## 3.5. Density operators

### 3.5.1. Def.

Def. A density operator $\rho$ on $\mathbb{H}$ is a linear operator on $\mathbb{H}$ that satisfies the following conditions

a) $\operatorname{tr}\rho = 1$

b) $\rho$: positive semidefinite

ex) $\rho = |\varphi\rangle\langle\varphi|$ $\left[\begin{array}{l} \operatorname{tr}\rho = \operatorname{tr}|\varphi\rangle\langle\varphi| = \langle\varphi|\varphi\rangle = 1 \\ \langle\psi|\rho|\psi\rangle = |\langle\varphi|\psi\rangle|^2 \geq 0. \end{array}\right.$

Def. A mixed state of the quantum state Q is a seq. $((p_0, |\psi_0\rangle), \cdots, (p_{l-1}, |\psi_{l-1}\rangle))$ where $l \in \mathbb{N}$. the $|\psi_i\rangle$ are quantum states in $\mathbb{H}$ for $0 \leq i < l$.

$p_i \in \mathbb{R}_{\geq 0}$, $\sum_{i=0}^{l-1} p_i = 1$

A pure state of the quantum system Q is a quantum state in its state space $\mathbb{H}$.

Prop 3.5.4.

Let $((p_0, |\psi_0\rangle), \cdots, (p_{l-1}, |\psi_{l-1}\rangle))$ be a mixed state of the quantum system Q. Then

$$\rho = \sum_{i=0}^{l-1} p_i |\psi_i\rangle\langle\psi_i|$$

is a density operator on the state space $\mathbb{H}$ of Q.

pf) $\operatorname{tr}\rho = \sum_{i=0}^{l-1} p_i \operatorname{tr}|\psi_i\rangle\langle\psi_i| = \sum_{i=0}^{l-1} p_i = 1$.

$\langle\xi|\rho|\xi\rangle = \langle\xi|\sum_{i=0}^{l-1} p_i|\psi_i\rangle\langle\psi_i|\xi\rangle = \sum_{i=0}^{l-1} p_i\langle\xi|\psi_i\rangle\langle\psi_i|\xi\rangle = \sum_{i=0}^{l-1} p_i|\langle\psi_i|\xi\rangle|^2 \geq 0$. ∎

Def. density operator of a mixed state $S = ((p_0, |\psi_0\rangle), \cdots, (p_{l-1}, |\psi_{l-1}\rangle))$ of Q $:= \rho_S = \sum_{i=0}^{l-1} p_i|\psi_i\rangle\langle\psi_i|$

density operator of a pure state $|\varphi\rangle \in \mathbb{H} := \rho_\varphi = |\varphi\rangle\langle\varphi|$.

### 3.5.2. Correspondence between mixed states and density operators.

Prop 3.5.8

Every density operator on $\mathbb{H}$ is the density operator of some mixed state of the quantum sys. Q.

i.e. $\forall\rho, \exists S$ s.t. $\rho = \rho_S$.

pf) $\rho$: density operator $\Rightarrow$ $\rho$: Hermitian.

$\Rightarrow \rho = \sum_{i=0}^{k-1} \lambda_i|b_i\rangle\langle b_i|$, $B = (|b_0\rangle, \cdots, |b_{k-1}\rangle)$ orthonormal basis of eigenvectors of $\rho$

$\lambda_i$: eigenvalue associated w/ $|b_i\rangle$ for all $i \in \mathbb{Z}_k$.

$\Rightarrow 1 = \operatorname{tr}\rho = \sum_{i=0}^{k-1}\lambda_i$, $((\lambda_0, |b_0\rangle), \cdots, (\lambda_{k-1}, |b_{k-1}\rangle))$ is the mixed state of the quantum state w/ $\rho$.

Prop 3.5.10

$S = (|\varphi_0\rangle, \cdots, |\varphi_{l-1}\rangle)$, $T = (|\psi_0\rangle, \cdots, |\psi_{l-1}\rangle) \in \mathbb{H}^l$

$\sum_{i=0}^{l-1}|\varphi_i\rangle\langle\varphi_i| = \sum_{i=0}^{l-1}|\psi_i\rangle\langle\psi_i|$ iff $\exists$ unitary matrix $U \in \mathbb{C}^{(l,l)}$ s.t. $T = SU$.

pf) ($\Leftarrow$) easy to show.

($\Rightarrow$) $\rho = \sum_{i=0}^{k-1}\lambda_i|b_i\rangle\langle b_i|$, $|b_i\rangle$: orthonormal seq. of eigenvectors of $\rho$.

