

## Chapter 2

# The Density Matrix

We are going to require a more general description of a quantum state than that given by a state vector. The density matrix provides such a description. Its use is required when we are discussing an ensemble of pure states or when we are describing a subsystem of a larger system.

### 2.1 Ensembles and Subsystems

Let us look at ensembles first. Suppose that we have a collection of objects, some of which are in the quantum state  $|\psi_1\rangle$ , some of which are in  $|\psi_2\rangle$ , and so on. In particular, if we choose an object from the ensemble, the probability that it is in state  $|\psi_j\rangle$  is  $p_j$ . We want to find the expectation value of some observable,  $Q$ , in this ensemble. We pick one of the objects in the ensemble and measure  $Q$ , pick another, and do the same. We repeat this process many times. If all of the objects were in the state  $|\psi_j\rangle$ , the expectation value of  $Q$  would be  $\langle\psi_j|Q|\psi_j\rangle$ , but in reality, objects with this state appear only with a probability  $p_j$ . Therefore, the expectation of  $Q$  in the ensemble is given by

$$\langle Q \rangle = \sum_j p_j \langle \psi_j | Q | \psi_j \rangle = \text{Tr}(Q\rho), \quad (2.1)$$

where we have defined the operator  $\rho$ , which is the density matrix corresponding to the ensemble, to be

$$\rho = \sum_j p_j |\psi_j\rangle \langle \psi_j|. \quad (2.2)$$

Now let us look at subsystems. Suppose we have a large system composed of two subsystems,  $A$  and  $B$ . The Hilbert spaces for the quantum states of the subsystems are  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , so that the Hilbert space for the entire system is  $\mathcal{H}_A \otimes \mathcal{H}_B$ . Let  $\{|m\rangle_A\}$  be an orthonormal basis for  $\mathcal{H}_A$  and  $\{|n\rangle_B\}$  be an orthonormal basis for  $\mathcal{H}_B$ .

Now if  $X_A$  is an observable on subsystem  $A$ , then the operator corresponding to it in the total Hilbert space is  $X_A \otimes I_B$ , where  $I_B$  is the identity on  $\mathcal{H}_B$ . If  $|\Psi\rangle$  is the state of the entire system, then the expectation value of  $X_A$  is given by

$$\begin{aligned}\langle X_A \rangle &= \langle \Psi | X_A \otimes I_B | \Psi \rangle \\ &= \sum_m \sum_n \langle \Psi | X_A \otimes I_B | m \rangle_A | n \rangle_B \rangle ({}_A \langle m | {}_B \langle n |) | \Psi \rangle \\ &= \sum_m {}_A \langle m | \left( \sum_n {}_B \langle n | \Psi \rangle \langle \Psi | n \rangle_B \right) X_A | m \rangle_A.\end{aligned}\quad (2.3)$$

If we now define

$$\rho_A = \sum_n {}_B \langle n | \Psi \rangle \langle \Psi | n \rangle_B = \text{Tr}_B(|\Psi\rangle\langle\Psi|), \quad (2.4)$$

then we have that

$$\langle X_A \rangle = \text{Tr}_A(\rho_A X_A). \quad (2.5)$$

The operator  $\rho_A$  is known as the reduced density operator for subsystem  $A$ , and it can be used to evaluate the expectation value of any observable that pertains only to subsystem  $A$ .

Now let us look at two examples. First, we have an ensemble in which half of the qubits are in the state  $|0\rangle$  and the other half are in the state  $|1\rangle$ . The density matrix for this ensemble is

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|. \quad (2.6)$$

Suppose we want to find the expectation value of  $\sigma_z$  in this ensemble, where  $\sigma_z|0\rangle = |0\rangle$  and  $\sigma_z|1\rangle = -|1\rangle$ . We have that

$$\langle \sigma_z \rangle = \text{Tr}(\sigma_z \rho) = 0. \quad (2.7)$$

Next, we have a two-qubit state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A |1\rangle_B + |1\rangle_A |0\rangle_B), \quad (2.8)$$

and we would like to find the reduced density matrix for subsystem  $A$ . We have that

$$\rho_A = \text{Tr}(|\Psi\rangle\langle\Psi|) = \frac{1}{2}I_A. \quad (2.9)$$

Defining  $\sigma_{zA} = \sigma_z \otimes I_B$ , we have that

$$\langle \sigma_{Az} \rangle = \text{Tr}(\sigma_{zA} \rho_A) = 0. \quad (2.10)$$

