§ 约化密度算符 reduced density operator

考虑一个子系统 A 与一个子系统 B 组成的系统，ρ^{AB}

定义 $\rho^{A} = tr_B(\rho^{AB})$ 　　Tr_B：部分迹

$$Tr_B\left(\underbrace{|a_1\rangle\langle a_2|}_{A\text{的态矢}} \otimes \underbrace{|b_1\rangle\langle b_2|}_{B\text{的态矢}}\right) = |a_1\rangle\langle a_2|\, Tr(|b_1\rangle\langle b_2|)$$

1. 复合系统的描述

System A. H_1 　　System B H_2. 　　比如两个原子.

复合系统 $H = H_1 \otimes H_2$.

例 H_1是 2D（自旋$\frac{1}{2}$）. 　H_2 是 3D.（自旋 1）.

$$|\psi\rangle_1 = \begin{pmatrix} a \\ b \end{pmatrix} = a|0\rangle + b|1\rangle,\quad |\phi\rangle_2 \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \alpha|0\rangle + \beta|1\rangle + \gamma|2\rangle$$

直乘

$$|\psi\rangle_1 \otimes |\phi\rangle_2 = \begin{pmatrix} a\alpha \\ b\alpha \\ a\beta \\ b\beta \\ a\gamma \\ b\gamma \end{pmatrix} = a\alpha|0\rangle_1 \otimes |0\rangle_2 + b\alpha|1\rangle_1 \otimes |0\rangle_2 + a\beta|0\rangle_1|1\rangle_2 + b\beta|1\rangle_1|1\rangle_2 + a\gamma|0\rangle_1|2\rangle_2 + b\gamma|1\rangle_1|2\rangle_2$$

对应基矢 $|0\rangle_1|0\rangle_2,\ |1\rangle_1|0\rangle_2,\ \cdots\cdots |1\rangle_1|2\rangle_2$

H空间上

- 单作用于系统1的算符：$X \otimes I$，作用于系统2的 $I \otimes Y$

矩阵：
$$X \otimes I = \begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \begin{matrix} x_1 & x_2 \\ x_3 & x_4 \end{matrix} & 0 & 0 \\ 0 & \begin{matrix} x_1 & x_2 \\ x_3 & x_4 \end{matrix} & 0 \\ 0 & 0 & \begin{matrix} x_1 & x_2 \\ x_3 & x_4 \end{matrix} \end{pmatrix}$$

- $\boxed{{}_1\langle 0|\,{}_2\langle 1|\,(X \otimes I)\,|1\rangle_1 |1\rangle_2 = {}_1\langle 0|X|1\rangle_1 \cdot {}_2\langle 1|I|1\rangle_2}$

部分迹：假设有：

$Tr_1(X \otimes Y) = \sum_n {}_1\langle n|X \otimes Y|n\rangle_1 = \sum_n {}_1\langle n|X|n\rangle_1 Y = Tr(X) \cdot Y$

$\cancel{= \sum_{n} {}_1\langle n|\,{}_2\langle m|X \otimes Y|m\rangle_2|n\rangle_1}$ 　　得到 H_2空间算符

$Z = X \otimes Y$，　$\boxed{Tr_1(Z) = Y \cdot Tr(X)}$

- $\boxed{Tr_2(X \otimes Y) = X\, Tr(Y)}$

例 $X \otimes Y = \begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \end{pmatrix} \otimes \begin{pmatrix} y_1 & y_2 & y_3 \\ y_4 & y_5 & y_6 \\ y_7 & y_8 & y_9 \end{pmatrix}$

$\cancel{= Tr(X)\, Y}$

$= \begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \end{pmatrix} \cdot (y_1 + y_5 + y_9)$

- $Tr[Tr_2(Z)] = (x_1 + x_4)(y_1 + y_5 + y_9) = Tr(Z)$

推广： $Z = X_1 \otimes Y_1 + X_2 \otimes Y_2$

$$Tr_1(Z) = Tr_1(X_1 \otimes Y_1 + X_2 \otimes Y_2) = Tr_1(X_1 \otimes Y_1) + Tr_1(X_2 \otimes Y_2)$$

$$= Y_1 Tr(X_1) + Y_2 Tr(X_2)$$

这是一个 H_2 空间上的算符.

☆ 部分迹将 $H = H_1 \otimes H_2$ 上算符映射到 H_1 或 H_2 上.

◎ ρ 是 H 上 density operater， $H = H_1 \otimes H_2$.

