Principles of Quantum Mechanics Pt. 5

PHYS 500 - Southern Illinois University

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The Partial Trace

The partial trace generates the density operator, or **reduced state**, for a subsystem given the density matrix for the total system:

\[
\rho^{ABC} \rightarrow \begin{cases} 
\rho^A = \text{tr}_{BC}(\rho^{ABC}) & \text{“System } A \text{ reduced state; trace out } B \text{ and } C” \\
\rho^B = \text{tr}_{AC}(\rho^{ABC}) & \text{“System } B \text{ reduced state; trace out } A \text{ and } C” \\
\rho^C = \text{tr}_{AB}(\rho^{ABC}) & \text{“System } C \text{ reduced state; trace out } A \text{ and } B” 
\end{cases}
\]

The partial trace is built from the **partial contraction** map. For a fixed state \( |\varphi\rangle^A \in \mathcal{H}^A \) and tripartite space \( \mathcal{H}^{ABC} \), the partial contraction \( A \langle \varphi | : \mathcal{H}^A \otimes \mathcal{H}^B \otimes \mathcal{H}^C \rightarrow \mathcal{H}^B \otimes \mathcal{H}^C \) is a linear map defined by

\[
A \langle \varphi |(| \psi \rangle^{ABC}) = A \langle \varphi | \left( \sum_i |a_i\rangle^A |\tilde{\psi}_i\rangle^{BC} \right) = \sum_i \langle \varphi |a_i\rangle\langle \tilde{\psi}_i |^{BC}
\]

for arbitrary basis \( \{|a_i\rangle\}_i \) for \( \mathcal{H}^A \) and \( |\psi\rangle^{ABC} = \sum_i |a_i\rangle^A |\tilde{\psi}_i\rangle^{BC} \).
The Partial Trace

Then for an arbitrary operator $T$ acting on $\mathcal{H}^A \otimes \mathcal{H}^B \otimes \mathcal{H}^C$, decompose as

$$T = \sum_{i,j} |a_i\rangle\langle a_j| A \otimes T_{ij}^{BC},$$

where $T_{ij}^{BC}$ is some operator acting on $\mathcal{H}^B \otimes \mathcal{H}^C$.

The $A$ partial trace of $T$, denoted by $\text{tr}_A(T)$, is defined as

$$\sum_{k=1}^{d_A} |a_k\rangle A \left( \sum_{i,j} |a_i\rangle\langle a_j| A \otimes T_{ij}^{BC} \right) |a_k\rangle A = \sum_{i,j} \text{tr}(|a_i\rangle\langle a_j|) T_{ij}^{BC} = \sum_k T_{kk}^{BC}.$$ 

Proposition

It $T$ is a density matrix, then so is $\text{tr}_A(T)$. 
The Partial Trace

Example

Compute $\text{tr}_A \rho^{AB}$ and $\text{tr}_B \rho^{AB}$ for

$$\rho = t_{00,00}|00\rangle \langle 00| + t_{00,01}|00\rangle \langle 01| + t_{01,00}|01\rangle \langle 00| + t_{01,01}|01\rangle \langle 00| + t_{00,10}|00\rangle \langle 10| + t_{00,11}|00\rangle \langle 11| + t_{01,10}|01\rangle \langle 10| + t_{01,11}|01\rangle \langle 10| + t_{10,00}|10\rangle \langle 00| + t_{10,01}|10\rangle \langle 01| + t_{11,00}|11\rangle \langle 00| + t_{11,01}|11\rangle \langle 00| + t_{10,10}|10\rangle \langle 10| + t_{10,11}|10\rangle \langle 11| + t_{11,10}|11\rangle \langle 10| + t_{11,11}|11\rangle \langle 10|. $$
The Partial Trace and Schmidt Decomposition

For bipartite pure states, computing the partial trace is easy once you know the Schmidt decomposition.

For $|\Psi\rangle^{AB} = \sum_i \sqrt{\lambda_i} |\alpha_i\rangle|\beta_i\rangle$, trace out in Schmidt basis:

$$\rho^A = \text{tr}_B \rho^{AB} = \sum_{i=1}^r \lambda_i |\alpha_i\rangle\langle\alpha_i|, \quad \rho^B = \text{tr}_A \rho^{AB} = \sum_{i=1}^r \lambda_i^r |\beta_i\rangle\langle\beta_i|.$$ 

Remarks

1. Schmidt basis vectors are the eigenvectors of $\rho^A$ and $\rho^B$!
2. Schmidt coefficients are eigenvalues of $\rho^A$ and $\rho^B$!
3. $\rho^A$ and $\rho^B$ have the same eigenvalue spectrum!
Purifications