Note that if  $\rho$  is a one-dimensional projection, i.e.,  $\rho = |\psi\rangle\langle\psi|$ , then for any observable  $Q$ ,

$$\langle Q \rangle = \text{Tr}(\rho Q) = \langle \psi | Q | \psi \rangle, \quad (2.11)$$

so that the density matrix corresponds to the system being in the state  $|\psi\rangle$ . If  $\rho$  is of this form we call it a pure state. If not, it is called a mixed state.

## 2.2 Properties

In order for an operator to be a density matrix, it must satisfy several properties. In fact, any operator satisfying these properties is a valid density matrix:

1.  $\text{Tr}(\rho) = 1$ .

This follows from the fact that

$$\text{Tr}(\rho) = \text{Tr} \left( \sum_j p_j |\psi_j\rangle\langle\psi_j| \right) = \sum_j p_j = 1. \quad (2.12)$$

2. A density matrix is hermitian,  $\rho = \rho^\dagger$ .
3. A density matrix is positive,  $\langle \psi | \rho | \psi \rangle \geq 0$  for all  $|\psi\rangle$ .

This follows from

$$\langle \psi | \rho | \psi \rangle = \sum_j p_j |\langle \psi | \psi_j \rangle|^2 \geq 0. \quad (2.13)$$

We also note that an operator is positive if and only if all of its eigenvalues are greater than or equal to zero, which implies that the eigenvalues of any density matrix must satisfy this property. In addition, because the trace of a density matrix is one and the trace is just the sum of the eigenvalues, we have that if  $\lambda_j$  is an eigenvalue of a density matrix, then  $0 \leq \lambda_j \leq 1$ .

We now want to use these requirements to find additional properties of the set of density matrices. The first is a simple way of identifying pure states.

**Theorem.** *The density matrix  $\rho$  is a pure state if and only if  $\text{Tr}(\rho^2) = 1$ .*

*Proof.* If  $\rho$  is pure, then  $\rho = |\psi\rangle\langle\psi|$ , and  $\rho^2 = \rho$ . This immediately implies that  $\text{Tr}(\rho^2) = 1$ . Now assume that  $\text{Tr}(\rho^2) = 1$ . Because  $\rho$  is hermitian, we can express it as

$$\rho = \sum_j \lambda_j P_j, \quad (2.14)$$

where  $\lambda_j$  are the nonzero eigenvalues of  $\rho$  and  $P_j$  are the corresponding spectral projections. This immediately implies that

$$\rho^2 = \sum_j \lambda_j^2 P_j. \quad (2.15)$$

Denoting the rank of  $P_j$  by  $n_j$  we have that

$$\begin{aligned}\mathrm{Tr}(\rho) &= 1 \Rightarrow \sum_j \lambda_j n_j = 1 \\ \mathrm{Tr}(\rho^2) &= 1 \Rightarrow \sum_j \lambda_j^2 n_j = 1,\end{aligned}\tag{2.16}$$

and subtracting these two equations gives us

$$\sum_j (\lambda_j - \lambda_j^2) n_j = 0.\tag{2.17}$$

Because each eigenvalue is between 0 and 1, each term in the above sum is greater than or equal to zero, which further implies that each term must be equal to zero. The only way this can happen is if each  $\lambda_j$  is equal to zero or one, and we have assumed that  $\lambda_j > 0$ , so that  $\lambda_j = 1$ . The only way that this can be consistent with the fact that the sum of the eigenvalues times their multiplicities is one is if only one of them is nonzero, and this eigenvalue has a multiplicity of one. Therefore,  $\rho$  is equal to a rank-one projection, which means that it is a pure state.  $\square$

### 2.3 Pure States and Mixed States of a Qubit

In the previous chapter we introduced the Bloch sphere as a convenient representation for state vectors of qubits, that is, qubit pure states. If we extend this representation to include the interior of the sphere, it can be used to represent mixed states of qubits as well. In order to see this we expand a general qubit density matrix, which is a  $2 \times 2$  matrix, in terms of the identity matrix and the Pauli matrices, which form a complete basis for the space of a set of  $2 \times 2$  matrices:

$$\rho = \frac{1}{2}(I + n_x \sigma_x + n_y \sigma_y + n_z \sigma_z).\tag{2.18}$$