约化密度算符 reduced density operator $\rho_1 \equiv Tr_2(\rho)$， $\rho_2 \equiv Tr_1(\rho)$. 部分迹 partial trace on H_1

设 X 是系统 1 的算符（力学量），

$$[X]_\rho = Tr[\rho(X \otimes I)] = Tr[Tr_2(\rho \cdot (X \otimes I))]$$

$$= \sum_{nm} {}_1\langle n|{}_2\langle m| \rho \cdot (X \otimes I) |m\rangle_2 |n\rangle_1$$

$$= \sum_{nm} {}_1\langle n|{}_2\langle m| \rho |m\rangle_2 \cdot (X) |n\rangle_1$$

$$= \sum_{n} {}_1\langle n| \rho_1 X |n\rangle_1 = Tr(\rho_1 X) = [X]_{\rho_1}$$

例子： $|\alpha\rangle = \dfrac{|0\rangle_A |1\rangle_B + |1\rangle_A |0\rangle_B}{\sqrt{2}}$ 纠缠态，纯态！

$$\rho = |\alpha\rangle\langle\alpha| =$$

$$= \frac{1}{2}\Big[|0\rangle_A |1\rangle_B \, {}_B\langle 1| {}_A\langle 0| + |0\rangle_A |1\rangle_B \, {}_B\langle 0| {}_A\langle 1| + |1\rangle_A |0\rangle_B \, {}_B\langle 1| {}_A\langle 0| + |1\rangle_A |0\rangle_B \, {}_B\langle 0| {}_A\langle 1|$$

$$= \frac{1}{2}\Big[|0\rangle_A\langle 0| \otimes |1\rangle_B\langle 1| + |0\rangle_A\langle 1| \otimes |1\rangle_B\langle 0| + |1\rangle_A\langle 0| \otimes |0\rangle_B\langle 1| + |1\rangle_A\langle 1| \otimes |0\rangle_B\langle 0|$$

$$\rho_A = Tr_B(|\alpha\rangle\langle\alpha|)$$

$$= \frac{1}{2}\Big[|0\rangle_A\langle 0| + |0\rangle_A\langle 1| \times 0 + |1\rangle_A\langle 0| \times 0 + |1\rangle_A\langle 1| \Big]$$

$$= \frac{1}{2} I$$ 这是一个混态系统!! $\vec{n} = 0$!

◎ 一个纯态，最好的确定状态，其子系统是个混态 → 不确定

更一般的 $|\alpha\rangle = (\sum_a c_a |a\rangle_A) \otimes (\sum_b c_b |b\rangle_B)$
$= |\psi\rangle_A \otimes |\phi\rangle_B$

$\rho = |\psi\rangle_A |\phi\rangle_B {}_B\langle\phi| {}_A\langle\psi| = |\psi\rangle_A\langle\psi| \otimes |\phi\rangle_B\langle\phi|$
$= \rho_A \otimes \rho_B$

但是．考虑 $|\alpha\rangle = |0\rangle_A |1\rangle_B$

$$\rho = |\alpha\rangle\langle\alpha| = |0\rangle_A |1\rangle_B {}_B\langle 1| {}_A\langle 0| = \underbrace{|0\rangle_A\langle 0|}_{\rho_A} \otimes \underbrace{|1\rangle_B\langle 1|}_{\rho_B}$$

$$\rho_A = Tr_B(\rho) = |0\rangle_A\langle 0|$$ 仍然是个纯态！

区别在哪里？一个是纠缠态 entangled，一个是直积态 product

- 怎样判断一个纯态是否纠缠？计算 $S(\rho_1)$ or $S(\rho_2)$．

$\boxed{\text{纠缠熵}}$ $E(|\alpha\rangle_{AB}) = S(\rho_A)$．

前面第1个例子，$S(\rho_A) = -Tr(\rho_A \ln \rho_A) = \ln 2$
第2个例子．$S(\rho_A) = 0$

- ~~反过来~~ 考虑 A系统的一个 mixed state．
我们总可以设想它与一个系统 F 纠缠．即：

设 $\rho_A = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|$， write

$$|\alpha\rangle_{AF} = \sum_k \sqrt{\lambda_k} |\phi_k\rangle_A |k\rangle_F$$

$|k\rangle_F$ 是F系统一组正交归一态

$$Tr_F(|\alpha\rangle_{AF}\langle\alpha|) = Tr_F\left(\sum_{kk'} \sqrt{\lambda_k}\sqrt{\lambda_{k'}} |\phi_k\rangle_A |k\rangle_F {}_F\langle k'| {}_A\langle\phi_{k'}|\right)$$

$$= Tr_F\left(\sum_{kk'} \sqrt{\lambda_k\lambda_{k'}} |\phi_k\rangle_A\langle\phi_{k'}| \otimes |k\rangle_F\langle k'|\right)$$

$$= \sum_{kk'} \sqrt{\lambda_k\lambda_{k'}} |\phi_k\rangle_A\langle\phi_{k'}| \delta_{kk'}$$

$$= \sum_k \lambda_k |\phi_k\rangle_A\langle\phi_k|$$

倒过来：Schmidt 分解！

纯态 $|\alpha\rangle_{AF} = \sum_i \lambda_i |i_A\rangle|i_B\rangle$，$\sum_i \lambda_i^2 = 1$

$\boxed{\lambda_i \to \text{schmidt number}}$

告诉我们 $\rho_A = \sum_i \lambda_i^2 |i_A\rangle\langle i_A|$，$\rho_B = \sum_i \lambda_i^2 |i_B\rangle\langle i_B|$ 本征值一样！