Mixed States and Density Matrices

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

- If there is only one possible state, i.e., $p_1 = 1$, then the system is in pure state.

- The expectation value (mean) of the measurement of the system corresponding to the observable described by the Hermitian matrix A is

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

where

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

is a density operator (matrix).

$|\psi\rangle$

$e^{i\theta}|\psi\rangle$

$e^{i\theta}|\psi\rangle\langle\psi|e^{-i\theta}$

Example $\frac{1}{2}(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2|) = \frac{1}{2}I_2$ is a maximally mixed state. It is the mixed state of $\frac{1}{2}(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2|)$ with

$$|e_1\rangle = (\cos\theta, \sin\theta)^t \quad \text{and} \quad |e_2\rangle = (\sin\theta, -\cos\theta)^t, \quad \theta \in [0, 2\pi).$$

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

Definition A (Hermitian) matrix $A \in M_n$ is positive semidefinite if

$$\langle x|A|x\rangle \geq 0 \text{ for all } |x\rangle \in \mathbb{C}^n.$$

Proposition Let $A \in M_n$.

(a) The matrix $A \in M_n$ is positive semidefinite if and only if it has nonnegative eigenvalues.

(b) The matrix A is a density matrix if and only if it is positive semi-definite with trace 1.

$A \quad \lambda_i \geq 0$

$=$

$\langle x_i| \sum^{n} \lambda_i |y_i\rangle\langle y_i| \, |x_i\rangle$

$\sum_{i=1}^{n} \lambda_i \, |\langle x|y_i\rangle|^2$

Proof. (a) Let $A = UDU^\dagger$. If A has a negative eigenvalues λ with unit eigenector $|\lambda\rangle$, then $\langle\lambda|A|\lambda\rangle = \lambda < 0$.

If A has nonnegative eigenvalues, then for any $|x\rangle \in \mathbb{C}^n$ we can let $|y\rangle = U^\dagger|x\rangle$ so that $\langle x|A|x\rangle = \langle y|D|y\rangle = \sum_{j=1}^n \lambda_j|y_j|^2 \geq 0$.

(b) If $A = \sum_{j=1}^r p_r|v_j\rangle\langle v_j|$ is a density matrix, then

$$\langle x|A|x\rangle = \sum_{j=1}^{r} p_r|\langle x|v_j\rangle|^2 \geq 0,$$

and $\operatorname{tr}(A) = \sum_{j=1}^r p_j \operatorname{tr}|v_j\rangle\langle v_j| = \sum_{j=1}^r p_j = 1$.

If A is positive semidefinite with trace 1, then

$$A = \sum_{j=1}^n \lambda_j|\lambda_j\rangle\langle\lambda_j| \text{ with } \sum_{j=1}^n \lambda_j = 1. \qquad \square$$

Postulates of a quantum system 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 $\langle A \rangle = \mathrm{tr}\,(\rho A)$.

After a measurement, the mixed state ρ will collapses to one of the eigenstate ρ_j with a probability of $p_j = \mathrm{tr}\,(\rho\rho_j)$. Note that $\sum_j p_j = 1$.

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.

$\rho = \sum p_i |x_i\rangle\langle x_i|$

$\sum \rho_i |y_i\rangle\langle y_i|$

$\sum \rho_i \langle y_i | A | y_i \rangle$

$x' = kx \sim e^{kt}$

$\boxed{U_t \rho U_t^\dagger}$

Theorem A state $\rho \in D_n$ is pure if and only if any one of the following condition holds.

D_n psd(n) M_n

(a) $\rho^2 = \rho$. (b) $\operatorname{tr} \rho^2 = 1$.

Proof. Suppose $\rho = |\psi\rangle\langle\psi|$ is a pure state.

Then $\rho^2 = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) = |\psi\rangle\langle\psi| = \rho$.

Thus, the condition (a) holds.

If (a) holds, then $\operatorname{tr} \rho^2 = \operatorname{tr} \rho = 1$. Thus, the condition (b) holds.

If (b) holds, and $\rho = \sum_{j=1}^n \lambda_j |\lambda_j\rangle\langle\lambda_j|$,

Tomography

low

where $\lambda_1 \geq \cdots \geq \lambda_n \geq 0$ and $\sum_{j=1}^n \lambda_j = 1$.

Then $\rho^2 = \sum_{j=1}^n \lambda_j^2 |\lambda_j\rangle\langle\lambda_j|$ has eigenvalues $\lambda_1^2, \ldots, \lambda_n^2$.

So, if $\operatorname{tr} \rho^2 = 1 = \operatorname{tr} \rho$, then

$$0 = \sum_{j=1}^n (\lambda_j - \lambda_j^2) = \sum_{j=1}^n \lambda_j (1 - \lambda_j)$$

so that all the nonnegative numbers $\lambda_j(1 - \lambda_j)$ is zero.

