

Chapter 2

The Reduced Density Matrix

We introduce the concept of reduced density matrix in the context of open quantum systems. We describe the general structure for operations on density matrices, which are distilled in the Kraus-Stinespring theorem. We show possible applications in the framework of two-level systems.

2.1 Open Quantum Systems, Partial Trace and the Reduced Density Matrix

One of the most important applications of the density matrix formalism is the description of the dynamics of a subsystem of a larger composite system, where one considers the interaction between the former and the later. This is called an open quantum system.

More formally, consider two quantum systems \mathcal{A} and \mathcal{B} , with associated Hilbert spaces $\mathbb{H}_{\mathcal{A}}$ and $\mathbb{H}_{\mathcal{B}}$, whose dimensions are respectively N and M . Let $\{|\phi_n^{\mathcal{A}}\rangle\}_{n=1}^N$ be a basis of $\mathbb{H}_{\mathcal{A}}$ and $\{|\phi_m^{\mathcal{B}}\rangle\}_{m=1}^M$ a basis of $\mathbb{H}_{\mathcal{B}}$. The Hilbert space associated to the composite system \mathcal{AB} is the tensor product space $\mathbb{H}_{\mathcal{A}} \otimes \mathbb{H}_{\mathcal{B}}$ of dimension $N \cdot M$, and a natural basis is the tensor product basis $\{|\phi_{nm}^{\mathcal{AB}}\rangle = |\phi_n^{\mathcal{A}}\rangle \otimes |\phi_m^{\mathcal{B}}\rangle\}_{n,m}$.

The statistical operator describing the state of the composite system has the general form

$$\hat{\rho}_{\mathcal{AB}} = \sum_{nmk\ell} \rho_{nm}^{k\ell} |\phi_{nm}^{\mathcal{AB}}\rangle \langle \phi_{k\ell}^{\mathcal{AB}}|, \quad (2.1)$$

and it can be represented by a $(N \cdot M) \times (N \cdot M)$ square density matrix with matrix elements $\rho_{nm}^{k\ell}$.

Suppose — and this is the crucial point in what follows — that we are interested only in the properties of subsystem \mathcal{A} . For example, this can be motivated by the fact that one cannot control or one does not have direct access to system \mathcal{B} . Then, the observable quantities we are interested in have the following form

$$\hat{A} \otimes \hat{\mathbb{1}}_{\mathcal{B}}, \quad (2.2)$$

where \hat{A} is an Hermitian operator pertaining to system \mathcal{A} , and $\hat{\mathbb{1}}_{\mathcal{B}}$ is the identity for system \mathcal{B} . The expectation value is:

$$\langle \hat{A} \rangle = \langle \hat{A} \otimes \hat{\mathbb{1}}_{\mathcal{B}} \rangle = \text{Tr} \left[(\hat{A} \otimes \hat{\mathbb{1}}_{\mathcal{B}}) \hat{\rho}_{\mathcal{AB}} \right] = \sum_n \langle \phi_n^{\mathcal{A}} | \hat{A} \left[\sum_m \langle \phi_m^{\mathcal{B}} | \hat{\rho}_{\mathcal{AB}} | \phi_m^{\mathcal{B}} \rangle \right] | \phi_n^{\mathcal{A}} \rangle, \quad (2.3)$$

where, in the last equality, we explicitly used the form in Eq. (2.2). The above relation can be written as:

$$\langle \hat{A} \rangle = \text{Tr}^{(\mathcal{A})} \left[\hat{A} \hat{\rho}^{(\mathcal{A})} \right], \quad (2.4)$$

where we defined the reduced density matrix

$$\hat{\rho}^{(\mathcal{A})} = \text{Tr}^{(\mathcal{B})} [\hat{\rho}_{\mathcal{AB}}] = \sum_m \langle \phi_m^{\mathcal{B}} | \hat{\rho}_{\mathcal{AB}} | \phi_m^{\mathcal{B}} \rangle, \quad (2.5)$$

and $\text{Tr}^{(\mathcal{B})} [\cdot]$ denotes the partial trace with respect to system \mathcal{B} .

