Mixed states and density matrices

A system is in a mixed state if there is a probability p_i that the system is in state $|x_i\rangle$ for $i = 1, \ldots, N$.

If $N = 1$, then the system is in pure state.

Consider an observable corresponds to the Hermitian matrix A.

- The mean value of the quantum system with quantum state $|x\rangle$ is given by $\langle A\rangle = \langle x|A|x\rangle$.
- The mean value of the quantum system with a mixed state $\sum_{j=1}^{N} p_j|x_j\rangle$ is given by

$$\langle A\rangle = \sum_{j=1}^{N} p_j\langle x_j|A|x_j\rangle = \mathrm{tr}\,(A\rho) = \mathrm{tr}\,(\rho A),$$

where

$$\rho = \sum_{j=1}^{N} p_j|x_j\rangle\langle x_j|$$

is a density operator (matrix).

Description of quantum systems in mixed states.

A1' A physical state is specified by a density matrix $\rho : \mathcal{H} \to \mathcal{H}$, which is positive semidefinite with trace equal to one.

A2' The mean value of an observable associate with the Hermitian matrix A is $\langle A\rangle = \mathrm{tr}\,(\rho A)$.

A3' The temporal evolution of the density matrix is given by the Liouville-von Neumann equation

$$i\hbar\frac{d}{dt}\rho = [H, \rho] = H\rho - \rho H,$$

where H is the system Hamiltonian.

$A = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$

$A = \dfrac{\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}}{\sqrt{2}}$

Multipartitle systems

- Let $\rho_1 \in M_{n_1}, \rho_2 \in M_{n_2}$ be mixed states. Then

$$\rho_1 \otimes \rho_2 \in M_{n_1} \otimes M_{n_2} \equiv M_{n_1 n_2}$$

  is a composite (uncorrelated) state in the bipartite system.

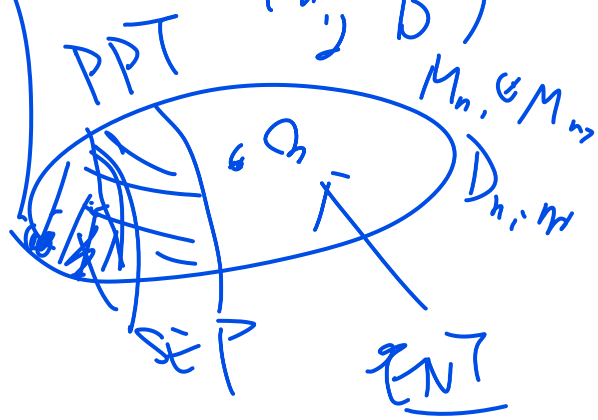
$= (A_{ij} B)$

- General states ρ in $M_{n_1} \otimes M_{n_2}$ are density matrices in $M_{n_1 n_2}$.

- Let ρ be a density matrix in the bipartite system $M_{n_1} \otimes M_{n_2}$. It is **separable** if it is a probabilistic (convex) combination of composite state, i.e.,

$$\rho = \sum_{j=1}^{N} p_j \sigma_j \otimes \tau_j$$

  with quantum states $\sigma_j \in M_{n_1}, \tau_j \in M_{n_2}$.



- Otherwise, it is **entangled**.

- Note that ρ is always a **linear combination** of composite states.

- Checking whether a state is separable is an NP-hard problem.

$M_2 \otimes M_2$

$\mathcal{B} := \left\{ \frac{I}{2}, \frac{\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}}{2}, \frac{\begin{pmatrix} & -i \\ i & \end{pmatrix}}{2}, \frac{\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}}{2} \right\}$

$\{ X \otimes Y \quad X, Y \in \mathcal{B} \}$

- A common test is to use the **partial transposes** defined by

$$(\rho_1 \otimes \rho_2)^{pt_1} = \rho_1^t \otimes \rho_2, \quad (\rho_1 \otimes \rho_2)^{pt_2} = \rho_1 \otimes \rho_2^t.$$

- If ρ is separable, then the partial transposes are also quantum states, i.e., positive semi-definite.

M_4

- If ρ is a state such that ρ^{pt_1} is positive semidefinite, we say that ρ is a ppt (positive partial trace) state.

$\rho^{pt_1} = \sum p_i (\sigma_i^t \otimes \tau_i)$

- One can extend the concepts to multipartite systems.

$|\psi_2\rangle$

$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \in M_2 \otimes M_2$

$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \frac{(1\,0\,0\,1)}{\sqrt{2}}$

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

$\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \to \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

is NOT PPT

Partial traces

- If ρ is quantum state in the bipartite system $M_{n_1} \otimes M_{n_2}$, the partial traces of ρ are defined by

$$\mathrm{tr}_1(\rho_1 \otimes \rho_2) = \mathrm{tr}(\rho_1)\rho_2 = \rho_2 \in M_{n_2},$$

$$\mathrm{tr}_2(\rho_1 \otimes \rho_2) = \rho_1 \mathrm{tr}(\rho_2) = \rho_1 \in M_{n_1}.$$

- One may regard ρ_1 lies in the principal system, and ρ_2 is the environment.

- There are many problems concerning partial traces.

