Notes for Lectures in Quantum Mechanics *

Density Matrix

A. K. Kapoor
http://0space.org/users/kapoor
akkapoor@cmi.ac.in; akkhcu@gmail.com

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1 Properties of density matrix

A mixed system is described by a density matrix ρ having properties (i) $Tr\rho = 1$ and (ii) ρ is a positive matrix. A matrix ρ represents a pure state if and only if $\rho^2 = \rho$.

We list some results about the density matrix.

1. The positivity property implies that the density matrix is hermitian.

2. Condition $\rho^2 = \rho$ implies that ρ has eigenvalues 0 and 1.

3. $\rho^2 = \rho$ together with $Tr\rho = 1$ implies that the eigenvalue 1 is non-degenerate. All other eigenvalues are zero. Hence spectral theorem implies that $\rho = |\psi\rangle\langle\psi|$, where $|\psi\rangle$ is the eigenvector corresponding to the eigenvalue 1. In this case the state is describe by vector $|\psi\rangle$ and is a pure state.

4. ρ being, a positive operator, is necessarily hermitian.

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5. A necessary and sufficient condition that ρ may represent a pure state is $Tr(\rho^2) = Tr(\rho^3) = Tr(\rho)$. Note that this is stated entirely in terms of traces of the density operator.
Question for you: Why do we need $Tr\rho^3 = Tr(\rho^2) = 1$. Give an example to show that the condition $Tr(\rho^2) = 1$ is not sufficient to restrict ρ to be a density operator. However $Tr\rho^3 = 1$ and $Tr\rho^2 = 1$ taken together are sufficient for ρ to be a density operator for a pure state.

2 Density matrix and ensemble of pure states

A mixed state can be thought of as an ensemble of pure states $\{|\psi_k\rangle\}$. If p_k is the probability of system being in state $|\psi_k\rangle$, then the density operator can be written as a convex linear combination of projection operators $|\psi_k\rangle\langle\psi_k|$

$$\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k| \ , \qquad p_k > 0. \tag{1}$$

with $\sum p_k = 1$. The representation (1) of a density operator in terms of ensemble of pure state is not unique.
To see a proof of this statement let $|\lambda_k\rangle$ denote normalized eigenvectors of ρ thus

$$\rho = \sum_{k=1}^{n} \lambda_k |\lambda_k\rangle\langle\lambda_k| \ , \qquad \sum \lambda_k = 1 \ , \tag{2}$$

where λ_k are eigenvalues of ρ. If we define

$$\sqrt{p_m}|\phi_m\rangle = \sum U_{mn}\sqrt{\lambda n}|\lambda_n\rangle \ . \tag{3}$$

Then it is easy to verify that

$$\sum p_m|\phi_m\rangle\langle\phi_m| = \sum \lambda_k|\lambda_k\rangle\langle\lambda_k| = \rho \, . \tag{4}$$

Thus there are infinite ways of interpreting the system as an ensemble of pure state $|\phi_i\rangle$, are for each unitary matrix.

We quote a result [Subahash] about restrictions on the probability distributions $\{p_i\}$ consistent with a given ρ. If the eigenvalues λ_i of ρ and the probabilities $\{p_i\}$ are arranged in descending order to obtain ordered sequences $\{\lambda_\alpha\}_\downarrow$ and $\{p_\alpha\}_\downarrow$, then the former sequence majorized the latter;

the partial sums of the first r entries of the form is greater than or equal to the corresponding sums of the latter for any r. Thus result shows, in particular, that uniform distribution - all p_r's equal is always admissible for any ρ.

Reference: Subash Chaturvedi, "Lecture Notes" (2013).

3 Partial Trace

Given a density matrix ρ for a composite system, having subsystems A and B, we ask what happens if we restrict our attention to one of the subsystems, say A (or B). The subsystems are described by taking partial trace of the density matrix ρ. The process of taking partial trace will be described now. Let ρ_A, ρ_B and ρ denote the density operators describing systems A, B and the composite system AB respectively. Let $\{|A_i\rangle\}$ and $\{|B_r\rangle\}$ denote orthonormal bases on $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively.

Recall that the trace of an operator $\hat{X}$ in a Hilbert space can be defined by writing its matrix representation $(\hat{X})_{mn}$ w.r.t. an orthonormal basis $\{|n\rangle\}$ and summing over diagonal elements

$$\begin{aligned} tr(\hat{X}) &= \sum_{m,n=1}^{N} \delta_{mn}(\hat{X})_{mn} \\ &= \sum_{m} (\hat{X})_{mn} \end{aligned} \tag{5}$$

In case of an operator an tensor product Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, we first form orthonormal basis in $\mathcal{H}_A \otimes \mathcal{H}_B$ as

$$|aA, \nu B\rangle = |aA\rangle \otimes |\nu B\rangle \tag{6}$$

where $\{|aA\rangle | \nu = 1, N\}$ and $\{|\nu B\rangle | \nu = 1 \cdots N\}$ are orthonormal bases in $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively. The partial traces of an operator $\mathscr{X}$ are defined as

$$\text{partial trace of } \mathscr{X} \text{ over } B = \sum_{\nu=1}^{N} \langle aA, \nu B | \hat{\mathscr{X}} | bA, \sigma B\rangle \delta_{\nu\sigma} \equiv (\mathscr{X}_A)_{ab} \tag{7}$$

$$\text{partial trace of } \mathscr{X} \text{ over } A = \sum_{a=1}^{N} \langle aA, \nu B | \hat{\mathscr{X}} | bA, \sigma B\rangle \delta_{ab} \equiv (\mathscr{X}_B)_{\nu\sigma} \tag{8}$$

These lead to matrices $(\mathscr{X}_A)_{ab}$ and $(\mathscr{X}_B)_{\nu\sigma}$ which represent operators in $\mathcal{A}$ and $\mathcal{H}_B$ respectively.

Thus we have

$$(\rho_A)_{ab} = \sum_{\nu=1}^{N} \langle aA, \nu B | \rho | bA, \nu B\rangle$$

and the partial trace of ρ over B can expressed in an operator form as

$$\begin{aligned}\rho_A &= \sum_{a,b}(\rho_A)_{ab}|a\rangle\langle b| \\ &= \sum_{a,b}\sum_{\nu}\langle aA,\nu B|\rho|bA,\nu B\rangle\langle a||b\rangle\end{aligned}$$

with similar expressions for partial trace of density operator ρ over A. It is obvious that $Tr(\rho) = Tr(\rho_A) = Tr(\rho_B)$, partial trace operation does not change the trace of the operators. However if ρ is a positive operator, the act of taking partial trace does not always lead to a positive operator in the subspace.

4 An example

The density operator for composite system in pure state in $\mathcal{H}_A \otimes \mathcal{H}_B$, after partial trace leads to density matrix which, in general, does not correspond to a pure state.

Example: Consider Bell state $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$ having density matrix

$$\begin{aligned}\rho &= \frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|) \\ &= \frac{1}{2}|00\rangle > \langle 001| + \frac{1}{2}|00\rangle\langle 11| + \frac{1}{2}|11\rangle\langle 00| + \frac{1}{2}|11\rangle\langle 11|\end{aligned}$$

ρ_A is then given by

$$\rho_A = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

and we compute

$$\rho_A^2 = \frac{1}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| \neq \rho_A$$

$\therefore$ The density operator ρ_A for the subsystem A does not correspond to a pure state.