In more formal terms, given the density matrix $\hat{\rho}_{\mathcal{AB}}$ acting on $\mathbb{H}_{\mathcal{AB}}$ as in Eq. (2.1), the partial trace with respect to \mathcal{B} is the map defined as

$$\text{Tr}^{(\mathcal{B})} [\cdot] : \hat{\rho}_{\mathcal{AB}} = \sum_{nmk\ell} \rho_{nm}^{k\ell} |\phi_{nm}^{\mathcal{AB}}\rangle \langle \phi_{k\ell}^{\mathcal{AB}}| \rightarrow \hat{\rho}^{(\mathcal{A})} = \sum_{nk} \sum_m \rho_{nm}^{km} |\phi_n^{\mathcal{A}}\rangle \langle \phi_k^{\mathcal{A}}|. \quad (2.6)$$

Contrary to the usual trace, which maps a square matrix into a number, the partial trace maps a density matrix of higher dimensionality into a density matrix of lower dimensionality. In our case, a density matrix of dimension $N \cdot M$, relative to the system \mathcal{AB} , into a density matrix of dimension N , relative to system \mathcal{A} alone. It can be easily shown that the above definition does not depend on the choice of basis $\{ |\phi_{nm}^{\mathcal{AB}}\rangle = |\phi_n^{\mathcal{A}}\rangle \otimes |\phi_m^{\mathcal{B}}\rangle \}_{n,m}$ or $\{ |\phi_m^{\mathcal{B}}\rangle \}_m$.

In order for $\hat{\rho}^{(\mathcal{A})}$ in Eq. (2.6) to represent a valid (reduced) density matrix, it should be a linear, positive operator with trace equal to 1. Linearity is obvious from the definition. Positivity is easily checked; given an arbitrary state $|\psi_{\mathcal{A}}\rangle \in \mathbb{H}_{\mathcal{A}}$:

$$\begin{aligned} \langle \psi_{\mathcal{A}} | \hat{\rho}^{(\mathcal{A})} | \psi_{\mathcal{A}} \rangle &= \langle \psi_{\mathcal{A}} | \text{Tr}^{(\mathcal{B})} [\hat{\rho}_{\mathcal{AB}}] | \psi_{\mathcal{A}} \rangle, \\ &= \sum_m \langle \psi_{\mathcal{A}} | \langle \phi_m^{\mathcal{B}} | \hat{\rho}_{\mathcal{AB}} | \phi_m^{\mathcal{B}} \rangle | \psi_{\mathcal{A}} \rangle \geq 0, \end{aligned} \quad (2.7)$$

since $\hat{\rho}_{\mathcal{AB}}$ is a positive operator. The trace of $\hat{\rho}^{(\mathcal{A})}$ is:

$$\begin{aligned} \text{Tr}^{(\mathcal{A})} [\hat{\rho}^{(\mathcal{A})}] &= \sum_n \langle \phi_n^{\mathcal{A}} | \hat{\rho}^{(\mathcal{A})} | \phi_n^{\mathcal{A}} \rangle = \sum_n \langle \phi_n^{\mathcal{A}} | \text{Tr}^{(\mathcal{B})} [\hat{\rho}_{\mathcal{AB}}] | \phi_n^{\mathcal{A}} \rangle, \\ &= \sum_{nm} \langle \phi_n^{\mathcal{A}} | \langle \phi_m^{\mathcal{B}} | \hat{\rho}_{\mathcal{AB}} | \phi_m^{\mathcal{B}} \rangle | \phi_n^{\mathcal{A}} \rangle = \text{Tr} [\hat{\rho}_{\mathcal{AB}}] = 1. \end{aligned} \quad (2.8)$$

This justifies the term reduced density matrix for $\hat{\rho}^{(\mathcal{A})}$.