This satisfies the condition  $\mathrm{Tr}(\rho) = 1$ , and the fact that  $\rho$  is hermitian implies that  $n_x$ ,  $n_y$ , and  $n_z$  are real. This equation implies that

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + n_z & n_x - in_y \\ n_x + in_y & 1 - n_z \end{pmatrix},\tag{2.19}$$

which further implies that  $\det \rho = (1 - |\mathbf{n}|^2)/4$ . The fact that  $\rho$  is positive means that its determinant must be greater than or equal to zero and, therefore,  $1 \geq |\mathbf{n}|$ . We represent the density matrix  $\rho$  by the vector  $\mathbf{n}$ , which lies in the unit ball.

We know that if  $\rho$  is a pure state, its corresponding vector will have its endpoint on the surface of the Bloch sphere. Let us show the converse. If  $|\mathbf{n}| = 1$  then  $\mathrm{Tr}(\rho) = 1$

and  $\det \rho = 0$ . This implies that one of the eigenvalues of  $\rho$  is zero and the other is one. If  $|u\rangle$  is the eigenvector with eigenvalue one, where  $\|u\| = 1$ , then  $\rho = |u\rangle\langle u|$ , and  $\rho$  is a pure state.

Given a qubit density matrix,  $\rho$ , we can easily find the vector corresponding to it. The identity  $\text{Tr}(\sigma_j \sigma_k) = \delta_{jk}$ , where  $j, k \in \{x, y, z\}$ , gives us that

$$n_j = \text{Tr}(\rho \sigma_j). \quad (2.20)$$

Most density matrices can correspond to many different ensembles. We give some examples. In the first example, we define the states

$$|\pm x\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle), \quad (2.21)$$

which are eigenstates of  $\sigma_x$ . Then we can write the density matrix of a maximally mixed state in two ways,

$$\rho = \frac{1}{2}I = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{1}{2}(|+x\rangle\langle +x| + |-x\rangle\langle -x|). \quad (2.22)$$

The first decomposition corresponds to an ensemble in which half of the elements are in the state  $|0\rangle$  and half in the state  $|1\rangle$ , and the second corresponds to an ensemble in which half of the elements are in the state  $|+x\rangle$  and half in the state  $|-x\rangle$ . These ensembles are different, but they are described by the same density matrix.

In the second example, we define the states

$$|u_{\pm}\rangle = \frac{1}{\sqrt{4 \pm 2\sqrt{2}}} \left[ (\sqrt{2} \pm 1)|0\rangle \pm |1\rangle \right]. \quad (2.23)$$

Then

$$\rho = \frac{1}{2}(|0\rangle\langle 0| + |+x\rangle\langle +x|) = \left( \frac{1}{2} + \frac{\sqrt{2}}{4} \right) \left( |u_+\rangle\langle u_+| + \left( \frac{1}{2} - \frac{\sqrt{2}}{4} \right) |u_-\rangle\langle u_-| \right), \quad (2.24)$$

again describing two different ensembles by the same density matrix.

In general, if  $\rho_1$  and  $\rho_2$  are density matrices, so is

$$\rho(\theta) = \theta \rho_1 + (1 - \theta) \rho_2, \quad (2.25)$$

where  $0 \leq \theta \leq 1$ . This implies that the set of density matrices is convex. Most density matrices can be expressed as a sum of other density matrices in many different ways, and each of these decompositions will, in general, correspond to a different ensemble. The two examples above were just special cases of this general statement. This, however, is not true for pure states; they have a unique

decomposition. To see this suppose that  $\rho = |\psi\rangle\langle\psi|$  is a pure state density matrix and that it can also be expressed as a convex sum of two other density matrices,  $\rho(\theta) = \theta\rho_1 + (1 - \theta)\rho_2$ . Then if  $|\psi_\perp\rangle$  satisfies  $\langle\psi_\perp|\psi\rangle = 0$ , then

$$0 = \langle\psi_\perp|\rho(\theta)|\psi_\perp\rangle = \theta\langle\psi_\perp|\rho_1|\psi_\perp\rangle + (1 - \theta)\langle\psi_\perp|\rho_2|\psi_\perp\rangle. \quad (2.26)$$

