

# Chapter 3

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## 1 Coupled density matrix

A two spin-1/2 particle system,  $\rho_A$  for the first one,  $\rho_B$  for the second. For example,

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

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 particle system, the overall state is described as

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

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

### Box 1.1: Examples of coupled 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

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

if  $|\psi_1\rangle = |00\rangle$ ,  $|\psi_2\rangle = |11\rangle$ ,  $|\psi_3\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ , for this case, because of entanglement of  $|\psi_3\rangle$ ,

$$\rho \neq \sum_i p_i \left( |\phi_i^{(1)}\rangle \otimes |\phi_i^{(2)}\rangle \right) \cdot \left( \langle\phi_i^{(1)}| \otimes \langle\phi_i^{(2)}| \right) \quad (3)$$

## 2 Dynamics

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

$$i\hbar \frac{\partial}{\partial t} |\psi_i(t)\rangle = H |\psi_i(t)\rangle \quad (4)$$

so

$$\dot{\rho} = \frac{d}{dt} \rho = \sum_i p_i \left( \frac{d}{dt} |\psi_i(t)\rangle \right) \langle \psi_i(t)| + \sum_i p_i |\psi_i(t)\rangle \left( \frac{d}{dt} \langle \psi_i(t)| \right) \quad (5)$$

$$= \sum_i p_i \frac{H}{i\hbar} |\psi_i(t)\rangle \langle \psi_i(t)| + \sum_i p_i |\psi_i(t)\rangle \langle \psi_i(t)| \frac{H}{-i\hbar} \quad (6)$$

$$= \frac{1}{i\hbar} \left[ H \cdot \left( \sum_i p_i |\psi_i(t)\rangle \langle \psi_i(t)| \right) - \left( \sum_i p_i |\psi_i(t)\rangle \langle \psi_i(t)| \right) \cdot H \right] \quad (7)$$

$$= \frac{1}{i\hbar} [H, \rho] \quad (8)$$

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

$$\Rightarrow \dot{\rho}_{\text{multi}} = \frac{1}{i\hbar} [H_{\text{multi}}, \rho_{\text{multi}}] \quad (9)$$

## 3 Trace

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

$$\text{tr}(\rho) = \sum_i \langle \psi_i | \rho | \psi_i \rangle \quad (10)$$

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

$$\text{tr}(\rho_{\text{multi}}) = \sum_i \langle \psi_i |_{\text{multi}} \rho_{\text{multi}} | \psi_i \rangle_{\text{multi}} \quad (11)$$

## 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

$$\text{tr}_A(\rho) = \sum_i (\langle \psi_i |^A \otimes I^B) \cdot \rho \cdot (| \psi_i \rangle^A \otimes I^B) \quad (12)$$

Here,  $|\psi_i\rangle$  is one of the basis of particle A, and  $\rho$  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,

$$\begin{aligned} \text{tr}_A(\rho) &= \sum_i (\langle \psi_i |^A \otimes I^B) \cdot \rho \cdot (| \psi_i \rangle^A \otimes I^B) \\ &= (\langle 0 |^A \otimes I^B) \cdot \rho \cdot (| 0 \rangle^A \otimes I^B) + (\langle 1 |^A \otimes I^B) \cdot \rho \cdot (| 1 \rangle^A \otimes I^B) \end{aligned} \quad (13)$$

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

$$(\langle 0 |^A \otimes I^B) \cdot (M_A \otimes M_B) \cdot (| 0 \rangle^A \otimes I^B) = \langle 0 | M_A | 0 \rangle \otimes (I^B \cdot M_B \cdot I^B) \quad (14)$$

$$= \langle 0 | M_A | 0 \rangle M_B \quad (15)$$

we can easily get that

$$(\langle 1 |^A \otimes I^B) \cdot M_A \otimes M_B \cdot (| 1 \rangle^A \otimes I^B) = \langle 1 | M_A | 1 \rangle M_B \quad (16)$$

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

$$| 0 \rangle^A \otimes I^B = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ 0 \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \quad (17)$$

So

$$\text{tr}_A(\rho) = \langle 0 | M_A | 0 \rangle M_B + \langle 1 | M_A | 1 \rangle M_B \quad (18)$$

$$= (\langle 0 | M_A | 0 \rangle + \langle 1 | M_A | 1 \rangle) M_B \quad (19)$$

$$= \text{tr}(M_A) M_B \stackrel{M_A \text{ be physical}}{=} M_B \quad (20)$$

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  $\rho^{AB}$ . The reduced density operator for system  $A$  is defined by

$$\rho^A \equiv \text{tr}_B(\rho^{AB}) \quad (21)$$

where  $\text{tr}_B$  is a map of operators known as the *partial trace* over system  $B$ . The partial trace is defined by

$$\text{tr}_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) \equiv |a_1\rangle\langle a_2| \text{tr}(|b_1\rangle\langle b_2|) \quad (22)$$

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 (22) 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  $\rho$  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  $\rho$  is a density operator for system  $A$ , and  $\sigma$  is a density operator for system  $B$ . Then

$$\rho^A = tr_B(\rho \otimes \sigma) = \rho tr(\sigma) = \rho \quad (23)$$

We want to proof that the two definitions are equivalent. For a matrix  $|a_1b_1\rangle\langle a_2b_2|$ , by definition 4.1, we have

$$tr(|a_1b_1\rangle\langle a_2b_2|) = \sum_i \langle i|^A I^B \cdot |a_1b_1\rangle\langle a_2b_2| \cdot |i\rangle^A I^B \quad (24)$$

$$= \sum_i \langle i|^A a_1\rangle\langle a_2|i\rangle^A \otimes I^B |b_1\rangle\langle b_2| I^B \quad (25)$$

$$= |b_1\rangle\langle b_2| tr(|a_1\rangle\langle a_2|) \quad (26)$$

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:

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|) \quad (27)$$

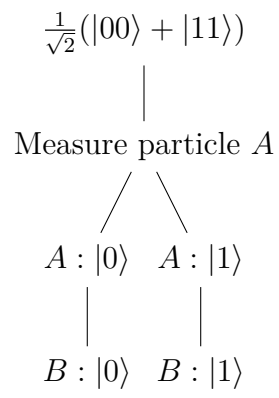
$$= \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) \quad (28)$$

by definition 4.1, we have

$$tr_A(\rho) = (\langle 0| \otimes I) \cdot \rho \cdot (|0\rangle \otimes I) + (\langle 1| \otimes I) \cdot \rho \cdot (|1\rangle \otimes I) \quad (29)$$

$$= \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{1}{2}I_B \quad (30)$$

which is a totally mixed state. It gives no information of particle  $B$ 's state.



$tr_A(\rho)$  means we discard information of  $A$ , and see what we left with  $B$ .