Chapter 3

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1 Coupled density matrix

For a two spin-1/2 particle, ρ_A for the first one, ρ_B for the second. For example,

$$\rho_A = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \; \rho_B = \frac{1}{2} I = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\Rightarrow \rho = \rho_A \otimes \rho_B = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

in general, for $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ of one particle, the physical meaning is there is a statistics, that there is a probability p_i for the particle at state $|\psi_i\rangle$. For 2 particles, the overall state is described as

$$\rho = \sum_i p_i |\psi_i^{(1)}\rangle\langle\psi_i^{(1)}| \otimes |\phi_i^{(2)}\rangle\langle\phi_i^{(2)}| \tag{1}$$

$$= \sum_i p_i \left(|\psi_i^{(1)}\rangle \otimes |\phi_i^{(2)}\rangle\right) \cdot \left(\langle\psi_i^{(1)}| \otimes \langle\phi_i^{(2)}|\right) \tag{2}$$

Box 1.1: Examples for density matrix

Pure state case:
particle 1 at $|0\rangle$, particle 2 at $|1\rangle$. Density matrix $\rho = |01\rangle\langle 01|$

Mixed state case:
For a two particle system, we have $\frac{1}{3}$ of chance two particles at $|\psi_1\rangle$, $\frac{1}{3}$ of chance two particles at $|\psi_2\rangle$, and $\frac{1}{3}$ of chance two particles at $|\psi_3\rangle$. The density matrix

$$\rho = \frac{1}{3}|\psi_1\rangle\langle\psi_1| + \frac{1}{3}|\psi_2\rangle\langle\psi_2| + \frac{1}{3}|\psi_3\rangle\langle\psi_3|$$

2 Dynamics

For 1 particle, $\rho = \sum_i p_i |\psi_i(t)\rangle\langle\psi_i(t)|$, the Shrödinger's equation

$$i\hbar \frac{\partial}{\partial t} |\psi_i(t)\rangle = H |\psi_i(t)\rangle \tag{3}$$

so

$$\dot{\rho} = \frac{d}{dt}\rho = \sum_i p_i \left(\frac{d}{dt} \right) \tag{4}$$

for multi particle system, we have $\rho_{\text{multi}}, H_{\text{multi}}$

$$\Rightarrow \dot{\rho}_{\text{multi}} = \frac{1}{i\hbar}[H_{\text{multi}}, \rho_{\text{multi}}] \tag{5}$$

3 Trace

Under basis $\{|\psi_i\rangle\}$,

$$tr(\rho) = \sum_i \langle\psi_i|\rho|\psi_i\rangle \tag{6}$$

for multi particles, we need a $\{|\psi_i\rangle_{\text{multi}}\}$ as a basis,

4 Partial trace

Definition 4.1: Partial trace for 2 particle system

Suppose we have a two particle system, then the partial trace on particle A is

$$tr_A(\rho) = \sum_i \left(\langle\psi_i|^A \otimes I^B \right) \cdot \rho \cdot \left(|\psi_i\rangle^A \otimes I^B \right) \tag{7}$$

Here, $|\psi_i\rangle$ is one of the basis of particle A, and ρ is the density matrix of the whole system. We can give an example below.

Box 4.1: An example of partial trace

$\rho = M_A \otimes M_B$, where M_A, M_B are matrixes. For spin-1/2 particles,

$$\begin{aligned} tr_A(\rho) &= \sum_i \left(\langle\psi_i|^A \otimes I^B \right) \cdot \rho \cdot \left(|\psi_i\rangle^A \otimes I^B \right) \\ &= \left(\langle 0|^A \otimes I^B \right) \cdot \rho \cdot \left(|0\rangle^A \otimes I^B \right) + \left(\langle 1|^A \otimes I^B \right) \cdot \rho \cdot \left(|1\rangle^A \otimes I^B \right) \end{aligned} \tag{8}$$

where $\rho = M_A \otimes M_B$, so

$$\left(\langle 0|^A \otimes I^B \right) \cdot (M_A \otimes M_B) \cdot \left(|0\rangle^A \otimes I^B \right) = \langle 0|M_A|0\rangle \otimes \left(I^B \cdot M_B \cdot I^B \right) \tag{9}$$

$$= \langle 0|M_A|0\rangle M_B \tag{10}$$

we can easily get that

$$\left(\langle 1|^A \otimes I^B\right) \cdot M_A \otimes M_B \cdot \left(|1\rangle^A \otimes I^B\right) = \langle 1|M_A|1\rangle M_B \tag{11}$$

