

# Chapter 3

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## 1 Coupled density matrix

For a two spin-1/2 particle,  $\rho_A$  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 particles, the overall state is described as

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

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

### Box 1.1: Examples 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

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

so

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

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

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

## 3 Trace

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

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

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

$$\text{tr}_A(\rho) = \sum_i (\langle \psi_i |^A \otimes I^B) \cdot \rho \cdot (|\psi_i\rangle^A \otimes I^B) \quad (7)$$

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,

$$\begin{aligned} \text{tr}_A(\rho) &= \sum_i (\langle \psi_i |^A \otimes I^B) \cdot \rho \cdot (|\psi_i\rangle^A \otimes I^B) \\ &= (\langle 0 |^A \otimes I^B) \cdot \rho \cdot (|0\rangle^A \otimes I^B) + (\langle 1 |^A \otimes I^B) \cdot \rho \cdot (|1\rangle^A \otimes I^B) \end{aligned} \quad (8)$$

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

$$(\langle 0 |^A \otimes I^B) \cdot M_A \otimes M_B \cdot (|0\rangle^A \otimes I^B) = \langle 0 | M_A | 0 \rangle \otimes (I^B \cdot M_B \cdot I^B) \quad (9)$$

$$= \langle 0 | M_A | 0 \rangle M_B \quad (10)$$

we can easily get that

$$(\langle 1|^A \otimes I^B) \cdot M_A \otimes M_B \cdot (|1\rangle^A \otimes I^B) = \langle 1|M_A|1\rangle M_B \quad (11)$$

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

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

So

$$\text{tr}_A(\rho) = \langle 0|M_A|0\rangle M_B + \langle 1|M_A|1\rangle M_B \quad (13)$$

$$= (\langle 0|M_A|0\rangle + \langle 1|M_A|1\rangle) M_B \quad (14)$$

$$= \text{tr}(M_A) M_B \xrightarrow{\text{M}_A \text{ be physical}} M_B \quad (15)$$

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, and 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

$$\rho^A \equiv \text{tr}_B(\rho^{AB}) \quad (16)$$

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

$$\text{tr}_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) \equiv |a_1\rangle\langle a_2| \text{tr}(|b_1\rangle\langle b_2|) \quad (17)$$

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  $\text{tr}(|b_1\rangle\langle b_2|) = \langle b_2|b_1\rangle$ . 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 (15) that the partial trace be linear in its input.

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

$$\rho^A = \text{tr}_B(\rho \otimes \sigma) = \rho \text{tr}(\sigma) = \rho \quad (18)$$

We want to proof that the 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:

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|) \quad (19)$$

$$= \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) \quad (20)$$

$$\Rightarrow tr_A(\rho) = (\langle 0| \otimes I). \quad (21)$$