# Density Matrix / Operator

Last time: composite system $\mathbb{C}^m \otimes \mathbb{C}^n$ $\quad |\varphi\rangle = \mathbb{C}^n \times \mathbb{C}^m$ a vector state

Do a partial measurement $A = A^* \in B(\mathbb{C}^m)$. $\quad \langle\varphi| A \otimes I |\varphi\rangle$.

E.g. $|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$ $\quad \langle\Phi^+| A \otimes I |\Phi^+\rangle = \frac{\langle 0|A|0\rangle}{2} + \frac{\langle 1|A|1\rangle}{2}$ (*)

$\mathbb{C}^2 \otimes \mathbb{C}^2$ $\quad \overset{?}{=} \langle\varphi|A|\varphi\rangle$ for some $|\varphi\rangle \in \mathbb{C}^2$?

No. Any $\alpha|1\rangle + \beta|0\rangle = |\varphi\rangle$ $\quad \langle\varphi|A|\varphi\rangle = |\alpha|^2 \underbrace{\langle 0|A|0\rangle}_{a_{00}} + |\beta|^2 \underbrace{\langle 1|A|1\rangle}_{a_{01}}$

$+ \alpha\bar{\beta} \underbrace{\langle 1|A|0\rangle}_{a_{10}} + \beta\alpha \underbrace{\langle 0|A|1\rangle}_{a_{11}}$

$$A = \begin{bmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{bmatrix}$$

Then what is the state for $\langle\Phi^+| A \otimes I |\Phi^+\rangle = \frac{1}{2}\langle 0|A|0\rangle + \frac{1}{2}\langle 1|A|1\rangle$

In general, the state of a quantum system can be described by

$\{p_i, |\psi_i\rangle\}$ ensemble of pure states. $p_i$ is the prob. system in $|\psi_i\rangle$

E.g. $\langle\Phi^+|A \otimes I|\Phi^+\rangle = \frac{1}{2}\langle 0|A|0\rangle + \frac{1}{2}\langle 1|A|1\rangle \rightsquigarrow \{(\frac{1}{2}, |0\rangle), (\frac{1}{2}, |1\rangle)\}$

Vector space $|\varphi\rangle \rightsquigarrow \{1, |\varphi\rangle\}$ single ensemble

Given an ensemble $\{p_i, |\varphi_i\rangle\}$, measurements

Expected value of $A = A^*$ : $\quad \sum_i p_i \langle\varphi_i|A|\varphi_i\rangle$

POVM $\{E_m\}$ : $\quad \sum_i p_i \langle\varphi_i|E_m|\varphi_i\rangle$ prob of outcome $m$

Unitary tranformation $\quad \{p_i, |\varphi_i\rangle\} \xrightarrow{U} \{p_i, U|\varphi_i\rangle\}$

However, in terms of measurement the ensemable representation is not unique

For any $A = A^*$ observable, $\frac{1}{2}\langle +|A|+\rangle + \frac{1}{2}\langle -|A|-\rangle = \frac{1}{2}\langle 0|A|0\rangle + \frac{1}{2}\langle 1|A|1\rangle$

So from phsysic measurement, we can not distinguish $\{(\frac{1}{2}, |0\rangle), (\frac{1}{2}, |1\rangle)\}$

and $\{(\frac{1}{2}, |+\rangle), (\frac{1}{2}, |-\rangle)\}$

What is really unique here is the notation of state (in Mathmatic)

$\varphi: \quad B(\mathbb{C}^n) \to \mathbb{C}, \quad \varphi(A) = \langle \Phi^+ | A \otimes I | \Phi^+ \rangle$

$\varphi$ is linear: So $\varphi \in L(B(\mathbb{C})^n, \mathbb{C}) = B(\mathbb{C})^*$

Recall that for a vector space $V$. the dual space $V^* = L(V, \mathbb{C})$

Example: $V = \mathbb{C}^n = \left\{ \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} \middle| \; u_i \in \mathbb{C} \right\}$

$$V^* \cong \mathbb{C}^n = \{ (v_1 \cdots v_n) \mid v_i \in \mathbb{C} \}$$

$(v_1 \cdots v_n) : \mathbb{C}^n \longrightarrow \mathbb{C}$

$(v_1 \cdots v_n) \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} = \sum_{i=1}^{n} v_i u_i$ linear functional

Given $e_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, e_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \cdots e_n = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$ basis

There exists $\{e_i^*\} \subseteq V^*$ dual basis s.t.

$$e_i^*(e_j) = \delta_{ij} = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$$

Indeed $e_1^* = (1, 0 \cdots 0)$.

