(or Density Operator)

⊛ Density Matrix → alternate formulation (to state vector formulation)

↳ Better language / formulation for some scenarios. Also easier in some contexts.

↳ A language for describing quantum systems whose state $|\psi\rangle$ is NOT known.

$\boxed{\rightarrow}$ $\{ p_i , \{|\psi_i\rangle\} \}$ → ensemble of "pure states"

⊛ Density operator for this system:

$$\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|$$ → Definition

Meaning? $\{p_i , |\psi_i\rangle\}$ → Quantum system is in one of the many states $|\psi_i\rangle$ with probability p_i

Note: $\sum_i p_i |\psi_i\rangle\langle\psi_i|$ → DO NOT CONFUSE THIS WITH QUANTUM SUPERPOSITION

This is simply a classical probability distribution, owing to our unsureness of which of the states $\{|\psi_i\rangle\}$ our system is in.

(ofcourse, $\sum_i p_i = 1$)

→ Pure state

Say for $i = i_0$, $p_{i_0} = 1$,

then $\forall\ i \neq i_0$, $p_i = 0$ $\left(\because \sum_i p_i = 1\right)$

$\Rightarrow \rho = |\psi_{i_0}\rangle\langle\psi_{i_0}|$ → Pure state density Matrix

→ We are sure about the System's state

$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

→ $\boxed{\text{Mixed state}}$

→ We are unsure about the system's state.

Examples: 1) $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \rightarrow$ A pure state system

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix}\alpha \\ \beta\end{pmatrix}\begin{pmatrix}\alpha^* & \beta^*\end{pmatrix} = \begin{pmatrix}|\alpha|^2 & \alpha\beta^* \\ \beta\alpha^* & |\beta|^2\end{pmatrix}$$

ρ also describes $|\psi\rangle$

We call 'ρ' as the state of the system in density matrix language.

Notice: $\text{Trace}(\rho) = tr(\rho) = |\alpha|^2 + |\beta|^2 = \underline{1}$

2) $$\Big\{ \big(\underbrace{|0\rangle}_{|\psi_1\rangle}, \underbrace{\tfrac{1}{4}}_{p_1}\big), \big(\underbrace{\tfrac{1}{\sqrt{2}}(|0\rangle + |1\rangle)}_{|\psi_2\rangle}, \underbrace{\tfrac{3}{4}}_{|p_2\rangle}\big) \Big\}$$

$\rightarrow$ A mixed state system.

$\rightarrow$ There's a 25% chance that state is $|0\rangle$ & 75% chance that it is $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$

$$\begin{pmatrix}1 \\ 0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0 \\ 0 & 0\end{pmatrix}$$

Now,

$$\rho = \frac{1}{4}|0\rangle\langle 0| + \frac{3}{4}|\psi_2\rangle\langle\psi_2|$$

$$= \frac{1}{4}\begin{pmatrix}1 & 0 \\ 0 & 0\end{pmatrix} + \frac{3}{4}\begin{pmatrix}1 & 1 \\ 1 & 1\end{pmatrix}\frac{1}{2} = \begin{pmatrix}5/8 & 3/8 \\ 3/8 & 3/8\end{pmatrix}$$

Notice again: $Tr(\rho) = 5/8 + 3/8 = \underline{1}$

Density Matrices were introduced for describing mixture/ensemble of quantum states

→ But we can give a complete description of quantum Mechanics using Density matrix language, which does NOT consider $|\psi\rangle$ (state vector) as the foundation.

ρ is NOT any Matrix. ρ satisfies:

→ $tr(\rho) = 1$

→ $\langle\psi_i|\rho|\psi_i\rangle \geq 0$ (positivity condition)

Reformulating quantum in Density Operator language:

1] Evolution of states:

(U: unitary)

Evolution in state vector language:

$$|\psi\rangle \xrightarrow{U} U|\psi\rangle = |\psi'\rangle \quad \Big| \quad \langle\psi| \xrightarrow{U} \langle\psi|U^{+} = \langle\psi'|$$

Evolution in density operator language:

$$\rho \xrightarrow{U} \sum_i p_i \left(U|\psi_i\rangle\right)\left(\langle\psi_i|U^{+}\right) = U\rho U^{+}$$

$$\boxed{*} \quad \rho \xrightarrow{U} \underline{U\rho U^{+}}$$ → Evolution in density operator language

2] Measurements :

