$|\psi\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$ $|a_1|^2$ $|a_2|^2$

Description of a quantum system in mixed states. $|\psi_1\rangle, |\psi_2\rangle$: p_1, p_2

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 $\langle A \rangle = \mathrm{tr}\,(\rho A)$. $\langle x|A|x\rangle$

$A|\psi\rangle$ $|u_1\rangle$ $|u_2\rangle$

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

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

$[\rho_{ij}(t)]$ $\frac{d}{dx}(|x\rangle\langle x|) =$

(mixed state) where H is the system Hamiltonian.

A density matrix ρ is pure iff $\rho = |\psi\rangle\langle\psi|$, i.e., ρ has eigenvalue $1, 0, 0, 0$. $\lambda_1, \cdots \lambda_n \geq 0$

Theorem 2.1 The following conditions are equivalent for a given state (density matrix) ρ.

(a) ρ is pure. (b) $\rho^2 = \rho$. (c) $\mathrm{tr}\,(\rho^2) = 1$.

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.,

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

$A = \lambda_1|\lambda_1\rangle\langle\lambda_1| + \lambda_2|\lambda_2\rangle\langle\lambda_2|$

Otherwise, it is **inseparable**.

In a quantum system with mixed states.

$p_1\ |\psi_1\rangle;\ p_2, |\psi_2\rangle \cdots p_k, |\psi_k\rangle \in \mathbb{C}^2$

$A(\quad) = \begin{cases} |\lambda_1\rangle \\ |\lambda_2\rangle \end{cases}$

$A|\psi\rangle <$ $|\lambda_1\rangle$ $|\lambda_2\rangle$

$\langle\lambda_1|A|\lambda_1\rangle$

$\langle\lambda_2|A|\lambda_2\rangle$

Probability of collapsing to $|\lambda_1\rangle$, $|\lambda_2\rangle$

depends on $\sum_{i=1}^{k} p_i \langle\psi_i|A|\psi_i\rangle = \mathrm{tr}\, A \left(\sum_{i=1}^{n} p_i |\psi_i\rangle\langle\psi_i|\right)$

ρ

Example

$p_i = \frac{1}{3}$, $i = 1, 2, 3$

$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $|\psi_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$

$\rho = \frac{1}{3}\begin{pmatrix} 1 \\ 0 \end{pmatrix}(1\ 0) + \frac{1}{3}\begin{pmatrix} 0 \\ 1 \end{pmatrix}(0\ 1) + \frac{1}{3}\cdot\frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} = \mu_1|\mu_1\rangle\langle\mu_1| + \mu_2|\mu_2\rangle\langle\mu_2|$

$\rho_1 = U\begin{pmatrix}\mu_1 & 0\\ 0 & \mu_m\end{pmatrix}U^+$ $\rho_1\otimes\rho_2$

$\rho_2 = V\begin{pmatrix}\mu_1 & 0\\ 0 & \mu_n\end{pmatrix}V^+$

Description 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.

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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.

Theorem 2.1 The following conditions are equivalent for a given state (density matrix) ρ.

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

Remarks

$\sum p_i \langle v|\psi_i\rangle\langle\psi_i|v\rangle \geq 0$

- A mixed state ρ is a Hermitian matrix with nonnegative eigenvalues (Exercise 2.3) summing up to one. Equivalently, $\langle v|\rho|v\rangle \geq 0$ for all vectors $|v\rangle$ and $\operatorname{tr}\rho = 1$.

  Note ρ is a nonnegative combination of Hermitian matrices so that it is Hermitian, and has real eigenvalues. If ρ has a negative eigenvalue λ_1, then ...

- A density matrix ρ is a pure state $\rho = |\psi\rangle\langle\psi|$, i.e., ρ has eigenvalues $1, 0, \ldots, 0$. This is the same as saying that $\operatorname{tr}\rho = 1$ (Exercise 2.4).

  Suppose ρ has eigenvalues $\lambda_1, \ldots, \lambda_n$. Then $\operatorname{tr}\rho^2 = \sum_{j=1}^n \lambda_j^2$.

$\mathbb{C}^m\otimes\mathbb{C}^n$ $\mathbb{C}^n\otimes\mathbb{C}^n$ M_n

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.,

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

$(|\psi_1\rangle\otimes|\xi_1\rangle)(\langle\psi_1|\otimes\langle\xi_1|)$

$\mathbb{C}^m$ $\mathbb{C}^n$

Otherwise, it is **inseparable**.

$= |\psi_1\rangle\langle\psi_1|\otimes|\xi_1\rangle\langle\xi_1|$

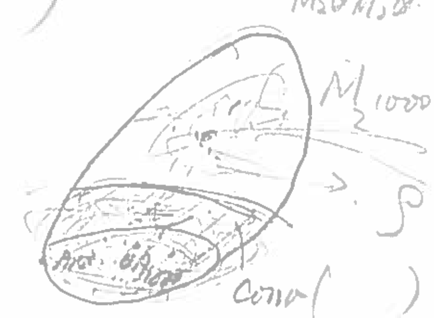
$(\sum|\psi_1\rangle\otimes\xi_1)(\quad)$

$= (\rho_{ij}),\ \rho_{ij}\in M_n.$

$\rho\in M_m(M_n)\cong M_{mn}$

$\|\qquad\qquad\|$

$M_m\otimes M_n = \text{Span}(M_m\otimes M_n)$



$M_m \otimes M_n$
$\cong$
$M_m(M_n)$

Partial transpose

Let $\rho = \sum_{j=1}^r c_j \rho_{1,j} \otimes \rho_{2,j} \in \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. The **partial transpose of** ρ **with respect to** $\mathcal{H}_2$ is

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

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{pmatrix} \quad \rho^{pt} = \begin{pmatrix} \rho_{11}^t & \rho_{12}^t & \rho_{13}^t \\ \rho_{21}^t & \rho_{22}^t & \rho_{23}^t \\ \rho_{31}^t & \rho_{32}^t & \rho_{33}^t \end{pmatrix}$$

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

Remark If ρ is separable, then so is ρ^{pt}. If ρ^{pt} has negative eigenvalues, which can be detected by $\boxed{N(A) = (\sum_j |\lambda_j(A)| - 1)/2}$ then it is not physical and ρ is not separable. Converse holds for $\mathbb{C}^r \otimes \mathbb{C}^s$ for $r + s \leq 5$.

See Example 2.5 and 2.6.

Remark: If $\rho = \sum_j p_j (\rho_{1,j} \otimes \rho_{2,j})$

then $\rho^{pt} = \sum_j p_j \rho_{1,j} \otimes \rho_{2,j}^t$.

is separable and in particular positive semidefinite

(a density matrix)

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

$$\rho^{pt} = \begin{pmatrix} a_{11}B^t & a_{12}B^t & a_{13}B^t \\ a_{21}B^t & a_{22}B^t & a_{23}B^t \\ a_{31}B^t & a_{32}B^t & a_{33}B^t \end{pmatrix} = (a_{ij}) \otimes B^t$$

$\therefore$ If ρ^{pt} is not positive semidefinite, then ρ is not separable.

Example

$$\rho = \frac{1}{2}\left[\begin{array}{cc|cc} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{array}\right] \in M_2 \otimes M_2$$

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

is not separable

because $$\rho^{pt} = \frac{1}{2}\left[\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right]$$ has e.v. 1, 1, 1, −1

$\lambda^2 + 0\lambda - 1$