Thus, $\lambda_j \in \{0, 1\}$. Since $\sum_{j=1}^n \lambda_j = 1$, we see that

$\lambda_1 = 1$ and $\lambda_j = 0$ for $j > 1$.

Thus, $\rho = |\lambda_1\rangle\langle\lambda_1|$ is a pure state. $\square$

Definition 2.1 Suppose $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. A state ρ is **uncorrelated** if $\rho = \rho_1 \otimes \rho_2$; it is **separable** if it is a **convex** combination of uncorrelated states, i.e.,

$$\rho = \sum_{j=1}^{r} p_j \rho_{1,j} \otimes \rho_{2,j}.$$

$\rho_1 \otimes \rho_2$

2×2 $\quad 4\times 4$

$D_m \quad D_n$

$\mathbb{C}^2 \otimes \mathbb{C}^4 \quad |u\rangle \otimes |v\rangle$

$D_2 \otimes D_4$

Otherwise, it is **inseparable** (or **entangled**).

Remark Every $A \in \mathcal{H}$ is a **linear** combination of product states with linear coefficient summing up to 1. But some of the coefficients may be negative.

Reason Suppose the basis $\mathcal{B}_1 \subseteq M_n$ contains the pure states:

$$|e_{1,j}\rangle\langle e_{1,j}|, 1 \le j \le m\}, \quad 1 \le j \le m,$$

and $\{|x\rangle\langle x|$ with

$$|x\rangle = \frac{1}{\sqrt{2}}(|e_{1,j} + |e_{1,k}\rangle)\rangle, \frac{1}{\sqrt{2}}(|e_{1,j} + i|e_{1,k}\rangle)\rangle, \quad 1 \le j < k \le m.$$

Then $\mathcal{B}_1$ is a basis for M_m. Similarly, there is a basis for M_n consisting of pure states. As a result, $\mathcal{B} = \{\rho_1 \otimes \rho_2 : \rho_j \in \mathcal{B}_j, j = 1, 2\}\}$ is a basis for $M_m \otimes M_n = M_{mn}$.

Remarks

The set of tensor states and separable states are small.

Separable states are closely related to product states.

Inseparable states are the resource for quantum computing.

Proposition Let $\rho \in D_{mn}$.

(a) Suppose ρ has rank one. Then ρ is separable if only only if $\rho = \rho_1 \otimes \rho_2$ for rank one matrices $\rho_1 \in D_m, \rho_2 \in D_n$.

(b) If $\rho \in D_{mn}$ is separable, then ρ is a convex combination of quantum states of the form $\rho_1 \in D_m, \rho_2 \in D_n$, where ρ_1, ρ_2 are pure states.

$|u\rangle \otimes |v\rangle \langle uv|$

$\sum s_i |u_i\rangle |v_i\rangle$

$|uv\rangle\langle uv|$

$|u\rangle\langle u| \otimes |v\rangle\langle v|$

Schmidt.

$\sum s_i |e_i\rangle |f_i\rangle$

Partial transpose - a tool to determine inseparable sates

The **partial transpose** with respect to $\mathcal{H}_2$ is defined by

$$\rho = (\rho_1 \otimes \rho_2)$$

$$\rho^{\text{pt}} = \rho_1 \otimes \rho_2^t.$$

Extend the map by linearity so that $\rho^{\text{pt}} = \sum_{j=1} c_j \rho_{1,j} \otimes \rho_{2,j}^t$ if $\rho = \sum_{j=1}^k c_j \rho_{1,j} \otimes \rho_{2,j}$.

$$\rho = (a_{ij}) \otimes B$$

In matrix form, if $\rho = (P_{ij}) \in M_m(M_n)$, then $\rho^{\text{pt}} = (P_{ij}^t)$.

$$\rho^t = (a_{ij}) \otimes B^t$$

Remark If ρ is separable, then so is ρ^{pt}.

If ρ^{pt} has negative eigenvalues, then ρ is not separable.

$$\boxed{\;} = \sum p_i (\rho_i \otimes \sigma_i)$$

If ρ is separable

then $\rho^t = \sum p_i \rho_i \otimes \sigma_i^t$

$p = \frac{2}{3}$

Define the **negativity** of $\rho \in \mathcal{H}_1 \otimes \mathcal{H}_2$ by

$$N(\rho) = \left(\sum_j |\lambda_i(\rho^{pt})| - 1\right)/2 \geq 0, \quad > 0$$

$$\begin{pmatrix} \frac{1-p}{4} & \frac{-p}{2} \\ \frac{-p}{2} & \frac{1-p}{4} \end{pmatrix}$$

Then ρ^{pt} has nonnegative eigenvalues if and only if $N(\rho) = 0$.