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad ; \quad |\alpha|^2 + |\beta|^2 = 1$$

$$\boxed{P(m) = \langle\psi| M_m^\dagger M_m |\psi\rangle \rightarrow \text{Postulate 3 of QM}}$$

↪ Probability that result 'm' occurs

Ex: Measurement operators for computational basis measurements.

$$M_0 = |0\rangle\langle 0| \qquad M_1 = |1\rangle\langle 1|$$

$$P(0) = \langle\psi| M_0^\dagger M_0 |\psi\rangle = |\alpha|^2$$

$$\text{III}^{ly} \quad P(1) = |\beta|^2$$

as expected

Note,

$$M_0|\psi\rangle = |0\rangle\langle 0| \left(\alpha|0\rangle + \beta|1\rangle\right)$$

$$= \alpha|0\rangle \rightarrow \text{Not Normalized}$$

⊛ State after Measurement,

$$|\psi^m\rangle = \frac{M_m|\psi\rangle}{\sqrt{\langle\psi| M_m^\dagger M_m |\psi\rangle}} \quad ⊛$$

(*) Measurement operators **MUST** satisfy completeness relation

$$\sum_m M_m^{+} M_m = I \rightarrow (*)$$

Reason: Probabilities **MUST** sum to 1.

Exercise: (1) check (*) for 'M_0' & 'M_1' defined earlier.

(2) Write down a valid set of measurement operators for Hadamard basis measurements.

(3) If (*) is True, check that Probabilities sum to 1.

i.e $$\sum_{m=0,1} P(m) = 1$$

Appendix: Completeness relation

let $|i\rangle$ be any orthonormal basis for vector space V, then any arbitrary vector $|v\rangle \in V$ can be written as, $|v\rangle = \sum_i v_i |i\rangle$

v_i are complex numbers and represent projection of $|v\rangle$ on $|i\rangle$.

How to get v_i's?

Inner product of $|v\rangle$ with $|i\rangle$

$$\langle i|v\rangle = \langle i| \sum_j v_j |j\rangle = \sum_j v_j \underbrace{\langle i|j\rangle}_{\delta_{ij}}$$

orthonormality of basis

$$\Rightarrow \underline{\langle i|v\rangle = v_i}$$

Appendix:

Now,

$$\left(\sum_i |i\rangle\langle i|\right)|v\rangle = \sum_i |i\rangle \underbrace{\langle i|v\rangle}_{v_i} = \sum_i v_i |i\rangle$$

$$= |v\rangle$$

Since the above is true for any $|v\rangle \in V$,

$$\sum_i |i\rangle\langle i| = I$$

Completeness relation.

The deep reason for why you can represent operators as outer products

Example: 1) $M_0, M_1 \rightarrow$ Measurement operators in computational basis

2) $Z = |0\rangle\langle 0| - |1\rangle\langle 1| \rightarrow$ Pauli-Z operator in computation basis

↪ check this is just $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

What about Pauli-X? $\rightarrow$ Homework

Appendix: Trace of an operator

By well-known definition,

$$\mathrm{Tr}(A) \equiv \sum_i A_{ii}$$ ↗ sum of diagonal elements.

$\{|i\rangle\}$ → orthonormal basis set

$$= \sum_i \langle i|A|i\rangle$$

$\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ → Trace is cyclic

$\mathrm{Tr}(A+B) = \mathrm{Tr}(B+A)$
$\mathrm{Tr}(zA) = z\,\mathrm{Tr}(A)$ → Trace is linear, $z \in \mathbb{C}$

We earlier saw how operators evolve under unitary transformation (U),

$$A \rightarrow U^{\dagger} A U$$

What is $\mathrm{tr}(U^{\dagger} A U)$?

$$\mathrm{tr}(U^{\dagger}(AU)) = \mathrm{tr}(AUU^{\dagger})$$ ↗ since trace is cyclic

$$= \underline{\underline{\mathrm{tr}(A)}}$$ ↘ Since $U^{\dagger}U = I$

Trace is invariant under Unitary Transformation

Appendix :

what is expectation of A ?

$$\langle A \rangle = \langle \psi | A | \psi \rangle$$ → we already know this

$$\langle \psi | A | \psi \rangle = \langle \psi | I A | \psi \rangle$$

$$= \sum_i \langle \psi | i \rangle \langle i | A | \psi \rangle$$

(Identity insertion from completeness relation)

$$= \sum_i \langle i | A | \psi \rangle \langle \psi | i \rangle$$

(since these are numbers & thus commute)

$$\boxed{\langle A \rangle = tr(A |\psi\rangle\langle\psi|)}$$

(By trace definition seen in previous page)

Using Appendix, we'll see how measurement can be described in density operator formalism.

