Mixed states, density matrices (lecture 6)

States of quantum mechanical systems:

unit vectors $|\psi\rangle \in \mathbb{C}^N$

it's more convenient if we can model probability distributions over states:

$|\psi_i\rangle$ with prob. p_i $\left(\sum_i p_i = 1,\ p_i \geq 0\right)$

instead of "random variable in $\{|\psi\rangle \in \mathbb{C}^N : \||\psi\|| = 1\}$

we will use <u>density matrices</u>

Def. a density matrix corresp. to $(|\psi_i\rangle, p_i)_i$ is

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

$|\psi_i\rangle\langle\psi_i|$: lin. transform $|\varphi\rangle \mapsto \underbrace{\langle\psi_i|\varphi\rangle}_{\text{inn. prod.} \in \mathbb{C}} |\psi_i\rangle$

i.e. $|\psi_i\rangle (|\psi_i\rangle)^\dagger$

if $|\psi_i\rangle = \begin{bmatrix} \alpha_0^{(i)} \\ \vdots \\ \alpha_{N-1}^{(i)} \end{bmatrix}$ $\rho = \sum_i \begin{bmatrix} \alpha_0^{(i)}\alpha_0^{(i)*} & \cdots & \alpha_0^{(i)}\alpha_{N-1}^{(i)*} \\ \vdots & & \\ \alpha_{N-1}^{(i)}\alpha_0^{(i)*} & \cdots & \alpha_{N-1}^{(i)}\alpha_{N-1}^{(i)*} \end{bmatrix}$

Ex. $p_i = \frac{1}{2}$, $|\psi_i\rangle = |i\rangle$ $(i = 0, 1)$

$|0\rangle\langle 0| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$, $|1\rangle\langle 1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ $\Rightarrow \rho = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \frac{I_2}{2}$

Prop. 1 $(|\psi_i\rangle)_{0 \leq i < N}$ orthonormal basis of $\mathbb{C}^N$.

$p_i = \frac{1}{N}$ $\Rightarrow$ $\rho = \frac{1}{N} I_N$ (<u>maximally mixed state</u>)

Proof. The claim is equiv. to $\rho|\varphi\rangle = \frac{1}{N}|\varphi\rangle$ $(|\varphi\rangle \in \mathbb{C}^N)$

i.e. we want $\sum_{0 \leq i < N} \frac{1}{N} \langle\psi_i|\varphi\rangle |\psi_i\rangle = \frac{1}{N}|\varphi\rangle$.

$(|\psi_i\rangle)_i$ basis $\Rightarrow$ $|\varphi\rangle = \sum_i \alpha_i |\psi_i\rangle$ for some $\alpha_i \in \mathbb{C}$

$\langle\psi_i|\psi_j\rangle = \delta_{i,j}$ $\Rightarrow$ $\alpha_i = \langle\psi_i|\varphi\rangle$. $\square$

Rem. one state $|\psi\rangle \in \mathbb{C}^N$ (pure state) corr. to

$\rho_\psi = |\psi\rangle\langle\psi|$.

- $\rho_\psi = \rho_{\alpha\psi}$ for $\alpha \in \mathbb{C}$, $|\alpha| = 1$.
- $\rho = \rho_\psi$ for some $|\psi\rangle \Leftrightarrow \mathrm{rank}\,\rho = 1$.

($|\psi\rangle$: unit vec. in the img of ρ).

Rem. unitary transform $|\psi\rangle \mapsto U|\psi\rangle$ corresp. to conjugation (adjoint) $\rho \mapsto U\rho U^\dagger$

- Measurement of mixed states

ρ density matrix from $(p_i, |\psi_i\rangle)_i$.

$|\varphi_j\rangle$ $(0 \le j < N)$ orthonormal basis for measurement

$\rightsquigarrow$ the prob. of observing $|\varphi_j\rangle$ for the meas. of ρ

is $P[\rho \rightsquigarrow |\varphi_j\rangle] = \langle\varphi_j|\rho|\varphi_j\rangle$

Compar. with prev. formalism

state $|\psi\rangle \rightsquigarrow$ obs. $|\varphi_j\rangle$ with prob. $|\alpha_j|^2$, $\alpha_j = \langle\varphi_j|\psi\rangle$

$\Downarrow$

$\rho_\psi = |\psi\rangle\langle\psi| \rightsquigarrow \langle\varphi_j|\rho_\psi|\varphi_j\rangle = \langle\varphi_j|\psi\rangle\langle\psi|\varphi_j\rangle = |\alpha_j|^2$.

Ex. max. mixed state $\rho = \frac{1}{N} I_N$ gives

$P[\rho \rightsquigarrow |\varphi_j\rangle] = \langle\varphi_j|\frac{1}{N} I_N|\varphi_j\rangle = \frac{1}{N}$.

- Characterization of density matrices (§6.1.2)

Prop 2. ρ : density matrix from $(p_i, |\psi_i\rangle)_i$

(1) $\mathrm{Tr}\,\rho = 1$.

(2) ρ is positive semidefinite.

(Hermitian $\rho = \rho^\dagger$, eigenvals ≥ 0)

Proof of 1) : $\mathrm{Tr}\,\rho = \sum_i \mathrm{Tr}(p_i|\psi_i\rangle\langle\psi_i|) = \sum p_i \mathrm{Tr}(|\psi_i\rangle\langle\psi_i|)$

by linearity. then $\mathrm{Tr}(|\psi_i\rangle\langle\psi_i|) = 1$.