Since both terms on the right-hand side are  $\geq 0$ , it follows that

$$\langle\psi_\perp|\rho_1|\psi_\perp\rangle = \langle\psi_\perp|\rho_2|\psi_\perp\rangle = 0. \quad (2.27)$$

This equation is true for any vector orthogonal to  $|\psi\rangle$ . Therefore,  $\rho_1 = \rho_2 = |\psi\rangle\langle\psi|$  and the representation of any pure state is unique. Pure states cannot be expressed as a sum of other density matrices. These are the only states with this property, because if  $\rho$  is mixed, it is given by  $\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$ , which is just a convex sum of pure states.

## 2.4 Pure State Decompositions and the Ensemble Interpretation

Next we turn our attention to the ways in which a density matrix can be decomposed into pure states. The main result is summarized in the following:

**Theorem.**  $\rho$  can be expressed as  $\sum_i p_i |\psi_i\rangle\langle\psi_i|$  and  $\sum_i q_i |\phi_i\rangle\langle\phi_i|$  iff

$$\sqrt{p_i}|\psi_i\rangle = \sum_j U_{ij}\sqrt{q_j}|\phi_j\rangle,$$

where  $U_{ij}$  is a unitary matrix and we “pad” whichever set of vectors is smaller with additional 0 vectors so that the sets have the same number of elements.

*Proof.* Let  $|\tilde{\psi}_i\rangle = \sqrt{p_i}|\psi_i\rangle$  and  $|\tilde{\phi}_i\rangle = \sqrt{q_i}|\phi_i\rangle$ . We first prove the if part, meaning that the condition is sufficient. To this end we suppose  $|\tilde{\psi}_j\rangle = \sum_i U_{ij}|\tilde{\phi}_i\rangle$  for  $U_{ij}$  unitary. Then

$$\begin{aligned} \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| &= \sum_{i,j,k} U_{ij}U_{ik}^* |\tilde{\phi}_j\rangle\langle\tilde{\phi}_k| = \sum_{j,k} \left( \sum_i U_{ki}^\dagger U_{ij} \right) |\tilde{\phi}_j\rangle\langle\tilde{\phi}_k| \\ &= \sum_{j,k} \delta_{jk} |\tilde{\phi}_j\rangle\langle\tilde{\phi}_k| = \sum_j |\tilde{\phi}_j\rangle\langle\tilde{\phi}_j|. \end{aligned} \quad (2.28)$$

To prove the only if part, that the condition is also necessary, is considerably more work. We now suppose

$$\rho = \sum_i^{N_1} |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum_i^{N_2} |\tilde{\phi}_i\rangle\langle\tilde{\phi}_i|, \quad (2.29)$$

and assume  $N_1 \geq N_2$ . Since  $\rho$  is a positive operator, it has the spectral representation

$$\rho = \sum_{k=1}^{N_k} \lambda_k |k\rangle\langle k| = \sum_{k=1}^{N_k} |\tilde{k}\rangle\langle\tilde{k}|, \quad (2.30)$$

where  $\langle k|k'\rangle = \delta_{k,k'}$  and  $|\tilde{k}\rangle = \sqrt{\lambda_k}|k\rangle$ . First, we want to show that  $|\tilde{\psi}_i\rangle$  lies in the subspace spanned by  $\{|k\rangle\}$ . To do this, let  $\mathcal{H}_k$  denote the space spanned by  $\{|k\rangle\}$ . Suppose  $|\psi\rangle \in \mathcal{H}_k^\perp$ , then

$$\langle\psi|\rho|\psi\rangle = 0 = \sum_{i=1}^{N_1} |\langle\tilde{\psi}_i|\psi\rangle|^2. \quad (2.31)$$

From here  $\langle\tilde{\psi}_i|\psi\rangle = 0$  follows and so  $|\tilde{\psi}_i\rangle \in (\mathcal{H}_k^\perp)^\perp = \mathcal{H}_k$ . Therefore, we can express  $|\tilde{\psi}_i\rangle$  as

$$|\tilde{\psi}_i\rangle = \sum_{k=1}^{N_k} c_{ik} |\tilde{k}\rangle. \quad (2.32)$$