  * Given quantum states $\rho_1 \in M_m, \rho_2 \in M_n$, determine

$$\mathcal{S}(\rho_1, \rho_2) = \{\rho \in D_{n_1 n_2} : \mathrm{tr}_1(\rho) = \rho_2, \mathrm{tr}_2(\rho) = \rho_1\}$$

  * Find a quantum state in $\mathcal{S}(\rho_1, \rho_2)$ with lowest rank.

  * Find a quantum state in $\mathcal{S}(\rho_1, \rho_2)$ with the lowest von Neumann entropy

$$S(\rho) = -\mathrm{tr}\,\rho \log \rho.$$

  * Find all possible eigenvalues of $\rho \in \mathcal{S}(\rho_1, \rho_2)$.

- One can extend the concepts to multipartite systems.

Research questions about quantum states

Quantum State tomography Determine $\rho = (\rho_{ij})$.

$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{12} & \rho_{22} \end{pmatrix}$

- For a Hermitian matrix $A = (a_{ij})$, we can determine $\mathrm{tr}\,(a_{ij})X$ for $X \in \mathcal{B}$, where

$$\boxed{\mathcal{B} = \{E_{rr} : 1 \le r \le n\} \cup \{E_{rs} + E_{sr} : 1 \le r < s \le n\} \cup \{i(E_{rs} - E_{sr}) : 1 \le r < s \le n\}.}$$

  Then $A = (a_{ij})$ is completely determined.

$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix}$

- If we know that $\mathrm{tr}\, A = 1$, we may skip the checking of $\mathrm{tr}\, AE_{nn}$.

$3 + 3 \times 2 = 3 + 6 = 9$

$4 + \frac{3 \times 4}{2}$

$= 16$

- If $\rho = (\rho_{ij}) = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} (\bar{x}_1, \dots, \bar{x}_n)$ is a pure state, we only need to get information for $\rho_{12}, \dots, \rho_{1n}$. If $x_1 > 0$, then we can solve x_1 in the equation

$\rho_{ij} = x_i \bar{x}_j$

$$x_1^2 + \sum_{j=2}^{n} |\rho_{1j}/x_1|^2 = 1.$$

  Thus, one only need to check $\mathrm{tr}\,\rho X$ for

$$X = E_{1j} + E_{j1},\ X = i(E_{1j} - E_{j1}),\ j = 2, \dots, n.$$

- Can we write a computer program to do that?
- Can we set up physical experiments to to that?
- Consider the Pauli matrices: $\sigma_0 = I_2$,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

  For an n-qubit states in M_{2^n}, the test set can be

$$\{T_1 \otimes \cdots \otimes T_n : T_j \in \{\sigma_0, \sigma_x, \sigma_y, \sigma_z\}\}.$$

$\sigma_0 \otimes \sigma_0 = I_4$

$= \mathrm{tr}\begin{pmatrix} a_{11} & 0 & 0 \\ \times & 0 & 0 \\ \times & 0 & 0 \end{pmatrix} = a_{11}$

$= 2\,\mathrm{Re}(a_{12})$

$= 2\,\mathrm{Im}(a_{12})$

- Suppose $\mathcal{S} \subseteq M_n$ is a special set of quantum states. Can we find a small test set $\mathcal{S}$ of observable to determine whether $\rho \in \mathcal{S}$ or not?
- For example, determine all ρ with specific norm, eigenvalues, specific the Renyi entropy

  $H_\alpha = \frac{1}{1-\alpha} \log \mathrm{tr}\, \rho^\alpha$ for $\alpha \in (0,1) \cup (1, \infty)$.

  For $\alpha = 2$, we get $\quad H_2(\rho) = -\mathrm{tr}\, \log \rho^2$.

  When $\alpha \to 1$, we get the von Neumann entropy $\quad H(\rho) = -\mathrm{tr}\,(\rho \log \rho)$.

$[\rho_{ij}]$ n^2

n

$= -\sum \lambda_i \log(\lambda_i)$

Multipartite states

Determine multipartite states with special properties.

- Let $\rho_1 \in M_{n_1}, \rho_2 \in M_{n_2}$. Determine the set

  $$\mathcal{S}(\rho_1, \rho_2) = \{\rho \in M_{n_1} \otimes M_{n_2} : \mathrm{tr}_1 \rho = \rho_2, \mathrm{tr}_1 \rho = \rho_2\}.$$

- One may consider the special case when $\rho_2 = I_{n_2}$.

- Determine all possible norms, eigenvalues, Renyi entropy of $\rho \in \mathcal{S}(\rho_1, \rho_2)$.

  Use projection methods to find the elements.

- Extend the problems to multipatite systems.

- For example, determine the set of states $\rho \in M_{n_1} \otimes M_{n_2} \otimes M_{n_3}$ with specific $\mathrm{tr}_1(\rho) = \rho_{23} \in M_{n_2} \otimes M_{n_3}$, and $\mathrm{tr}_3(\rho) = \rho_{12} \in M_{n_1} \otimes M_{n_2}$.

- If the set is non-empty, determine all possible norms, eigenvalues, Renyi entropy of $\rho \in \mathcal{S}(\rho_1, \rho_2)$.