Thm: $V \cong V^*$ as $\mathbb{C}$ vector space if $\dim(V) < \infty$.

Now consider $V = B(\mathbb{C})^n \cong M_n$. What is $V^*$ ?

Recall the trace functional:

$$tr((a_{ij})) = \sum a_{ii}$$

equivalently $tr(A) = \sum_i \langle e_i | A | e_i \rangle$

① Independence of basis

② Tracial Property.

(Tracial property) ① $\forall A, B \in M_n(\mathbb{C})$ $\quad tr(AB) = tr(BA)$

② $\forall U$ unitary, $\quad tr(U^* A U) = tr(A)$

③ $tr(A) = \sum_i \langle \varphi_i | A | \varphi_i \rangle$ for any O.N.B. $|\varphi_i\rangle$.

<u>Proof</u>: ① $\quad A = (a_{ij}) \quad B = (b_{ij})$

$$AB = \left(\sum_k a_{ik} b_{kj}\right)_{ij}$$

$$BA = \left(\sum_l b_{il} a_{lj}\right)_{i,j}$$

$$tr(AB) = \sum_{i,k=1}^{n} a_{ik} b_{ki}$$

$$tr(BA) = \sum_{i,l=1}^{n} b_{il} a_{li}$$

lemma: $M_n \cong M_n^*$ by the following bijection

$f \in M_n^* \longleftrightarrow$ a operator $X_f$ s.t. $f(A) = tr(AX)$.

How to see it in an elementary way?

Consider $\{E_{ij} = |i\rangle\langle j|\} \subseteq M_n$ basis

$\{f_{ij}(e_{kl}) = \delta_{(ij)(kl)}\}$ is $M_n^*$ dual basis

$f_{ij} \longleftrightarrow E_{ji} \in M_n$ basis $\quad f_{ij}(A) = tr(A\, |j\rangle\langle i|)$

$= tr(\sum a_{kl} |k\rangle\langle l|\, |j\rangle\langle i|)$

$= a_{ij}$

$Span\{E_{ji}\} = M_n \cong M_n^*$

Now for $|\varphi\rangle \in \mathbb{C}^n \otimes \mathbb{C}^m$,

$\varphi(A) = \langle\varphi| A \otimes I |\varphi\rangle$ corresponds to a operator $\rho$. s.t. $\varphi(A) = tr(A\rho)$

What property $\varphi$ have?

① if $A \geq 0$, $A \otimes I \geq 0$, then $\varphi(A) \geq 0$

② $\varphi(I) = \langle\varphi| I \otimes I |\varphi\rangle = \langle\varphi|\varphi\rangle = 1$

A linear function satisfy ① + ② is called a state.

What property should the operator. $\rho$ have?

① $tr(\rho A) = \langle\varphi| A \otimes I |\varphi\rangle \geq 0 \Rightarrow \rho \geq 0$ (choose $A = |h\rangle\langle h|$, $|h\rangle \in \mathbb{C}^n$)

② $tr(\rho \cdot I) = tr(\rho) = 1$

$\rho \geq 0 \Rightarrow \rho = \sum p_i |\psi_i\rangle\langle\psi_i|$, $p_i \geq 0$ (by orthogonal decomposition)

$tr(\rho) = 1 \Rightarrow \sum p_i = 1$ (by basis independence of trace)

A state of a quantum system $\mathbb{C}^n$ can be equivalently described by one of the following

① An ensemble of pure state $\{p_i, |\psi_i\rangle\}$ $\sum p_i = 1$. $p_i \geq 0$ $|\psi_i\rangle \in \mathbb{C}^n$

② A density operator $\rho \in B(\mathbb{C}^n)$ s.t. $\rho \geq 0$, $tr(\rho) = 1$

③ A linear functional $\varphi: B(\mathbb{C})^n \to \mathbb{C}$ s.t. $\varphi(I) = 1$ and $\varphi(A) \geq 0$ if $A \geq 0$