Note that $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ → A Mixed state

If the state was $|\psi_i\rangle$, then probability of getting result 'm' is

$$P(m|i) = \langle\psi_i| M_m^\dagger M_m |\psi\rangle$$

$$= tr\left(M_m^\dagger M_m |\psi_i\rangle\langle\psi_i|\right)$$

Saw these results earlier

But 'ρ' contains mixture of $|\psi_i\rangle$, what is $P(m)$?

$$P(m) = \sum_i P(m|i)\, P(i)$$ → Total law of probability

$$= \sum_i tr\left(M_m^\dagger M_m |\psi_i\rangle\langle\psi_i|\right) p_i$$

$$= tr\left(M_m^\dagger M_m \sum_i p_i |\psi_i\rangle\langle\psi_i|\right)$$

Due to linearity of Trace

$$\boxed{P(m) = tr\left(M_m^\dagger M_m \rho\right)}$$

* State after Measurement (in density Matrix language)

$$\rho_m = \sum_i p(i|m)\, |\psi_i^m\rangle\langle\psi_i^m|$$

($|\psi_i\rangle$ changes to $|\psi_i^m\rangle$ after Measurement)

$$\rho_m = \sum_i p(i|m) \frac{M_m|\psi_i\rangle\langle\psi_i|M_m^\dagger}{\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle}$$

$p(m|i)$ → seen earlier

↳ We saw the expression for $|\psi_i^m\rangle$ earlier

$$= \sum_i \frac{p(i|m)}{p(m|i)} M_m|\psi_i\rangle\langle\psi_i|M_m^\dagger$$

$$= \sum_i \frac{p(i)}{p(m)} M_m|\psi_i\rangle\langle\psi_i|M_m^\dagger$$

From probability theory,

$$p(i|m) = \frac{p(m|i)p(i)}{p(m)}$$

↳ (Bayes Theorem)

$$\boxed{\rho_m = \frac{M_m \rho M_m^\dagger}{tr(M_m^\dagger M_m \rho)}}$$

→ $p(m)$ derived earlier & used $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

3] Expectation value

$\langle A \rangle = \langle \psi | A | \psi \rangle$ → In state vector language.

We saw in an earlier Appendix,

$\langle A \rangle = tr(A\, |\psi\rangle\langle\psi|)$

$\langle A \rangle = tr(A\rho)$ → In density operator language.

Likewise, you can reformulate everything in QM from state vector to density Matrix language.

Fun Exercise:

Schrödinger equation in state vector language

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \hat{H} |\psi\rangle$$ {Describes time evolution of $|\psi\rangle$}

How will this equation look in the density operator language?

(Note: State is 'ρ' in this language)

Ok, so QM can be expressed in 'ρ' rather than $|\psi\rangle$. But is there any deep application of 'ρ' which is hard in the state vector language?

Yes!

(*) <u>Reduced</u> <u>Density</u> <u>Operator</u> : (RDO)

↳ Tool to describe subsystems of a composite system.

let ρ^{AB} describe density operator for composite systems consisting of A & B.

(subsystems)

RDO for system A is,

$$\rho^A \equiv tr_B(\rho^{AB})$$

This describes the system 'A' in the composite system 'AB'

Partial Trace over system 'B'

Reason

Because RDO provides correct description of measurement statistics for observations on subsystem 'A' {This can be neatly proved, refer Box 2.6 of Nielsen & Chuang}

Definition of Partial Trace:

$$\boxed{tr_B\left(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|\right) \equiv |a_1\rangle\langle a_2|\, tr\left(|b_1\rangle\langle b_2|\right)}$$

Say $\rho^{AB} = \underbrace{|a\rangle\langle a|}_{\text{System A}} \otimes \underbrace{|b\rangle\langle b|}_{\text{System B}}$.

(Assuming composite system is in a product state i.e NOT entangled)

$$tr_B(\rho^{AB}) = |a\rangle\langle a|\, tr(|b\rangle\langle b|)$$

$$= \rho^A \underbrace{tr(\rho^B)}_{1 \text{ (by def}^n \text{ of } \rho)} = \underline{\underline{\rho^A}}$$

$\Rightarrow$ $tr_B(\rho^{AB})$ separated out system 'A' from composite 'AB'.