Here, $|0\rangle^A \otimes I^B$ means that

$$|0\rangle^A \otimes I^B = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ 0 \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{12}$$

So

$$\begin{aligned} tr_A(\rho) &= \langle 0|M_A|0\rangle M_B + \langle 1|M_A|1\rangle M_B & (13) \\ &= \left(\langle 0|M_A|0\rangle + \langle 1|M_A|1\rangle\right) M_B & (14) \\ &= tr(M_A)M_B \xlongequal{M_A \text{ be physical}} M_B & (15) \end{aligned}$$

The definition here is a bit complicated, we can refer to *Quantum Computation and Quantum Information, Michael A. Nielsen* and read the corresponding section. In that book, the author introduce the *reduced density operator* and the *partial trace* at the same time. Here is the definition in the book.

Definition 4.2: Reduced density operator and partial trace

Suppose we have physical systems A and B, whose state is described by a density operator ρ^{AB}. The reduced density operator for system A is defined by

$$\rho^A \equiv tr_B(\rho^{AB}) \tag{16}$$

where tr_B is a map of operators known as the *partial trace* over system B. The partial trace is defined by

$$\operatorname{tr}_B\left(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|\right) \equiv |a_1\rangle\langle a_2| \operatorname{tr}\left(|b_1\rangle\langle b_2|\right) \tag{17}$$

where $|a_1\rangle$ and $|a_2\rangle$ are any two vectors in the state space of A, and $|b_1\rangle$ and $|b_2\rangle$ are any two vectors in the state space of B. The trace operation appearing on the right hand side is the usual trace operation for system B, so $tr(|b_1\rangle\langle b_2|) = \langle b_2|b_1\rangle$. We have defined the partial trace operation only on a special subclass of operators on AB; the specification is completed by requiring in addition to Equation (17) that the partial trace be linear in its input.

It means that $tr_A(|a_1b_1\rangle\langle a_2b_2|) = |b_1\rangle\langle b_2| \cdot tr(|a_1\rangle\langle a_2|)$. Due to $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$, we can always decompose ρ such that $\rho = \sum_{i,j,i',j'} c_{i,j,i',j'}|\phi_i^A\phi_j^B\rangle\langle\phi_{i'}^A\phi_{j'}^B|$. Specifically, suppose a quantum system is in the product state $\rho^{AB} = \rho \otimes \sigma$, where ρ is a density operator for system A, and σ is a density operator for system B. Then

$$\rho^A = \mathrm{tr}_B(\rho \otimes \sigma) = \rho\,\mathrm{tr}(\sigma) = \rho \tag{18}$$

We want to proof that the two definitions are equivalent. For a matrix $|a_1 b_1\rangle\langle a_2 b_2|$, by definition 4.1, we have

$$tr(|a_1 b_1\rangle\langle a_2 b_2|) = \sum_i \langle i|^A I^B \cdot |a_1 b_1\rangle\langle a_2 b_2| \cdot |i\rangle^A I^B \tag{19}$$

$$= \sum_i \langle i|^A a_1\rangle\langle a_2|i\rangle^A \otimes I^B|b_1\rangle\langle b_2|I^B \tag{20}$$

$$= |b_1\rangle\langle b_2| tr(|a_1\rangle\langle a_2|) \tag{21}$$

so these two definitions are equivalent.

4.1 Partial trace and entangled state

If we have $\rho = |\psi\rangle\langle\psi|$, where $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ is an entangled state, then what is $tr_A(\rho)$? First, we can calculate the density matrix as follows:

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|) \tag{22}$$

$$= \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) \tag{23}$$

$$\Rightarrow tr_A(\rho) = ((\langle 0| \otimes I)\cdot \tag{24}$$