④ A state vector $|\varphi\rangle \in \mathbb{C}^n \times \mathbb{C}^m$ for some $m$

$$\{p_i, |\psi_i\rangle\} \underset{\text{orthogonal decomposition}}{\overset{\sum p_i |\psi_i\rangle\langle\psi_i|}{\rightleftarrows}} \rho \overset{\varphi(A) = tr(\rho A)}{\longleftrightarrow} \varphi \underset{\text{partil trace}}{\overset{\text{purification}}{\rightleftarrows}} |\varphi\rangle$$

density operator — State (unital positive linear function) — pure state on larger system

## Examples

① Pure state = Vector state: $|\varphi\rangle \leftrightarrow \varphi(A) = \langle\varphi|A|\varphi\rangle \longleftrightarrow \rho = |\varphi\rangle\langle\varphi|$ density operator

② A mixed state $\rho = \sum p_i |\varphi_i\rangle\langle\varphi_i|$ $\{|\varphi_i\rangle\}$ orthonormal set
$\sum p_i = 1$ $p_i \geq 0$

Mixed state are convex combination of pure state

If $p_i = 1$, $p_j = 0$ $\forall j \neq i$ $\Rightarrow$ $\rho = |\varphi_i\rangle\langle\varphi_i|$ pure state

For $\mathbb{C}^n$, $p_i = \frac{1}{n}$, $\rho = \sum \frac{1}{n} |\varphi_i\rangle\langle\varphi_i| = \frac{1}{n} I$, completely mixed state

like uniform distribution $(\frac{1}{n}, \frac{1}{n} \cdots \frac{1}{n})$

③ Flat state: $P$ projection. $\rho = \frac{P}{tr(P)} = \frac{1}{k} \sum_{i=1}^{k} |\varphi_i\rangle\langle\varphi_i|$ $\{|\varphi_i\rangle\}$ O.N.B of $Ran(P)$.

$k = tr(P) \in \mathbb{N}$

④ Ensemable of pure states $\{p_i, |\varphi_i\rangle\} \to \rho = \sum p_i |\varphi_i\rangle\langle\varphi_i|$

e.g. $\frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{I}{2} = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -|$

## Product state

Let $\rho \in D(\mathbb{C}^n)$ and $\sigma \in D(\mathbb{C}^m)$. Then $\rho \otimes \sigma \in D(\mathbb{C}^{n \times m})$

Fact: $tr(A \otimes B) = tr(A)\, tr(B)$.

Then $tr(\rho \otimes \sigma) = tr(\rho)\, tr(\sigma) = 1$

$\rho \geq 0$. $\sigma \geq 0 \Rightarrow \rho \otimes \sigma \geq 0$

## Joint States / density operator

Denote $H_A = \mathbb{C}^n$ and $H_B = \mathbb{C}^m$, A density operator $\rho_{AB} \in B(H_A \otimes H_B)$ is called a joint density operator / states over joint system AB.

Examples: 1. Product state $\rho \otimes \sigma$ $\quad \rho \in D(H_A) \quad \sigma \in D(H_B)$

$\rho = \frac{1}{4}|0\rangle\langle 0| + \frac{3}{4}|1\rangle\langle 1| = \begin{bmatrix} \frac{1}{4} & 0 \\ 0 & \frac{3}{4} \end{bmatrix}$ $\qquad \sigma = \frac{1}{3}|+\rangle\langle +| + \frac{2}{3}|-\rangle\langle -| = \begin{bmatrix} \frac{1}{2} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{1}{2} \end{bmatrix}$

$$\rho \otimes \sigma = \begin{bmatrix} \frac{1}{4}\cdot\sigma & 0\sigma \\ 0\cdot\sigma & \frac{3}{4}\cdot\sigma \end{bmatrix} = \begin{bmatrix} \frac{1}{8} & -\frac{1}{24} & 0 & 0 \\ -\frac{1}{24} & \frac{1}{8} & 0 & 0 \\ 0 & 0 & \frac{3}{8} & -\frac{1}{8} \\ 0 & 0 & -\frac{1}{8} & \frac{3}{8} \end{bmatrix}$$

2. Seperable state $\omega = \sum_i \lambda_i\, \rho_i \otimes \sigma_i$ $\qquad \sum \lambda_i = 1 \quad \lambda_i \geq 0$