Example 2.1

Let us consider a factorized state for \mathcal{A} and \mathcal{B} :

$$\hat{\rho}_{\mathcal{AB}} = \hat{\rho}_{\mathcal{A}} \otimes \hat{\rho}_{\mathcal{B}}.$$

Then, the partial trace with respect to \mathcal{B} gives:

$$\hat{\rho}^{(\mathcal{A})} = \text{Tr}^{(\mathcal{B})} [\hat{\rho}_{\mathcal{AB}}] = \text{Tr}^{(\mathcal{B})} [\hat{\rho}_{\mathcal{A}} \otimes \hat{\rho}_{\mathcal{B}}] = \hat{\rho}_{\mathcal{A}} \cdot \text{Tr}^{(\mathcal{B})} [\hat{\rho}_{\mathcal{B}}] = \hat{\rho}_{\mathcal{A}}.$$

As it will become clearer in what follows, the reduced density matrix is meant to encode the information about system \mathcal{A} , when system \mathcal{B} is not accessible. The previous example confirms this: when \mathcal{A} and \mathcal{B} are uncorrelated, i.e. their states are factorized, the reduced density matrix $\hat{\rho}^{(\mathcal{A})}$ returns the density matrix $\hat{\rho}_{\mathcal{A}}$ of system \mathcal{A} . A more interesting case is when \mathcal{A} and \mathcal{B} are entangled, as the following example shows.

Example 2.2

Let us consider two qubits \mathcal{A} and \mathcal{B} , in the following entangled state:

$$|\psi_+\rangle = \frac{|0_{\mathcal{A}}\rangle |0_{\mathcal{B}}\rangle + |1_{\mathcal{A}}\rangle |1_{\mathcal{B}}\rangle}{\sqrt{2}}.$$

The associated density matrix $\hat{\rho}_{\mathcal{AB}}$ is

$$\begin{aligned}\hat{\rho}_{\mathcal{AB}} &= |\psi_+\rangle \langle \psi_+|, \\ &= \frac{1}{2} [|0_{\mathcal{A}}\rangle |0_{\mathcal{B}}\rangle \langle 0_{\mathcal{A}}| \langle 0_{\mathcal{B}}| + |0_{\mathcal{A}}\rangle |0_{\mathcal{B}}\rangle \langle 1_{\mathcal{A}}| \langle 1_{\mathcal{B}}| + |1_{\mathcal{A}}\rangle |1_{\mathcal{B}}\rangle \langle 0_{\mathcal{A}}| \langle 0_{\mathcal{B}}| + |1_{\mathcal{A}}\rangle |1_{\mathcal{B}}\rangle \langle 1_{\mathcal{A}}| \langle 1_{\mathcal{B}}|].\end{aligned}$$

Then, the partial trace over qubit \mathcal{B} returns the following reduced density matrix for qubit \mathcal{A} :

$$\begin{aligned}\hat{\rho}^{(\mathcal{A})} &= \text{Tr}^{(\mathcal{B})} [\hat{\rho}_{\mathcal{AB}}] = \langle 0_{\mathcal{B}} | \hat{\rho}_{\mathcal{AB}} | 0_{\mathcal{B}} \rangle + \langle 1_{\mathcal{B}} | \hat{\rho}_{\mathcal{AB}} | 1_{\mathcal{B}} \rangle, \\ &= \frac{1}{2} [|0_{\mathcal{A}}\rangle \langle 0_{\mathcal{A}}| + |1_{\mathcal{A}}\rangle \langle 1_{\mathcal{A}}|] = \frac{1}{2} \hat{\mathbb{1}}_{\mathcal{A}}.\end{aligned}$$

In the example above, the two qubits \mathcal{A} and \mathcal{B} are in a pure state $\hat{\rho}_{\mathcal{AB}}$, while the reduced density matrix $\hat{\rho}^{(\mathcal{A})}$ of qubit \mathcal{A} represents a statistical mixture (the same is true for the reduced density matrix $\hat{\rho}^{(\mathcal{B})}$ of qubit \mathcal{B}). This shows that the partial trace can transform pure states into statistical mixtures, a property with far reaching consequences, which in many respects is the essence of the theory of open quantum systems.

Equation (2.4) states a very important property: when computing physical predictions regarding subsystem \mathcal{A} alone, neglecting \mathcal{B} , it is not necessary to consider the full density matrix $\hat{\rho}_{\mathcal{AB}}$; it is sufficient to consider the smaller reduced density matrix $\hat{\rho}^{(\mathcal{A})}$. In other words, $\hat{\rho}^{(\mathcal{A})}$ contains all physical information about subsystem \mathcal{A} , when we are not interested in the properties of subsystem \mathcal{B} , which is expressed by the mathematical fact that the observables have the form $\hat{A} \otimes \hat{\mathbb{1}}_{\mathcal{B}}$. It is also important to remark that what said above holds true only if observations are limited to the system \mathcal{A} alone. This is not the only possibility. It is always possible, at least in principle, to consider both systems and measure correlations among them. To do this, the full density matrix $\hat{\rho}_{\mathcal{AB}}$ is needed. Indeed, the physical predictions cannot be derived only from the two reduced density matrices $\hat{\rho}^{(\mathcal{A})}$ and $\hat{\rho}^{(\mathcal{B})}$.