We can use this representation in Eq. (2.29) to obtain

$$\rho = \sum_{i=1}^{N_1} |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum_{k,k'=1}^{N_k} \left( \sum_{i=1}^{N_1} c_{ik} c_{ik'}^* \right) |\tilde{k}\rangle\langle\tilde{k}'| = \sum_{k=1}^{N_k} |\tilde{k}\rangle\langle\tilde{k}|. \quad (2.33)$$

Since the operators  $|\tilde{k}\rangle\langle\tilde{k}'|$  are linearly independent we have that  $\sum_{i=1}^{N_1} c_{ik} c_{ik'}^* = \delta_{kk'}$ . Thus  $c_{ik}$  form  $N_k$  orthogonal vectors of dimension  $N_1$  and  $N_1 \geq N_k$ . In other words,  $c_{ik}$  ( $k = 1, \dots, N_k$ ) form the first  $N_k$  columns of a matrix containing  $N_1$  rows that can be extended to an  $N_1 \times N_1$  unitary matrix in the following way. Find  $N_1 - N_k$  orthonormal vectors of dimension  $N_1$  that are orthogonal to the vectors  $c_{ik}$  and call them  $c'_{ik}$ , where  $i = 1, \dots, N_1$  and  $k = N_k + 1, \dots, N_1$ . Obviously, the matrix

$$C_{ik} \equiv \begin{cases} c_{ik} & \text{for } k = 1, \dots, N_k \\ c'_{ik} & \text{for } k = N_k + 1, \dots, N_1 \end{cases} \quad (2.34)$$

for  $i = 1, \dots, N_1$  is an  $N_1 \times N_1$  unitary matrix. If we introduce the vectors

$$\begin{pmatrix} |\tilde{\psi}\rangle \end{pmatrix} = \begin{pmatrix} |\tilde{\psi}_1\rangle \\ \vdots \\ |\tilde{\psi}_{N_1}\rangle \end{pmatrix}, \quad (2.35)$$

and

$$\begin{pmatrix} |\tilde{k}_{N_1}\rangle \end{pmatrix} = \begin{pmatrix} |\tilde{k}_1\rangle \\ \vdots \\ |\tilde{k}_{N_k}\rangle \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad (2.36)$$

where the last  $N_1 - N_k$  elements of  $(|\tilde{k}_{N_1}\rangle)$  are 0, we can write

$$\begin{pmatrix} |\tilde{\psi}\rangle \end{pmatrix} = \begin{pmatrix} \ddots & & \\ & C_{ik} & \\ & & \ddots \end{pmatrix} \begin{pmatrix} |\tilde{k}_{N_1}\rangle \end{pmatrix}, \quad (2.37)$$

or, formally,

$$|\tilde{\psi}\rangle = C|\tilde{k}_{N_1}\rangle. \quad (2.38)$$

In an entirely similar way, we can show that  $|\tilde{\phi}_i\rangle$  also lies in the subspace spanned by  $\{|k\rangle\}$ . Therefore, we can express  $|\tilde{\phi}_i\rangle$  as

$$|\tilde{\phi}_i\rangle = \sum_{k=1}^{N_k} d_{ik} |\tilde{k}\rangle. \quad (2.39)$$

We can use this representation in Eq. (2.29) to obtain

$$\rho = \sum_{i=1}^{N_2} |\tilde{\phi}_i\rangle \langle \tilde{\phi}_i| = \sum_{k,k'=1}^{N_k} \left( \sum_{i=1}^{N_2} d_{ik} d_{ik'}^* \right) |\tilde{k}\rangle \langle \tilde{k}'| = \sum_{k=1}^{N_k} |\tilde{k}\rangle \langle \tilde{k}|. \quad (2.40)$$