WTS: $V = \mathrm{span}(|b_0\rangle, \cdots, |b_{m-1}\rangle) = V' = \mathrm{span}(|\varphi_0\rangle, \cdots, |\varphi_{l-1}\rangle)$

$\lambda_i|b_j\rangle = \rho|b_j\rangle = \sum \langle\varphi_i|b_j|\varphi_i\rangle \Rightarrow V \subset V'$.

set $|\xi_i\rangle = \sqrt{\lambda_i}\,|b_i\rangle$. then $\rho = \sum |\xi_i\rangle\langle\xi_i|$.

↳ orthonormal basis of $V$.

$|\psi\rangle \in V^\perp$, then $\langle\psi|\rho|\psi\rangle = 0$.

$\Rightarrow \sum |\langle\varphi_i|\psi\rangle|^2 = 0 \Rightarrow {}^\forall |\psi\rangle \in V^\perp,\ |\varphi_i\rangle \in (V^\perp)^\perp = V$.

$\Rightarrow V = V',\ m \le l$.

$\Rightarrow |\varphi_j\rangle = \sum_{i=0}^{m-1} u_{ij}|\xi_i\rangle$

$(u_{ij}) = U,\ \sum_{p=0}^{m-1} |\xi_p\rangle\langle\xi_p| = \sum_{i,j=0}^{m-1} \underbrace{\left(\sum_{p=0}^{l-1} u_{ip}u^*_{ij}\right)}_{=\delta_{ij}} |\xi_p\rangle\langle\xi_j|$

Set $|\xi_m\rangle, \cdots, |\xi_{l-1}\rangle = 0$.

$\Rightarrow (|\varphi_0\rangle, \cdots, |\varphi_{l-1}\rangle) = (|\xi_0\rangle, \cdots, |\xi_{l-1}\rangle)U$, $(|\psi_0\rangle, \cdots, |\psi_{l-1}\rangle) = (|\xi_0\rangle, \cdots, |\xi_{l-1}\rangle)U'$.

$\Rightarrow$ we can get $U^* U'$. ∎

Thm 3.5.11

↗ $|\varphi\rangle\langle\varphi| = ((1, |\varphi\rangle))$

(1) The density operators of two pure states of $Q$ are same iff these states are equal up to a global phase factor.

(2) $((p_0, |\varphi_0\rangle), \cdots, (p_{l-1}, |\varphi_{l-1}\rangle))$, $((q_0, |\psi_0\rangle), \cdots, (q_{l-1}, |\psi_{l-1}\rangle))$ are same iff $\exists$ unitary $U \in \mathbb{C}^{(l,l)}$ s.t.

$(\sqrt{p_0}|\varphi_0\rangle, \cdots, \sqrt{p_{l-1}}|\varphi_{l-1}\rangle) = (\sqrt{q_0}|\psi_0\rangle, \cdots, \sqrt{q_{l-1}}|\psi_{l-1}\rangle)U$.

Thm 3.5.13

The set $R$ of all pairs of mixed states of $Q$ w/ same density operator $\rho$ is an equiv. relation on the sets of all mixed states of $Q$.

pf) By thm 3.5.11, it holds.

Thm 3.5.15

(1) $\rho$: density operator of a pure state iff $\rho^2 = \rho$.

(2) $\rho$: not density operator of a pure state iff $\rho^2 \neq \rho$.

## 3.6. The quantum postulates for mixed states.

### 3.6.1. State Space Postulate.

Postulate - State Space Postulate (density operator ver)

Associated w/ any physical system is Hilbert space, called the state space of the system.

The system is completely described by a density operator on the state space.

- Composite System Postulate (density operator ver)

The state space of the composition of finitely many physical systems in the tensor product of the state spaces of the component physical systems.

Moreover, if we have systems numbered $0 \sim m-1$,

and if system $i$ is in the state $\rho_i$, $\rho_i$: density operator on the state space

then the composite system is in the state $\rho_0 \otimes \cdots \otimes \rho_{m-1}$.

- Evolution

the state of the system at the time $t$ is described by the density operator $\rho$ on $\mathbb{H}$.

" $t'$ " $\rho'$,

$\rho' = U\rho U^*$, $U$ unitary.

- Measurement

A projective measurement is described by an observable $O$ that is a Hermitian operator on the state space of the system being observed. Let $O = \sum \lambda P_\lambda$ be the spectural decomposition of $O$.

