# **2.4 Density operator/matrix**

Ensemble of *pure states* gives a *mixed state* 



The *density operator* or *density matrix*  $\rho$  for the ensemble or mixture of normalized states  $|\psi_i\rangle$  with probabilities  $p_i$  is given by

$$\rho = \sum_{i} p_i |\psi_i\rangle \langle \psi_i| \qquad \sum_{i} p_i = 1$$

Note: The set of states  $|\psi_i\rangle$  and probabilites  $p_i$  are not unique:

$$\rho = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| = \frac{1}{2}[|a\rangle\langle a| + |b\rangle\langle b|] \quad |a/b\rangle = \frac{1}{2}\left[\sqrt{3}|0\rangle \pm |1\rangle\right]$$

### **Composition**

If we have systems numbered 1 through n, and system i is in state  $\rho_i$  , the state of the total system is

 $\rho_1 \otimes \rho_2 \otimes \ldots \otimes \rho_n$ 

## General properties

An operator  $\rho$  is a density operator if (and only if):

- 1)  $\rho$  has trace equal to one.
- 2)  $\rho$  is Hermitian
- 3)  $\rho$  is a positive operator.

**Derivation:** Show general properties from  $\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|$ .

**Example:** General single qubit density matrix, decomposition.

**Derivation:** Exercise 2.71, purity of a state  $\rho$ .

### Time development

For an individual state  $|\psi_i
angle$ , with U the unitary time evolution operator

$$|\psi_i\rangle \to U|\psi_i\rangle \implies$$
$$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i| \to \sum_i p_i U|\psi_i\rangle \langle\psi_i| U^{\dagger} = U\rho U^{\dagger}$$

<u>Measurement</u>

We perform a general measurement described by  $M_m$ . If the system is in state  $|\psi_i\rangle$ , the (conditional) probability to get m is

$$p(m|i) = \langle \psi_i | M_m^{\dagger} M_m | \psi_i \rangle = \operatorname{tr}(M_m^{\dagger} M_m | \psi_i \rangle \langle \psi_i |)$$

The total probability to get m when measuring on  $\rho$  is then

$$\sum_{i} p_{i} p(m|i) = \sum_{i} p_{i} \operatorname{tr}(M_{m}^{\dagger} M_{m} |\psi_{i}\rangle \langle \psi_{i}|) = \operatorname{tr}(M_{m}^{\dagger} M_{m} \rho)$$

#### Post-measurement state

For an initial state  $|\psi_i\rangle$ , the state after measuring m is

$$|\psi_i^m\rangle = \frac{M_m|\psi_i\rangle}{\sqrt{\langle\psi_i|M_m^{\dagger}M_m|\psi_i\rangle}}$$

The total state after measuring m on  $\rho$  is

$$\rho_m = \sum_i \frac{p_i p(m|i) |\psi_i^m \rangle \langle \psi_i^m|}{p(m)}$$

The normlization condition  $tr(\rho_m) = 1$  gives the denominator

$$p(m) = \sum_{i} p_{i} p(m|i)$$

Inserting known expressions, this gives

$$\rho_m = \sum_i p_i \frac{M_m |\psi_i\rangle \langle \psi_i | M_m^{\dagger}}{\operatorname{tr}(M_m^{\dagger} M_m \rho)} = \frac{M_m \rho M_m^{\dagger}}{\operatorname{tr}(M_m^{\dagger} M_m \rho)}$$

Reduced density operator/matrix

The composite, total system AB is in the state  $\rho_{AB}.$ 

The *reduced density operator* of system A is by definition

 $\rho_A = \operatorname{tr}_B\left(\rho_{AB}\right)$ 



where the *partial trace* over B is defined by

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

with  $|a_1\rangle$ ,  $|a_2\rangle$  ( $|b_1\rangle$ ,  $|b_2\rangle$ ) any vectors in A (B), and the linearity property of the trace.

The reduced density operator describes completely all the properties/outcomes of measurements of the system A, given that system B is left unobserved ("tracing out" system B)

**Derivation:** Properties of reduced density operator. **Derivation:** Reduced density matrix for Bell state  $|\psi\rangle = \frac{1}{\sqrt{2}} [|00\rangle + |11\rangle]$ 

# 2.5 Schmidt decomposition and purification

## Schmidt decomposition

For a pure state  $|\psi\rangle$  in the composite system AB, there exists orthonormal bases  $|i_A\rangle$  and  $|i_B\rangle$  (Schmidt bases) for systems A and B, such that

$$|\psi\rangle = \sum_{i} \lambda_{i} |i_{A}\rangle |i_{B}\rangle$$

with  $\lambda_i$  the real, non-negative Schmidt coefficients and

$$\sum_i \lambda_i^2 = 1$$
 for  $|\psi\rangle$  normalized,  $\langle \psi |\psi\rangle = 1.$ 

## **Properties**

The reduced density matrices  $\rho_A, \rho_B$  have the same eigenvalues

$$\rho_A = \operatorname{tr}_B\left(|\psi\rangle\langle\psi|\right) = \sum_i \lambda_i^2 |i_A\rangle\langle i_A| \qquad \rho_B = \sum_i \lambda_i^2 |i_B\rangle\langle i_B|$$

The Schmidt number is the number of non-zero Schmidt coefficients.

## **Purification**

Consider a system A in state  $\rho_A$ .

It is possible to introduce an additional system R and to define a pure state  $|AR\rangle$ , such that the reduced density operator for A is

$$\operatorname{tr}_R(|AR\rangle\langle AR|) = \rho_A$$

This is called *purification*.

We can construct  $|AR\rangle$  by first noting that we can spectrally decompose

$$\rho_A = \sum_i p_i |i_A\rangle \langle i_A|$$

By taking R to have the same dimensions as A we can define

$$|AR\rangle = \sum_{i} \sqrt{p_i} |i_A\rangle |i_R\rangle$$

This then gives

$$\operatorname{tr}_{R}(|AR\rangle\langle AR|) = \sum_{ij} \sqrt{p_{i}p_{j}} |i_{A}\rangle\langle j_{A}|\operatorname{tr}(|i_{R}\rangle\langle j_{R}|) = \sum_{i} p_{i}|i_{A}\rangle\langle i_{A}| = \rho_{A}$$