Definition

A **purification** of a mixed state $\rho^S$ acting on $\mathcal{H}^S$ is any pure state $|\psi\rangle^{SA} \in \mathcal{H}^S \otimes \mathcal{H}^A$ for some auxiliary system $A$ such that

$$\rho^S = \text{tr}_A(|\psi\rangle\langle\psi|^S).$$

An easy way to construct a purification:

$$\begin{cases}
\text{Spectral decomposition} & 
\rho^S = \sum_i p_i |v_i\rangle\langle v_i| \iff \text{Purification} \ |\psi\rangle^{SA} = \sum_i \sqrt{p_i} |v_i\rangle^S |i\rangle^A.
\end{cases}$$

Lemma

Purifications are not unique! Two states $|\psi\rangle^{SA}$ and $|\psi'\rangle^{SA}$ purify $\rho^S$ iff

$$|\psi\rangle = I^S \otimes U^A |\psi'\rangle$$

for some unitary $U$ acting on $\mathcal{H}^A$. 


Representing Density Matrices by Different Ensembles

Let $\rho^S = \sum_{i=1}^r p_i |v_i\rangle\langle v_i|$ be a spectral decomposition and $|\psi^{SA}\rangle = \sum_{i=1}^r \sqrt{p_i} |v_i⟩^S |i⟩^A$ a purification, where $\mathcal{H}^A$ has dimension $d_A$.

Apply an arbitrary unitary on $\mathcal{H}^A$:

$$U^A : |i⟩^A \rightarrow |\kappa_i⟩^A = \sum_{j=1}^{d_A} u_{ij} |j⟩^A.$$ 

Then $$(\mathbb{I} \otimes U^A)|\psi⟩^{SA} = \sum_{i=1}^r \sum_{j=1}^{d_A} \sqrt{p_i} u_{ij} |v_i⟩^S |j⟩^A = \sum_{j=1}^{d_A} \sqrt{q_j} |\varphi_j⟩^S |j⟩^A,$$

where $\sqrt{q_j} |\varphi_j⟩ = \sum_{i=1}^r \sqrt{p_i} u_{ij} |v_i⟩$ for $j = 1 \cdots, d_A$. 
Then \( \rho^S = \sum_{i=1}^S p_i |v_i\rangle\langle v_i| = \sum_{i=1}^{d_A} \sqrt{q_i} |\varphi_i\rangle\langle \varphi_i| \).

**Theorem**

Two ensembles \( \mathcal{E}_1 = \{|\psi_i\rangle, p_i\}_{i=1}^{l_1} \) and \( \mathcal{E}_2 = \{|\varphi_i\rangle, q_i\}_{i=1}^{l_2} \) generate the same density matrix iff there exists an \( l_0 \times l_0 \) unitary matrix with elements \( u_{ij} \), where \( l_0 = \max\{l_1, l_2\} \) such that

\[
\sqrt{q_j} \varphi_j = \sqrt{p_i} u_{ij} |\psi_i\rangle \quad \text{for } j = 1 \cdots l_0
\]

**Example**

Consider the two bipartite ensembles \( \mathcal{E}_1 = \{|00\rangle, 1/2\}; (|11\rangle, 1/2) \) and \( \mathcal{E}_2 = \{|\Phi^+\rangle, 1/2\}; (|\Phi^-\rangle, 1/2) \).
The Partial Trace and Generalized Measurements

Let $U$ be any unitary applied to $\mathcal{H}^S \otimes \mathcal{H}^A$, where $A$ is an arbitrary ancilla system. Then we can always decompose

$$U = \sum_{j=1}^{d_A} M_j^S \otimes |j\rangle \langle 0|^A + \hat{U}$$

where $\hat{U} (|\psi\rangle^S |0\rangle^A) = 0$ for all $|\psi\rangle^S \in \mathcal{H}^S$, and $\sum_{j=1}^{d_A} M_j^\dagger M_j 1 = \mathbb{I}^S$.

For an arbitrary $|\psi\rangle^S$ acting on $\mathcal{H}^S$, the unitary evolution is

$$|\psi\rangle^S \otimes |0\rangle^A \rightarrow U \left( |\psi\rangle^S \otimes |0\rangle^A \right) = \sum_{j=1}^{d_A} M_j |\psi\rangle^S |j\rangle^A.$$
Let $\{S_k\}_{k=1}^N$ be a disjoint partitioning of $\{1, 2, \cdots, d_A\}$; i.e. $S_j \cap S_k = \emptyset$ for $j \neq k$ and $\bigcup_k S_k = \{1, 2, \cdots, d_A\}$.