The possible outcomes of the measurement are eigenvalues of the observable.

when measuring the state $\rho$ the probability of getting the result corresponding to $\lambda$ is $Pr(\lambda) = tr(P_\lambda \rho)$. If this outcome occurs, the state immediately after the measurement is $\frac{P_\lambda \rho P_\lambda}{Pr(\lambda)}$

Def. the expectation value of this measurement is defined as $tr(O\rho)$

$O$: observable of a quantum sys. w/ state space $\mathbb{H}$.

we measure this observable when the system is in a state described by the density operator $\rho$.

Prop 3.6.7

Suppose that we measure the quantum system in the orthonormal basis $B = (|b_0\rangle, \cdots, |b_{k-1}\rangle)$ when in the mixed state.

Then measuring the observable $\sum \lambda |\lambda_j\rangle\langle\lambda_j|$ gives $\lambda \in \mathbb{Z}_k$ w/ probability $Pr(\lambda) = \sum_{i=0}^{k-1} p_i |\langle b_\lambda|\varphi_i\rangle|^2$.

Immediately after this measurement, the quantum system is in the state $|b_\lambda\rangle\langle b_\lambda|$

pf) $\rho = \sum_{i=0}^{k-1} p_i |\varphi_i\rangle\langle\varphi_i|$

$\forall \lambda \in \mathbb{Z}_k$, $P_\lambda \rho = \sum_{i=0}^{k-1} p_i \langle b_\lambda|\varphi_i\rangle |b_\lambda\rangle\langle\varphi_i|$.

By prop 2.4.29, $Pr(\lambda) = tr(P_\lambda \rho) = \sum_{i=0}^{k-1} p_i |\langle b_\lambda|\varphi_i\rangle|^2$.

when the measurement outcomes is $\lambda$, then immediately after the measurement the quantum system is in the state $\frac{P_\lambda \rho P_\lambda}{Pr(\lambda)} = \frac{1}{Pr(\lambda)} \left( \sum_{i=0}^{k-1} p_i |b_\lambda\rangle\langle b_\lambda|\varphi_i\rangle\langle\varphi_i|b_\lambda\rangle\langle b_\lambda| \right)$ ☐

3.7. Partial trace and reduced density operators

$\mathrm{tr}_J(\otimes \xi_j) = \prod_{j\in J} \mathrm{tr}\, \xi_j \otimes \xi_j$

Setting : quantum system $A, B$

state space $\mathbb{H}_A, \mathbb{H}_B \to$ orthonormal basis $(|a_0\rangle, \cdots, |a_{M-1}\rangle), (|b_0\rangle, \cdots, |b_{N-1}\rangle)$

dimension $M, N$ (WLOG $M \le N$)

composition of $A$ and $B$ by $AB$, $\mathbb{H}_{AB} = \mathbb{H}_A \otimes \mathbb{H}_B$

Prop 3.7.1.

Let $U \in \mathrm{End}(\mathbb{H}_{AB})$, $U = \sum_{\substack{i,j \in \mathbb{Z}_M \\ k,l \in \mathbb{Z}_N}} u_{i,j,k,l} |a_i\rangle\langle a_j| \otimes |b_k\rangle\langle b_l|$

Then $\mathrm{tr}_B(U) = \sum_{k \in \mathbb{Z}_N} U_k$,

$U_k = \sum_{i,j \in \mathbb{Z}_M} u_{i,j,k,k} |a_i\rangle\langle a_j|$.

Prop 3.7.4.

Let $\varphi \in \mathbb{H}_{AB}$, $|\varphi\rangle = \sum_{i=0}^{k-1} r_i |\psi_i\rangle |\xi_i\rangle$ be a Schmidt decomposition of $\varphi$. Thm 2.5.18

Then we have $\mathrm{tr}_B(|\varphi\rangle\langle\varphi|) = \sum_{i=0}^{k-1} r_i^2 |\psi_i\rangle\langle\psi_i|$

pf) $\mathrm{tr}_B(|\varphi\rangle\langle\varphi|) = \mathrm{tr}_B\left(\sum_{i,j=0}^{k-1} r_i^2 |\psi_i\rangle|\xi_i\rangle\langle\psi_j|\langle\xi_j|\right)$

$= \sum_{i,j=0}^{k-1} r_i^2\, \mathrm{tr}_B(|\psi_i\rangle\langle\psi_j| \otimes |\xi_i\rangle\langle\xi_j|) = \sum_{i,j=0}^{k-1} r_i^2 |\psi_i\rangle\langle\psi_j| \delta_{i,j} = \sum_{i=0}^{k-1} r_i^2 |\psi_i\rangle\langle\psi_i|$

Prop 3.7.5

If $U \in \mathrm{End}(\mathbb{H}_{AB})$ is positive semidefinite, then $\mathrm{tr}_B U$ is positive semidefinite.

pf) $U_{k,l} = \sum_{i,j \in \mathbb{Z}_M} u_{i,j,k,l} |a_i\rangle\langle a_j| \Rightarrow U = \sum U_{k,l} \otimes |b_k\rangle\langle b_l|$

Let $|\varphi\rangle \in \mathbb{H}_A$, $|\varphi_x\rangle = |\varphi\rangle \otimes |b_x\rangle$.