We conclude the section by showing that the partial trace is the only way of defining a physically appropriate reduced density matrix. The result is contained in the following theorem.

Theorem 2.1. *Consider two quantum systems \mathcal{A} and \mathcal{B} , with associated Hilbert spaces $\mathbb{H}_{\mathcal{A}}$ and $\mathbb{H}_{\mathcal{B}}$ respectively, whose dimensions are N and M . Consider a generic map between the space of density matrices of the composite systems \mathcal{AB} , and the space of density matrices of the subsystem \mathcal{A} :*

$$\hat{\rho}_{\mathcal{AB}} \rightarrow F(\hat{\rho}_{\mathcal{AB}}), \quad (2.9)$$

such that, for any observable \hat{A} of \mathcal{A} :

$$\text{Tr}^{(\mathcal{A})} [\hat{A} F(\hat{\rho}_{\mathcal{AB}})] = \text{Tr} [(\hat{A} \otimes \hat{\mathbb{1}}_{\mathcal{B}}) \hat{\rho}_{\mathcal{AB}}]. \quad (2.10)$$

Then, the map $F(\hat{\rho}_{\mathcal{AB}})$ is unique and corresponds to the partial trace defined in Eq. (2.5), i.e. $F(\hat{\rho}_{\mathcal{AB}}) = \hat{\rho}^{(\mathcal{A})}$, with $\hat{\rho}^{(\mathcal{A})}$ being the reduced density matrix.

Proof. The space of the bounded Hermitian operators is a Hilbert-Schmidt space $\mathbb{B}(\mathbb{H})$ associated to the Hilbert space \mathbb{H} , where \mathbb{B} stands for bounded operators space. $\mathbb{B}(\mathbb{H})$ is defined as

$$\mathbb{B}(\mathbb{H}) = \mathbb{H} \otimes \mathbb{H}^*,$$

where \mathbb{H}^* is the dual Hilbert space associated to \mathbb{H} . In $\mathbb{B}(\mathbb{H})$ the inner product is defined as

$$\langle X, Y \rangle = \text{Tr} [XY],$$

Let $\{M_n\}_n$ be a basis of $\mathbb{B}(\mathbb{H}_{\mathcal{A}})$, so we can decompose $F(\hat{\rho}_{\mathcal{AB}})$ with respect to this basis:

$$F(\hat{\rho}_{\mathcal{AB}}) = \sum_n \hat{M}_n \text{Tr} [\hat{M}_n F(\hat{\rho}_{\mathcal{AB}})]. \quad (2.11)$$

Then, Eq. (2.10) sets $\text{Tr}^{(A)} [\hat{M}_n F(\hat{\rho}_{AB})] = \text{Tr} [(\hat{M}_n \otimes \hat{\mathbb{1}}_B) \hat{\rho}_{AB}]$ and we can write:

$$F(\hat{\rho}_{AB}) = \sum_n \hat{M}_n \text{Tr} [(\hat{M}_n \otimes \hat{\mathbb{1}}_B) \hat{\rho}_{AB}]. \quad (2.12)$$

Therefore, given the basis $\{\hat{M}_n\}_n$, the coefficients $\text{Tr} [(\hat{M}_n \otimes \hat{\mathbb{1}}_B) \hat{\rho}_{AB}]$ are uniquely identified by $\hat{\rho}_{AB}$, which in turn uniquely identify the map $F(\hat{\rho}_{AB})$. Clearly, the mapping is independent from the chosen basis. By construction, Eq. (2.10) is satisfied for any operator \hat{A} . We have proved that the map $F(\hat{\rho}_{AB})$ satisfying Eq. (2.10) is unique. The partial trace defined in Eq. (2.5) satisfies Eq. (2.10), and therefore it is the only map with this property.