(to see this for ex. $|\psi_i\rangle = \sum_j \alpha_j^{(i)} |j\rangle$;
$\sum_j |\alpha_j^{(i)}|^2 = \|\psi_i\| = 1$, $|\psi_i\rangle\langle\psi_i| = \begin{pmatrix} \alpha_0^{(i)} \alpha_0^{(i)*} & & \cdots \\ & \ddots & \\ \alpha_{N-1}^{(i)} \alpha_0^{(i)*} & & \alpha_{N-1}^{(i)} \alpha_{N-1}^{(i)*} \end{pmatrix}$)

Proof of 2) $\rho = \rho^\dagger$ from $(|\psi_j\rangle\langle\psi_j|)^\dagger = |\psi_j\rangle\langle\psi_j|$

eigenval ≥ 0 : suppose $|\varphi\rangle$ is an eigenvec.

$\rho|\varphi\rangle = \lambda|\varphi\rangle$ for some $\lambda \in \mathbb{C}$ ($\in \mathbb{R}$ by $\rho = \rho^\dagger$)

$\lambda \underbrace{\|\varphi\|^2}_{>0} = \langle\varphi|\rho|\varphi\rangle \Rightarrow$ enough to check RHS ≥ 0

$\langle\varphi|\rho|\varphi\rangle = \sum_i p_i \langle\varphi|\psi_i\rangle\langle\psi_i|\varphi\rangle = \sum_i p_i |\langle\varphi|\psi_i\rangle|^2$

Th'm the conditions of Prop 2 characterize desity matrices. i.e ρ sat. (1) & (2) $\Leftrightarrow$ $\rho = \sum_i \alpha_i |\psi_i\rangle\langle\psi_i|$

Proof $\Rightarrow$: take the eigenvecs $|\varphi_j\rangle$, corresp. eigenvals α_j $(0 \leq j < N)$

$Tr(\rho) = \sum \alpha_j \Rightarrow \sum \alpha_j = 1$ by (1), $\alpha_j \geq 0$ by (2)

$\langle\varphi_i|\varphi_j\rangle = \delta_{i,j}$ by (2) so $\rho = \sum_i \alpha_i |\varphi_i\rangle\langle\varphi_i|$
(agree on basis $(|\varphi_j\rangle)_j$)

- Partial trace (partial meas. (§ 6.1.3))

Suppose we have the state space $\mathbb{C}^{N_A} \otimes \mathbb{C}^{N_B}$ $(\simeq \mathbb{C}^{N_A N_B})$

ρ : density matrix on this space.

Def. The <u>partial</u> <u>trace</u> $(Tr_A \otimes id)(\rho)$ is

$\rho^B = \sum_{0 \leq i < N_A} (\langle i| \otimes I_{N_B}) \rho (|i\rangle \otimes I_{N_B})$ ($N_B \times N_B$ matrix)

also say reduced density mat. / local density mat.

Rem $(Tr_A \otimes id)(S \otimes T) = Tr_A(S)\, T$ $\quad S \in M_{N_A}$, $T \in M_{N_B}$

$\underbrace{Tr_B}_{\text{tr. on } \mathbb{C}^{N_B}} ((Tr_A \otimes id)(\rho)) = \underbrace{Tr_{AB}}_{\text{trace on } \mathbb{C}^{N_A} \otimes \mathbb{C}^{N_B}} (\rho)$.

Ex. $N_A = N_B = 2$, $|\varphi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ max. entangled ~~st.~~

(cont.) $\rho_\varphi = |\varphi\rangle\langle\varphi| = \frac{1}{2} \sum_{i,j=0,1} |ii\rangle\langle jj|$

$$(\mathrm{Tr}_A \otimes id)(\rho_\varphi) = \sum_{i=0,1} (\langle i| \otimes I_2)\left(\frac{1}{2}\sum_{j,k} |jj\rangle\langle kk|\right)(|i\rangle \otimes I_2)$$

$$\underset{\text{only } j=k=i \text{ survives}}{=} \sum_i \frac{1}{2} |i\rangle\langle i| = \frac{1}{2} I_2 .$$

Interpretation : Alice and Bob shares the state $|\varphi\rangle$

Alice can obs. the first qubit $\mathbb{C}^{N_A}$ $(= \mathbb{C}^2)$

Bob ~ second ~ $\mathbb{C}^{N_B}$ $(= \mathbb{C}^2)$

to Bob (who cannot see what Alice observes)

the system looks like $(\mathrm{Tr}_A \otimes id)(\rho_\varphi) = \frac{1}{2} I_2$

$|0\rangle, |1\rangle$ meas $\rightsquigarrow$ eq. prob.

(or any other orthnorm basis like $|+\rangle, |-\rangle$)

Operation on Alice's side

generally : trace-preserving completely pos. map.

$\Phi : M_{N_A} \to M_{N_A'}$ $\quad \Phi(\rho) = \sum_i (V_i \otimes I_{N_B})^\dagger \rho (V_i \otimes I_{N_B})$

$V_i \in M_{N_A' \times N_A}$, $\sum V_i V_i^\dagger = I_{N_A}$

ρ density mat $\Rightarrow$ $\Phi(\rho)$ density mat.

<u>No-communication theorem</u> : $(\mathrm{Tr}_A \otimes id)(\Phi(\rho)) = (\mathrm{Tr}_A \otimes id)(\rho)$

for any density mat on $\mathbb{C}^{N_A} \otimes \mathbb{C}^{N_B}$.

So : operations on Alice's side cannot change the reduced density mat for Bob.

<u>But</u> Alice can know what Bob will observe

measurement for $|0\rangle, |1\rangle$ basis

observed $|0\rangle \rightsquigarrow$ Bob has $(\langle 0| \otimes I)\, \rho\, (|0\rangle \otimes I)$

~ $|1\rangle \rightsquigarrow$ ~ $(\langle 1| \otimes I)\, \rho\, (|1\rangle \otimes I)$

these can be pure states