$0 \le \sum_{x \in \mathbb{Z}_N} \langle\varphi_x|U|\varphi_x\rangle = \sum_{x \in \mathbb{Z}_N} \sum_{k,l \in \mathbb{Z}_N} \langle\varphi|U_{k,l}|\varphi\rangle \langle b_x|b_k\rangle\langle b_l|b_x\rangle$

$= \sum \langle\varphi|U_{x,x}|\varphi\rangle = \langle\varphi|\mathrm{tr}_B U|\varphi\rangle$.

Prop 3.7.6.

$\rho$: density operator of $\mathbb{H}_{AB} \Rightarrow \mathrm{tr}_B(\rho)$ is a density operator on $\mathbb{H}_A$.

Def. $\rho$: density operator on $\mathbb{H}_{AB}$,

$\mathrm{tr}_B(\rho)$ is called the reduced density operator of $\rho$ on the subsystem $A =: \rho^A$

Thm 3.7.8

(1) $O_A$ : observable of system $A$. $O_{AB} = O_A \otimes I_B$

$\rho$: state of $O_{AB}$

expectation value of $O_{AB}$ is same as the expectation value of $O_A$. i.e. $\mathrm{tr}(O_{AB}\rho) = \mathrm{tr}(O_A \rho^A)$.

(2) $\mathrm{End}(\mathbb{H}_{AB}) \to \mathrm{End}(\mathbb{H}_A)$

$\rho \mapsto \rho^A = \mathrm{tr}_B(\rho)$ is the only linear map s.t. $\mathrm{tr}(O_{AB}\rho) = \mathrm{tr}(O_A\rho^A)$

for all observables $O_A$ of $A$ and all states $\rho$ of $AB$.

pf) $\mathrm{tr}(O_{AB}\rho) = \mathrm{tr}((O_A \otimes I_B)(S_i \otimes T_j))$

$= \mathrm{tr}(O_A S_i \otimes T_j) = \mathrm{tr}(\mathrm{tr}_B(O_A S_i \otimes T_j)) = \mathrm{tr}(O_A S_i\, \mathrm{tr}\, T_j) = \mathrm{tr}(O_A \rho^A)$.

ex) $|\varphi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

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

$$\rho^A = tr_B(\rho) = \frac{1}{2}(tr_B(|00\rangle\langle 00|) + tr_B(|00\rangle\langle 11|) + tr_B(|11\rangle\langle 00|) + tr_B(|11\rangle\langle 11|))$$

$$= \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \Rightarrow ((\tfrac{1}{2}, |0\rangle), (\tfrac{1}{2}, |1\rangle)).$$

Prop 3.7.10

Let $L \in \mathbb{N}$ and for $0 \le i \le L-1$, $|\varphi_i\rangle, |\psi_i\rangle$ : orthogonal quantum states in $\mathbb{H}_A, \mathbb{H}_B$.

$\rho$ = density operator of the state $|\xi\rangle = \frac{1}{\sqrt{L}}\sum_{i=0}^{L-1}|\varphi_i\rangle|\psi_i\rangle$.

$\Rightarrow \rho^A$ : density operator of $((\frac{1}{L}, |\varphi_0\rangle), \cdots, (\frac{1}{L}, |\varphi_{L-1}\rangle))$.

Cor. 3.7.12

Assume that composite system AB is in the state $\rho = |\xi\rangle\langle\xi|$ where $|\xi\rangle = |\varphi\rangle|\psi\rangle$ with $|\varphi\rangle \in \mathbb{H}_A, |\psi\rangle \in \mathbb{H}_B$.
Then $\rho^A = |\varphi\rangle\langle\varphi|$.

Thm. 3.7.13.

$|\varphi\rangle$ : state of the composite system AB

$\rho = |\varphi\rangle\langle\varphi|$ density operator of $|\varphi\rangle$.

$\Rightarrow |\varphi\rangle$ is entangled with respect to the decomposition of AB into the subsystems A and B iff $\rho^A$ is not the density operator of a pure state.