Then $\{P_k\}_{k=1}^N$ is a complete set of orthogonal projectors, where

$$P_k = \sum_{i \in S_k} |i\rangle \langle i|.$$ 

Apply the projective measurement $\{P_k\}$ to system $A$ when entangled with $S$ in state $U(|\psi\rangle^S \otimes |0\rangle^A)$. The transformation is

$$U(|\psi\rangle^S \otimes |0\rangle^A) \rightarrow \frac{1}{\sqrt{p_k}} \sum_{j=1}^{d_A} M_j |\psi\rangle^S \otimes P_k |j\rangle^A = \frac{1}{\sqrt{p_k}} \sum_{j \in S_k} M_j |\psi\rangle^S \otimes |j\rangle^A$$

with probability $p_k = \sum_{j \in S_k} \langle \psi | M_j^\dagger M_j |\psi\rangle$. 

The Partial Trace and Generalized Measurements

Now trace out system $A$:

$$|\psi\rangle\langle\psi| \rightarrow \frac{1}{p_k} \sum_{j\in S_k} M_j |\psi\rangle\langle\psi| M_j^\dagger.$$ 

The completion relation

$$I = \sum_{k=1}^{N} \sum_{j\in S_k} M_j^\dagger M_j$$

implies that

$$\langle\psi|I|\psi\rangle = \sum_{k=1}^{N} \sum_{j\in S_k} \langle\psi|M_j^\dagger M_j|\psi\rangle \geq \sum_{j\in S_k} \langle\psi|M_j^\dagger M_j|\psi\rangle \quad \forall |\psi\rangle, \forall k.$$ 

This is sometimes expressed as the **operator inequality**

$$I \geq \sum_{j\in S_k} M_j^\dagger M_j.$$
Generalized Measurements on the Density Matrix

Suppose that the state of system $S$ is described by an ensemble $\{|\psi_i\rangle, q_i\}$. If this unitary + measurement process is performed on the system, then each $|\psi_i\rangle$ would transform as $|\psi_i\rangle\langle\psi_i| \rightarrow \frac{1}{p_k} \sum_{j \in S_k} M_j |\psi_i\rangle\langle\psi_i| M_j^\dagger$. Hence the ensemble average transforms as

$$\sum_i q_i |\psi_i\rangle\langle\psi_i| \rightarrow \frac{1}{p_k} \sum_{j \in S_k} M_j \left( \sum_i q_i |\psi_i\rangle\langle\psi_i| \right) M_j^\dagger.$$

Summary

By combining unitary evolution and projective measurements on an ancilla system, the density of matrix can undergo the stochastic transformation

$$\rho \rightarrow \frac{1}{p_k} \sum_{j \in S_k} M_j \rho M_j^\dagger \otimes |k\rangle\langle k|^M$$

such that

$$\left\{ \begin{array}{l} p_k = \sum_{j \in S_k} \text{tr}[M_j^\dagger M_j \rho] \\ \| = \sum_{k=1}^N \sum_{j \in S_k} M_j^\dagger M_j \end{array} \right.$$
Let $\mathcal{B}(\mathcal{H}^S)$ be the space of bounded linear operators on $\mathcal{H}^S$. A linear map acting on $\mathcal{B}(\mathcal{H}^S)$ is called a **superoperator**.

A superoperator $\mathcal{M}$ is **positive** if $\mathcal{M}(T) \geq 0$ whenever $T \geq 0$.

A superoperator $\mathcal{M}$ on $\mathcal{B}(\mathcal{H}^S)$ is called **completely positive** if for any auxiliary system $A$, $\mathcal{M} \otimes \mathcal{I}^A(T^{SA}) \geq 0$ whenever $T^{SA} \geq 0$, where $\mathcal{I}^A$ is the identity on $\mathcal{H}^A$.

**Example**

The transpose map is a positive but not completely positive map.
Completely Positive Maps

Theorem
A superoperator $\mathcal{M}$ is completely positive iff it can be represented as

$$\mathcal{M}(T) = \sum_k M_k T M_k$$

for some operators $\{M_k\}_k$.

A superoperator $\mathcal{M}$ is called **trace-preserving** if $\text{tr}[\mathcal{M}(T)] = \text{tr}[T]$ for all $T \in \mathcal{B(H^S)}$.

A **quantum channel** is a completely-positive trace-preserving (CPTP) map. Any CPTP map $\mathcal{E}$ can be written as

$$\mathcal{E}(T) = \sum_k M_k^\dagger T M_k \quad \text{where} \quad \sum_k M_k^\dagger M_k = \mathbb{I}.$$