Since the operators  $|\tilde{k}\rangle \langle \tilde{k}'|$  are linearly independent we have that  $\sum_{i=1}^{N_2} d_{ik} d_{ik'}^* = \delta_{kk'}$ . Thus  $d_{ik}$  form  $N_k$  orthogonal vectors of dimension  $N_2$  and  $N_1 \geq N_2 \geq N_k$ . In other words,  $d_{ik}$  ( $k = 1, \dots, N_k$ ) form the first  $N_k$  columns of a matrix containing  $N_2$  rows that can be extended to an  $N_2 \times N_2$  unitary matrix in the following way. Find  $N_2 - N_k$  orthonormal vectors of dimension  $N_2$  that are orthogonal to the vectors  $d_{ik}$  and call them  $d'_{ik}$ , where  $i = 1, \dots, N_2$  and  $k = N_k + 1, \dots, N_1$ . Obviously, the matrix

$$D'_{ik} \equiv \begin{cases} d_{ik} & \text{for } k = 1, \dots, N_k \\ d'_{ik} & \text{for } k = N_k + 1, \dots, N_2 \end{cases} \quad (2.41)$$

for  $i = 1, \dots, N_2$  is an  $N_2 \times N_2$  unitary matrix. Then we introduce the vector

$$\begin{pmatrix} |\tilde{\phi}\rangle \end{pmatrix} = \begin{pmatrix} |\tilde{\phi}_1\rangle \\ \vdots \\ |\tilde{\phi}_{N_2}\rangle \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad (2.42)$$



where the last  $N_1 - N_2$  elements are 0 and unitarily extend  $D'_{ik}$  into an  $N_1 \times N_1$  matrix  $D_{ik}$  by the following definition:

$$D = \begin{pmatrix} \ddots & & & \\ & D'_{ik} & & 0 \\ & & \ddots & \\ 0 & & & I \end{pmatrix}, \quad (2.43)$$

so that it is Eq. (2.41) for the first  $N_2$  dimensions and identity for the remaining  $N_1 - N_2$  dimensions. With these definitions we can now write

$$\begin{pmatrix} |\tilde{\phi}\rangle \end{pmatrix} = \begin{pmatrix} \ddots & & & \\ & D'_{ik} & & 0 \\ & & \ddots & \\ 0 & & & I \end{pmatrix} \begin{pmatrix} |\tilde{k}_{N_1}\rangle \end{pmatrix}, \quad (2.44)$$

or, formally,

$$|\tilde{\phi}\rangle = D|\tilde{k}_{N_1}\rangle. \quad (2.45)$$

Comparing Eqs. (2.38) and (2.45), we finally obtain

$$|\tilde{\psi}\rangle = CD^\dagger|\tilde{\phi}\rangle. \quad (2.46)$$

Since the matrix  $U = CD^\dagger$  is unitary by construction, this completes the proof.  $\square$

## 2.5 A Mathematical Aside: The Schmidt Decomposition of a Bipartite State

In the previous section we have looked at the possible decompositions of the density matrix in terms of convex sums of pure state density matrices. The decomposition is not unique, but the possible decompositions of the same density matrix are connected via the theorem proved in the previous section. Namely, the renormalized pure states, with appropriate zero vectors included if their numbers are different, are connected via a unitary transformation. Each of these decompositions gives rise to a different ensemble interpretation. The ensembles are not unique, but the various decompositions cannot be discriminated.

In this section we want to take a look at the other possible interpretation in which the mixed state density matrix emerges as the state of the subsystem of a larger system that itself is in a pure state. Therefore, we now examine the different ways

in which a given density matrix  $\rho$  can be represented as the reduced density matrix for part of a pure bipartite state. To do this, we first need to derive the Schmidt decomposition of a bipartite state.

Let  $|\psi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$ , and  $\{|u_i\rangle_A\}$  be an orthonormal basis for  $\mathcal{H}_A$  and  $\{|v_j\rangle_B\}$  be an orthonormal basis for  $\mathcal{H}_B$ . Then an arbitrary bipartite state can be expanded as a double sum over the product basis  $\{|u_i\rangle|v_j\rangle\}$ , as

$$|\psi\rangle_{AB} = \sum_{i,j} c_{ij} |u_i\rangle_A |v_j\rangle_B. \quad (2.47)$$

It is easy to see that this double sum expression can be written as a single sum,

$$|\psi\rangle_{AB} = \sum_i |u_i\rangle |\tilde{v}_i\rangle_B, \quad (2.48)$$

where we introduced  $|\tilde{v}_i\rangle = \sum_j c_{ij} |v_j\rangle_B$ . The price to pay is that  $\{|\tilde{v}_i\rangle_B\}$  are not, in general, orthonormal. Therefore, it is somewhat surprising that for bipartite states, there exists a single sum expansion where only diagonal elements of a product basis,  $\{|u_i\rangle|w_i\rangle\}$ , enter.

