The Framework of Quantum Mechanics Pt. 2

PHYS 500 - Southern Illinois University

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Ensembles of Pure States and the Density Operator

Definition

An *ensemble of pure states* (or just “ensemble of states”) is a collection of pure states with a probability distribution. That is, a pure state ensemble has the form \( \mathcal{E} = \{ |\psi_i\rangle, p_i \} \) where \( p_i \) is the probability associated with state \( |\psi_i\rangle \).

Definition

For a given pure state ensemble \( \mathcal{E} = \{ |\psi_i\rangle, p_i \} \) with \( |\psi_i\rangle \in \mathcal{H}^S \), its **ensemble average** is the operator acting on \( \mathcal{H}^S \) defined as

\[
\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i |,
\]

which is also called the **density operator**, **density of states**, or **density matrix**.
Ensembles of Pure States and the Density Operator

Pure state ensembles are useful when describing quantum measurements. Let $X = \sum_{k=1}^{n} \lambda_k P_k$ be some quantum observable for system $A$.

According to the Measurement Axiom, this observable generates the stochastic transformation

$$|\psi\rangle \rightarrow |\psi_k\rangle := \frac{1}{\sqrt{p_k}} P_k |\psi\rangle \text{ w/ prob. } p_k = \langle \psi | P_{\lambda_k} |\psi\rangle.$$

Associated with this measurement is the post-measurement ensemble $\mathcal{E} = \{|\psi_k\rangle^A, p_k\}$ and the density matrix

$$\rho = \sum_k p_k |\psi_k\rangle \langle \psi_k |^A.$$
Interpretation of the Density Operator

Density operators are useful for computing measurement probabilities on a system when you are unable to assign a definite state vector to the system or when making such an assignment is unimportant.

There are various reasons why you may be unable to assign a state vector to a quantum system. Perhaps a measurement has occurred and you do not know the outcome. Or perhaps you have forgotten the outcome. Or maybe the system is entangled with another system so that it is not possible to assign state vectors to the individual subsystems.

It is common practice to say that the density matrix is the system’s “state.” This language is useful as far as the word “state” refers to the mathematical object \( \rho = \sum_i p_i |\psi_i\rangle\langle \psi_i| \). But assigning any further ontological meaning to the density matrix is a controversial endeavor.
Properties of the Density Operator

If a system is in state $|\psi\rangle$, then it is described by a trivial ensemble of states $\mathcal{E} = \{|\psi\rangle, 1\}$. Hence, the density operator for $|\psi\rangle$ is $\rho = |\psi\rangle\langle\psi|$. 

Definition

Any rank-one density operator, i.e. $\rho = |\psi\rangle\langle\psi|$, is called a pure state. Any density operator of higher rank is called a mixed state.

Proposition

Every density operator is a trace one, positive operator. Conversely, for every trace one, positive operator $P$, there exists an ensemble of pure states $\mathcal{E}$ whose density operator is $P$.

Proof
Purifications

Definition

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

$$\rho^A = \text{tr}_B(|\psi\rangle\langle\psi|^{AB}).$$

An easy way to construct a purification:

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

Lemma

Purifications are not unique! Two states $|\psi\rangle^{AB}$ and $|\psi'\rangle^{AB}$ purify $\rho^A$ iff $|\psi\rangle = I^A \otimes U^B |\psi'\rangle$ for some unitary $U$ acting on $\mathcal{H}^B$. 
Representing Density Matrices by Different Ensembles

Let \( \rho^A = \sum_{i=1}^r p_i |v_i\rangle \langle v_i| \) be a spectral decomposition and 
\( |\psi\rangle^{AB} = \sum_{i=1}^r \sqrt{p_i} |v_i\rangle^A |i\rangle^B \) a purification, where \( \mathcal{H}^B \) has dimension \( d_B \).

Apply an arbitrary unitary on \( \mathcal{H}^B \):

\[
U^B : |i\rangle^B \rightarrow |\kappa_i\rangle^B = \sum_{j=1}^{d_B} u_{ij} |j\rangle^B.
\]

Then 
\[
(\mathbb{I} \otimes U^B) |\psi\rangle^{AB} = \sum_{i=1}^r \sum_{j=1}^{d_B} \sqrt{p_i u_{ij}} |v_i\rangle^S |j\rangle^B = \sum_{j=1}^{d_B} \sqrt{q_j} |\phi_j\rangle^A |j\rangle^B,
\]

where 
\[
\sqrt{q_j} |\phi_j\rangle = \sum_{i=1}^r \sqrt{p_i u_{ij}} |v_i\rangle \quad \text{for} \ j = 1 \cdots d_B.
\]
Representing Density Matrices by Different Ensembles

Then \[ \rho^A = \sum_{i=1}^{S} p_i |v_i\rangle \langle v_i| = \sum_{i=1}^{d_B} \sqrt{q_i} |\varphi_i\rangle \langle \varphi_i|. \]

**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 \( \mathcal{E}_2 = \{(|\Phi^+\rangle, 1/2); (|\Phi^-\rangle, 1/2)\} \).