hat{I}_B\right)\right) = \mathrm{Tr}(\hat{\rho}_A\hat{O}_A)$$

9 entanglement

Entanglement is based on multi-system situation. We have said any state can be written as

$$|\Psi\rangle_{AB} = \sum_{n,m} a_{nm} |n\rangle_A |m\rangle_B \quad \text{where} \sum_{n,m} |a_{nm}|^2 = 1$$

This is just like one-system situation, where mixed state and pure state are distinguished but can also be interpreted in the same form. So let's take a look at how pure state and mixed state look like in multi-system situation.

A pure state: $|\Psi\rangle_{AB} = |\psi\rangle_A |\phi\rangle_B$
Then we have

$$\hat{\rho}_A = \mathrm{Tr}_B(\hat{\rho}_{AB}) = \mathrm{Tr}_B(|\psi\rangle_A\langle\psi| \otimes |\phi\rangle_B\langle\phi|) = |\psi\rangle_A\langle\psi|$$

Another kind of pure state is

$$|\Psi\rangle_{AB} = \sum_k p_k |\psi_k\rangle |\phi_k\rangle$$

This pure state is entangled, i.e. it cannot be written as a product of states of A and B.

$$\begin{cases} \text{this pure state is entangled} \iff \hat{\rho}_A \text{is mixed} \\ \text{this pure state is not entangled} \iff \hat{\rho}_A \text{is pure} \end{cases}$$

for pure states of two systems, a measure of entanglement is the entropy of the reduced density operator of either A or B(both give the same number):

$$E(|\Psi\rangle_{AB}) = S(\hat{\rho}_A) = S(\hat{\rho}_B)$$

I don't know how to proof this. The von Neumann entropy is too abstract for me.
Maybe for any pure states of two system,

This is a very vague description. I need more details about the pure state and mixed state of two systems.

10 make a mixed state of one system as entangled with some ficitious auxiliary system F

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First, write it in its diagonal form: $\hat{\rho}_A = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|$.

Then write: $|\Psi\rangle_{AF} = \sum_k \sqrt{\lambda_k} |\phi_k\rangle_A |\psi_k\rangle_F$, where $\{|\psi_k\rangle\}$ is a set of basis of system F. Then, we have $\mathrm{Tr}_F(\hat{\rho}_{AF}) = \hat{\rho}_A$

$$\begin{aligned}\hat{\rho}_{AF} &= |\Psi\rangle_{AF}\langle\Psi| \\ &= \sum_{k,l} \sqrt{\lambda_k}\sqrt{\lambda_l} |\phi_k\rangle_A |\psi_k\rangle_F \langle\psi_l|_F \langle\phi_l|_A\end{aligned}$$

$$\begin{aligned}\mathrm{Tr}_F(\hat{\rho}_{AF}) &= \sum_m \langle\psi_m|_F \left(\sum_{k,l} \sqrt{\lambda_k}\sqrt{\lambda_l} |\phi_k\rangle_A |\psi_k\rangle_F \langle\psi_l|_F \langle\phi_l|_A\right) |\psi_m\rangle_F \\ &= \sum_{k,l,m} \sqrt{\lambda_k}\sqrt{\lambda_l} \left(\langle\psi_m|_F |\psi_m\rangle_F\right) \left(|\phi_k\rangle_A\langle\phi_l|_A\right) \left(\langle\psi_k|_F |\psi_l\rangle_F\right) \\ &= \sum_n \lambda_n |\phi_n\rangle_A\langle\phi_n|_A \\ &= \hat{\rho}_A\end{aligned}$$

11 a mixed state can be written in infinitely many different ways as mixtures of pure states. Here, mixed state and pure state are both for single system.

To achieve this conclusion, we need the help of the last section, making a mixed state of one system as entangled with some ficitious auxiliary system.

$$\hat{\rho}_A = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|$$

$$|\Psi\rangle_{AF} = \sum_k \sqrt{\lambda_k} |\phi_k\rangle_A |k\rangle_F, \text{where } \{|k\rangle\} \text{ is a set of basis of system} F$$

Now we change basis $\{|k\rangle\}$ to another basis $|\psi_m\rangle$, using

$$|\psi_m\rangle = \sum_k U_{mk} |k\rangle$$

So

$$\begin{aligned}
|\Psi\rangle_{AF} &= \sum_k \sqrt{\lambda_k}\,|\phi_k\rangle_A\,|k\rangle_F \\
&= \sum_k \sqrt{\lambda_k}\,|\phi_k\rangle_A \left(\sum_m U^*_{mk}\,|\psi_m\rangle\right) \\
&= \sum_k \sum_m U^*_{mk}\sqrt{\lambda_k}\,|\phi_k\rangle_A\,|\psi_m\rangle
\end{aligned}$$

To make the subscript back to one, set

$$\left|\tilde{\phi}_m\right\rangle = \frac{\sum\limits_k U^*_{mk}\sqrt{\lambda_k}\,|\phi_k\rangle}{\sqrt{\sum\limits_k \lambda_k U_{mk} U^*_{mk}}} \equiv \frac{\sum\limits_k U^*_{mk}\sqrt{\lambda_k}\,|\phi_k\rangle}{\sqrt{p_m}}$$

Then

$$|\Psi\rangle_{AF} = \sum_m \sqrt{p_m}\left|\tilde{\phi}_m\right\rangle|\psi_m\rangle$$

So $\hat{\rho}_A = \sum\limits_m p_m \left|\tilde{\phi}_m\rangle\langle\tilde{\phi}_m\right|$, instead of $\hat{\rho}_A = \sum\limits_k \lambda_k\,|\phi_k\rangle\langle\phi_k|$.