Theorem If $\rho \in \mathcal{H}_1 \otimes \mathcal{H}_2$ is separable, then $N(\rho) = 0$. The converse holds if $\dim \mathcal{H}_1 + \dim \mathcal{H}_2 \leq 5$.

Open problem Find a simple proof!

$= \sum$

Example Let $\left(\begin{array}{cc|cc} \frac{1-p}{4} & 0 & 0 & 0 \\ 0 & \frac{1+p}{4} & \frac{-p}{2} & 0 \\ \hline 0 & \frac{-p}{2} & \frac{1+p}{4} & 0 \\ 0 & 0 & 0 & \frac{1-p}{4} \end{array}\right)$. $= \rho$.

$\frac{1-p}{4} \geq \frac{p}{2}$

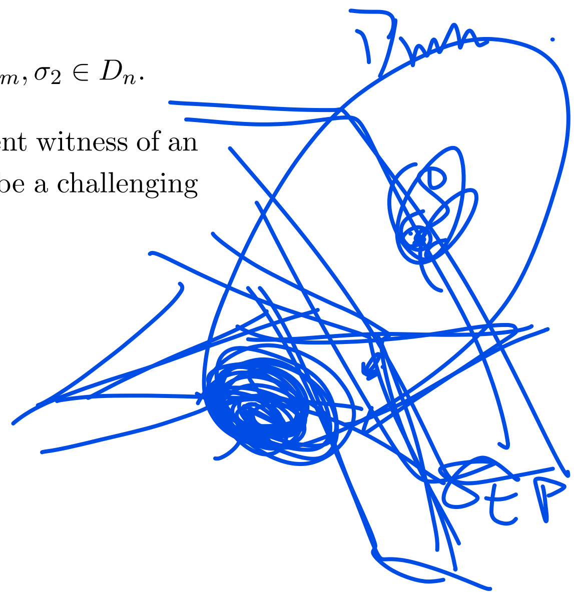
$1 \geq 3p$

$$\begin{pmatrix} \frac{1+p}{4} & \frac{-p}{2} \\ \frac{-p}{2} & \frac{1+p}{4} \end{pmatrix} \quad 0 \leq 1$$

Theorem Let $\rho \in M_m \otimes M_n$. Then ρ is inseparable if and only if there is an entanglement witness F such that

$$\operatorname{tr}(F\rho) > 0 \geq \operatorname{tr}(F(\sigma_1 \otimes \sigma_2)) \qquad \text{for all } \sigma_1 \in D_m, \sigma_2 \in D_n.$$

It should be remarked that finding an entanglement witness of an inseparable state or showing the nonexistence could be a challenging problem.



Partial traces and Purification

Partial trace

Let $C = A \otimes B = (A_{ij}B) \in M_m \otimes M_n$.

$\sum p_i A_i$

(1) One can take the partial trace of the first system to get the matrix B in the second system by simply summing the diagonal blocks of C resulting in $A_{11}B + \cdots + A_{mm}B = (\operatorname{tr} A)B = B$.

$p_1, \dots, p_r \geq 0$

$\sum p_i = 1$

(2) One can take the partial trace of the second system to get the matrix A in the first system by simply taking the trace of all the blocks of C resulting in $(A_{ij}\operatorname{tr}(B)) = (A_{ij}) = A$.

$\frac{1+i}{2} A_1 + \frac{1-i}{2} A_2$

$c_1 A_1 + \cdots + c_r A_r$

For a general state $\rho = (T_{rs})_{1 \leq r,s \leq m}$ with $T_{rs} \in M_n$ for all r, s, the first partial trace and second partial traces are

$$\operatorname{tr}_1(\rho) = T_{11} + \cdots + T_{mm} \in M_n \quad \text{and} \quad \operatorname{tr}_2(\rho) = (\operatorname{tr} T_{ij}) \in M_m.$$

$c_1 + \cdots + c_r = 1$

Let $A \in \mathcal{H}_1 \otimes \mathcal{H}_2$. The partial trace of A over $\mathcal{H}_2$ is an operator acting on $\mathcal{H}_1$ defined by

$$A_1 = \operatorname{tr}_2 A = \sum_{k=1}^{n} (I_m \otimes \langle e_{2,k}|) A (I_m \otimes |e_{2,k}\rangle),$$

where m, n are the dimension of $\mathcal{H}_1$ and $\mathcal{H}_2$.

In matrix form, if $\rho = (P_{ij}) \in M_m(M_n)$, then $\operatorname{tr}_2(\rho) = (\operatorname{tr} P_{ij}) \in M_n$. One can define $\operatorname{tr}_1(\rho_{ij}) = \rho_{11} + \cdots + \rho_{mm}$, which corresponds to

$$A_2 = \operatorname{tr}_1 A = \sum_{k=1}^{m} (\langle e_{1,k}| \otimes I_n) A (|e_{1,k}\rangle \otimes I_n).$$