$\rho_i \in D(H_A)$. $\sigma_i \in D(H_B)$

$\omega = \sum \lambda_i |i\rangle\langle i| \otimes \sigma_i$ $\qquad \sigma_i \in D(H_B)$ $\quad \sum \lambda_i = 1 \ \lambda_i \geq 0$ $\qquad$ classical-quantum state

3. Pure joint state: $|\varphi\rangle \in H_A \otimes H_B$ unit vector

$\varphi = |\varphi\rangle\langle\varphi|$ is the joint density

e.g. $|\varphi\rangle = |0\rangle \otimes |0\rangle$ $\qquad \varphi = |00\rangle\langle 00| = |0\rangle\langle 0| \otimes |0\rangle\langle 0|$ product state

$|\varphi\rangle = \frac{|0\rangle|0\rangle + |1\rangle|1\rangle}{\sqrt{2}}$

$\varphi = |\varphi\rangle\langle\varphi| = \frac{1}{2}\left(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\right)$

Using $|00\rangle \to |1\rangle$ $|01\rangle \to |2\rangle$ $|10\rangle \to |3\rangle$ $|11\rangle \to |4\rangle$

$$\begin{bmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

Is this a seperable state?

Definition: A joint state $\rho_{AB}$ is called entangled if it is not seperable

Important concept! A lot more to explore later.

Marginal state / Reduced density

Given a joint state $\rho_{AB} \in B(H_{AB})$. it induce a state on $A$.

$\varphi_A : B(H_A) \to \mathbb{C}$. $\quad \varphi_A(x) = tr_{AB}\left((x_A \otimes I_B)\,\rho_{AB}\right)$

$= tr_A(x_A \rho_A)$ for some $\rho_A$

$\rho_A = Id \otimes tr_B(\rho_{AB})$

e.g. $\rho_{AB} = \sum a_{ij,kl}\, e_{ij} \otimes e_{kl}$

$id_A \otimes tr_B(\rho_{AB}) = \sum a_{ij,kl}\, Id(e_{ij}) \otimes tr_B(e_{kl})$

$= \sum_{k,ij} a_{ij,kk}\, e_{ij}$

For example: ① $\omega_{AB} = \rho_A \otimes \sigma_B \Rightarrow \omega_A = id_A \otimes tr_B = \rho_A\, tr_B(\sigma_B) = \rho_A$

$\omega_B = \sigma_B$

② $\omega_{AB} = \sum \lambda_i |i\rangle\langle i| \otimes \sigma_i \qquad \omega_A = \sum \lambda_i |i\rangle\langle i| \qquad \omega_B = \sum \lambda_i \sigma_i$

③ $\omega_{AB} = |\varphi\rangle\langle\varphi|$. $\quad |\varphi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \qquad \omega_A = \omega_B = \frac{1}{2}$

# Purification.

Given a mixed state $\rho \in D(H_A)$

① Does there exises a joint state $\omega_{AB}$ such that $\omega_A = \rho$?

② . . . . . . . a pure joint state $\varphi_{AB} = |\varphi\rangle\langle\varphi|$ such that $\varphi_A = \rho$?

Such $|\varphi\rangle$ is called a purification of $\rho$.

① Yes. $\omega_{AB} = \rho_A \otimes \sigma_B$

② Given $\rho = \sum p_i |\varphi_i\rangle\langle\varphi_i|$. Define $|\varphi\rangle_{AA'} = \sum_i \sqrt{p_i}\, |\varphi_i\rangle \otimes |i\rangle$ $\quad A \cong A'$

Then $\varphi = |\varphi\rangle\langle\varphi|$ has reduced density $\rho$ on $A$.

$$id_A \otimes tr_{A'} (|\varphi\rangle\langle\varphi|) = id_A \otimes tr_{A'} \left( \sum_{i,j} \sqrt{p_i}\sqrt{p_j}\, |\varphi_i\rangle\langle\varphi_j| \otimes |i\rangle\langle j| \right)$$
$$= \sum_i p_i |\varphi_i\rangle\langle\varphi_i| = \rho.$$

Theorem (Ulmann): Let $|\psi\rangle_{AC}$ be any purification of $\rho$. Then there exises a isometry $V \in L(H_{A'}, H_C)$ such that $V|\varphi\rangle = |\psi\rangle$.