Now, let our composite system consist of entangled subsystems, say Maximally entangled $\rightarrow$ Bell state,

$$\rho = \underbrace{\left(\frac{|00\rangle + |11\rangle}{\sqrt{2}}\right)}_{|\psi_{AB}\rangle}\underbrace{\left(\frac{\langle 00| + \langle 11|}{\sqrt{2}}\right)}_{\langle\psi_{AB}|}$$

(Clearly A & B are entangled here)

Is 'ρ' a pure state?
'Yes', as there are NO p_i's

What is $tr_B(\rho)$?

$$\frac{1}{2}\Big[tr_B\left(|00\rangle\langle 00|\right) + tr_B\left(|00\rangle\langle 11|\right) + tr_B\left(|11\rangle\langle 00|\right) + tr_B\left(|11\rangle\langle 11|\right)\Big]$$

use the definition of $tr_B(\rho^{AB})$

to show that above expression evaluates to,

$$tr_B(\rho) = \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2} \rightarrow \text{A Mixed State}$$

Quite remarkable! The joint system (ρ) is Pure (i.e state is exactly known), whereas the subsystem is Mixed (i.e NOT exactly known)

Thus the language of 'ρ' gives us a nice perspective on entanglement
(& strange too)

↓

State of composite (or joint) system can be "exactly" known, yet a subsystem can be in mixed state. (known only with certain probabilities & are not "exactly" known)

Purity of states (ρ):

For a density operator ρ,

$\boxed{tr(\rho^2) \leq 1}$; equality if 'ρ' is a pure state & inequality if 'ρ' is a mixed state.

Exercise: Let $\rho = \frac{1}{2} |1\rangle\langle 1| + \frac{1}{2} |\psi\rangle\langle\psi|$

where $|\psi\rangle = \sqrt{3/4}\, |0\rangle + \sqrt{1/4}\, |1\rangle$.

Show that $tr(\rho^2) < 1$ implying 'ρ' is mixed

✱ Other uses of 'ρ':

→ 'ρ' is used to describe 'statistical' distribution of quantum states ($\{p_i, |\psi_i\rangle\}$) in a system. Hence, they can be used to describe states (& their evolution) of open quantum systems (these are dissipative quantum system & are in permanent contact with the environment)

(This is a useful thing to know while working on Quantum Error Correction)

→ Quantifying distance between two states 'ρ' & 'σ' (These are density operators)

(Basically asking the question, how much different are 2 states 'ρ' & 'σ', if they are very close or not much different they would have similar measurement statistics)

Trace distance:

$$D(\rho, \sigma) = \frac{1}{2} \mathrm{tr} \, |\rho - \sigma|$$

where $|A| = \sqrt{A^{\dagger} A}$

Fidelity:

$$F(\rho, \sigma) = \mathrm{tr} \sqrt{\rho^{1/2} \sigma \rho^{1/2}}$$

These are some useful distance measures.

Entropy Measures

- Von Neumann entropy of quantum state ρ, $S(\rho) \equiv -\mathrm{tr}[\rho \log \rho] = \sum_x \lambda_x \log \lambda_x$

quantifies uncertainty associated with learning the state of the quantum system 'ρ'

λ_x: eigen values of ρ

If 'ρ' is pure, $S(\rho) = 0$, as we exactly know the state $\Rightarrow$ No uncertainty

Exercise: What do you think is the state for which $S(\rho)$ is Maximal?

Entanglement Entropies (EE): several types → Von-Neumann EE, Renyi Entropies, log-negativity, etc...

↓

Measures | quantifies quantum entanglement b/n 2 subsystems of a composite system.

→ For composite system ρ^{AB}, the von Neumann entropy of the subsystem $[S(\rho^A)$ or $S(\rho^B)]$ is used to quantify entanglement. → Von-Neumann EE.

Exercise:

Earlier we found ρ^A (or ρ^B) for a system made of Bell entangled subsystems. For this, find $S(\rho^A)$ (or $S(\rho^B)$).

This is the Maximum value $S(\rho)$ can have → hence Bell states are Maximally entangled

→ Bulk - Boundary correspondence

(or AdS - CFT correspondence)

↓

A beautiful story for some other day . . .