In order to show this, suppose that  $\{|u_i\rangle\}$  is the basis in which  $\rho_A = \text{Tr}_B(|\psi\rangle_{AB} \langle \psi|)$  is diagonal,

$$\rho_A = \sum_i \lambda_i |u_i\rangle \langle u_i|, \quad (2.49)$$

where  $0 \leq \lambda_i \leq 1$ . But we also have

$$\rho_A = \text{Tr}_B[\sum_{(i,j)} (|u_i\rangle_A |\tilde{v}_i\rangle_B) ({}_A\langle u_j| {}_B\langle \tilde{v}_j|)] = \sum_{(i,j)} {}_B\langle \tilde{v}_j | \tilde{v}_i \rangle_B |u_i\rangle_A \langle u_j|. \quad (2.50)$$

Therefore, we must have  ${}_B\langle \tilde{v}_j | \tilde{v}_i \rangle_B = \delta_{ij} \lambda_i$  and hence  $\{|\tilde{v}_i\rangle\}$  are orthogonal.

Let  $\{|u_i\rangle_A \mid i = 1, \dots, N, \text{ where } N \leq \dim \mathcal{H}_A\}$  correspond to nonzero values of  $\lambda_i$  and set  $|w_i\rangle_B = \frac{1}{\sqrt{\lambda_i}} |\tilde{v}_i\rangle_B$ . Hence  $\{|w_i\rangle_B\}$  are orthonormal. Then

$$|\psi\rangle_{AB} = \sum_{i=1}^N \sqrt{\lambda_i} |u_i\rangle_A |w_i\rangle_B, \quad (2.51)$$

where  $N \leq \dim \mathcal{H}_A$  and by a similar argument  $N \leq \dim \mathcal{H}_B$ . Note that

$$\rho_B = \text{Tr}_A(|\psi\rangle_{AB} \langle \psi|) = \sum_{i=1}^N \lambda_i |w_i\rangle_B \langle w_i|, \quad (2.52)$$

so that  $\{|w_i\rangle\}$  are eigenstates of  $\rho_B$  having nonzero eigenvalues and  $\rho_A$  and  $\rho_B$  have the same nonzero eigenvalues. The double sum expansion in Eq. (2.47) always exists. It is somewhat surprising that the single sum expansion of Eq. (2.51), in terms of orthonormal basis vectors, also exists for bipartite systems. This later is called the Schmidt decomposition.

## 2.6 Purification, Reduced Density Matrices, and the Subsystem Interpretation

Equipped with the Schmidt decomposition, we now look at purifications. Suppose, we have a density matrix

$$\rho_A = \sum_{i=1}^N p_i |\psi_i\rangle_{AA} \langle \psi_i|, \quad (2.53)$$

where  $|\psi_i\rangle \in \mathcal{H}_A$ . We want to find a state  $|\Phi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$  on a larger space so that

$$\rho_A = \text{Tr}_B(|\Phi\rangle_{AB} \langle \Phi|). \quad (2.54)$$

$|\Phi\rangle_{AB}$  is called a purification of  $\rho_A$ .

One way to do this is to choose  $\dim(\mathcal{H}_B) \geq N$  and let  $\{|u_i\rangle\}$  be an orthonormal basis for  $\mathcal{H}_B$ . Then

$$|\Phi\rangle_{AB} = \sum_i \sqrt{p_i} |\psi_i\rangle_A |u_i\rangle_B \quad (2.55)$$

is called a purification of  $\rho_A$ .

Purifications are not unique. But if two purifications are in the same Hilbert space, we can still say something about their mutual relationship. Suppose we have two different states,  $|\Phi_1\rangle_{AB}$  and  $|\Phi_2\rangle_{AB}$ , both of which are in  $\mathcal{H}_A \otimes \mathcal{H}_B$  and both of which are purifications of  $\rho_A$ . How are they related? To answer this question, we use the Schmidt decomposition,  $|\Phi_1\rangle_{AB} = \sum_k \sqrt{\lambda_k} |u_k\rangle_A |v_k\rangle_B$  and  $|\Phi_2\rangle_{AB} = \sum_k \sqrt{\lambda_k} |u_k\rangle_A |w_k\rangle_B$ . A part of both states, eigenvalues and eigenvectors of  $\rho_A$ , is the same.  $\{|v_k\rangle_B\}$  and  $\{|w_k\rangle_B\}$  form orthonormal sets, so there is at least one unitary operator on  $\mathcal{H}_B$ , which we call  $U_B$ , such that

$$|w_k\rangle_B = U_B |v_k\rangle_B. \quad (2.56)$$

Then  $|\Phi_2\rangle_{AB} = (I_A \otimes U_B) |\Phi_1\rangle_{AB}$ .

## 2.7 Problems

1. This problem combines elements from Chaps. 1 and 2 as it uses circuits with mixed states. We shall consider a complicated quantum circuit, one consisting of three qubits and four C-NOT gates. One of its uses is as a “quantum cloner.” The operator for this circuit is given by  $U = D_{ca} D_{ba} D_{ac} D_{ab}$  (remember that  $D_{ab}$  is a C-NOT gate with  $a$  as the control qubit and  $b$  as the target qubit).

(a) Find  $U(|\psi\rangle_a |\Psi_+\rangle_{bc})$ , where

$$|\Psi_+\rangle_{bc} = \frac{1}{\sqrt{2}}(|0\rangle_b |0\rangle_c + |1\rangle_b |1\rangle_c),$$

and  $U(|\psi\rangle_a |0\rangle_b |x\rangle_c)$ . What you should find is that in the first case  $|\psi\rangle$  comes out of output  $a$  and in the second case it comes out of output  $b$ .

(b) Now find

$$|\Phi\rangle_{abc} = U|\psi\rangle_a(c_1|\Psi_+\rangle_{bc} + c_2|0\rangle_b|x\rangle_c),$$

and find the condition on the constants  $c_1$  and  $c_2$  so that the input state is normalized. The idea here is that by combining the effects of the two input states in part (a), some of the information about  $|\psi\rangle$  will end up in qubit  $a$  and some will end up in qubit  $b$ . How much ends up in each qubit depends on the values of  $c_1$  and  $c_2$ .

(c) Find the reduced density matrixes for the outputs of qubits  $a$  and  $b$ , i.e., find

$$\rho_a = \text{Tr}_{bc}(|\Phi\rangle_{abc}\langle\Phi|) \quad \rho_b = \text{Tr}_{ac}(|\Phi\rangle_{abc}\langle\Phi|)$$

In both cases your answer should be of the form

$$\rho = s|\psi\rangle\langle\psi| + \frac{1-s}{2}I,$$

where  $0 \leq s \leq 1$ . Find  $s$  in the case that  $\rho_a = \rho_b$ . Notice that what this device does is to produce two imperfect copies of the state  $|\psi\rangle$ .

2. The Schmidt representation for states of a bipartite system is extremely convenient, and so it is natural to ask if such a representation exists for tripartite systems. Unfortunately, the answer is no. Show that there exist three-qubit states that cannot be written in the form

$$|\Psi\rangle_{abc} = \sum_{j=0}^1 \sqrt{\lambda_j} |u_j\rangle_a |v_j\rangle_b |w_j\rangle_c,$$

where  $\{u_j|j=0,1\}$ ,  $\{v_j|j=0,1\}$ , and  $\{w_j|j=0,1\}$  are orthonormal bases.

3. Suppose that Alice can prepare a density matrix only in the computational basis. She prepares a bipartite state of the form

$$\rho = \sum_{j,k=0}^1 p_{jk} |j\rangle\langle j| \otimes |k\rangle\langle k|.$$

She sends one qubit to Bob and one qubit to Charlie. If Bob and Charlie do not measure in the computational basis, the correlations they can obtain are limited. Show that if they measure in the  $|\pm x\rangle$  basis their results will be uncorrelated, that is, they are equally likely to get the same result as opposite results.

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