

Density operators and quantum operations

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We cannot always assign a definite state vector to a quantum system. It may be that the system is part of a composite system that is in an entangled state. Or it may be that our knowledge of the preparation of a particular system is insufficient to determine its state. For example, someone may prepare a particle in one of the states $|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_n\rangle$, choosing with probabilities p_1, p_2, \dots, p_n . Nevertheless, in either case we are able to make statistical predictions about the outcomes of measurements performed on the system using a more general description of quantum states *density operators*.

I. MIXTURES

Suppose the state of some system arises by a random process, so that the state $|\psi_j\rangle$ is prepared with probability p_j . The states $|\psi_j\rangle$ need not be orthogonal. We call this situation a mixture of states $|\psi_j\rangle$, or a mixed state for short. A measurement performed on this mixture gives a specific outcome, corresponding to some projector P , with the probability

$$\langle P \rangle = \sum_j p_j \langle \psi_j | P | \psi_j \rangle = \text{Tr} P \left(\sum_j p_j |\psi_j\rangle \langle \psi_j| \right).$$

We now define the density operator ρ to be

$$\rho = \sum_j p_j |\psi_j\rangle \langle \psi_j|.$$

It depends on the constituent states $|\psi_j\rangle$ and their probabilities, but not on the operators describing measurements. In particular, if we can assign a state vector $|\psi\rangle$ to a quantum system then the corresponding density operator is the projector on this state, $|\psi\rangle \langle \psi|$. This is particular case is called a pure state. As always, if we choose a particular basis operators become matrices. For example, the two density matrices below represent a qubit in the pure state $\alpha|0\rangle + \beta|1\rangle$ and in the equally weighted mixture of $\alpha|0\rangle \pm \beta|1\rangle$,

$$\begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}, \quad \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}.$$

Here, the diagonal elements, called populations, are the probabilities that a measurement in the standard basis will yield 0 or 1. In general, the diagonal matrix elements $\rho_{nn} = \langle n | \rho | n \rangle$ are the probabilities that a measurement in the chosen basis will yield the result n . This implies that the diagonal elements must be always nonnegative, $\langle v | \rho | v \rangle \geq 0$ for any $|v\rangle$, and that they should add up to one, $\text{Tr} \rho = 1$. The off-diagonal elements are called coherences. They tell us to what extent we are dealing with a superposition of $|0\rangle$ and $|1\rangle$ rather than with a probabilistic mixture of the two states. The coherences attain their maximal absolute value $|\rho_{ij}| = \sqrt{\rho_{ii}\rho_{jj}}$ for pure states and drop to zero for statistical mixtures.

Different mixtures of states can lead to the same density operator. For example, for a qubit a mixture of any

pair of orthogonal states taken with equal probabilities gives $\rho = \frac{1}{2} \mathbb{1}$. Mixtures with the same density operator behave identically under any physical investigation. For example, you cannot tell the difference between the equally weighted mixture of $\alpha|0\rangle \pm \beta|1\rangle$ and a mixture of $|0\rangle$ and $|1\rangle$ with probabilities $|\alpha|^2$ and $|\beta|^2$ respectively. The two preparations may be different but they are described by the same density operator. In general, many different preparations can lead to the same quantum state, as described by a density matrix.

Mathematically speaking,

- Density operator ρ on a finite dimensional Hilbert space is any positive operator $\rho \geq 0$ (meaning $\langle v | \rho | v \rangle \geq 0$ for any $|v\rangle$) with trace equal to one.
- Given a quantum system in state ρ , the measurement described by projectors $\{P_k\}$ gives outcome n with probability $\text{Tr} P_n \rho$.

At a more fundamental level mixed states arise as a consequence of entanglement. In order to see the relationship between the two consider the entangled state of a composite system AB,

$$|\psi_{AB}\rangle = \sum_{j=1}^n \sqrt{p_j} |\psi_j\rangle |b_j\rangle.$$

The states $|\psi_j\rangle$ pertain to part A and orthonormal vectors $|b_j\rangle$ to part B. If we measure part B and obtain result b_n , which happens with probability p_n , we “collapse” the state of A to $|\psi_n\rangle$. This way system A is effectively prepared in a mixture of $|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_n\rangle$, with probabilities p_1, p_2, \dots, p_n . Now, suppose B is very far away from A, so that in the absence of any superluminal communication, the measurement at B should have no effect whatsoever on any physical process at A. In other words, regardless whether the measurement at B is performed or not the quantum state of A is described by the density operator $\rho = \sum_j p_j |\psi_j\rangle \langle \psi_j|$.

Given orthonormal bases $\{|a_i\rangle\}$ and $\{|b_j\rangle\}$ any pure entangled state $|\psi_{AB}\rangle$ of a composite system AB can be written as

$$|\psi_{AB}\rangle = \sum_{ij} c_{ij} |a_i\rangle |b_j\rangle = \sum_j |\psi_j\rangle |b_j\rangle$$

where $|\psi_j\rangle = \sum_i c_{ij} |a_i\rangle$ are usually neither normalised nor orthogonal. Again, by the previous argument, the density operator of system A is a mixture,

$$\rho = \sum_j |\psi_j\rangle\langle\psi_j| = \sum_j \langle\psi_j|\psi_j\rangle |\bar{\psi}_j\rangle\langle\bar{\psi}_j|.$$

Vectors $|\bar{\psi}_j\rangle$ are the normalised versions of $|\psi_j\rangle$ and the normalisation factors $\langle\psi_j|\psi_j\rangle$ play the role of probabilities, p_j . Sometimes it more convenient to write density operators in terms of projectors on states which are not normalised; here the expression $\rho = \sum_j |\psi_j\rangle\langle\psi_j|$ is more compact and as long as the original entangled state is properly normalised, that is $\sum_{ij} |c_{ij}|^2 = 1$, we will always get a legal density operator pertaining to subsystem A. Needless to say, the same method can be used to obtain the density operator pertaining to subsystem B.

II. PARTIAL TRACE

We know now how to construct a density operator for any subsystem of a composite system that is in a pure state. However, there is an elegant mathematical method which allows us to construct density operators for any subsystem regardless whether it is part of a bigger system that is in a pure or in a mixed state. The basic tool is called the partial trace.

Given a composite system AB the partial trace over B and A are defined on a tensor product of two operators $A \otimes B$ as

$$\text{Tr}_B A \otimes B = A (\text{Tr} B), \quad \text{Tr}_A A \otimes B = (\text{Tr} A) B,$$

and then extended to any operator on AB by linearity. Given any density operator ρ_{AB} of the composite system AB we obtain reduced density operators by taking partial traces

$$\rho_A = \text{Tr}_B \rho_{AB}, \quad \rho_B = \text{Tr}_A \rho_{AB}$$

In particular,

$$\begin{aligned} \rho_A &= \text{Tr}_B |\psi_{AB}\rangle\langle\psi_{AB}| = \text{Tr}_B \sum_{ij} |\psi_j\rangle\langle\psi_i| \otimes |b_j\rangle\langle b_i| \\ &= \sum_{ij} |\psi_j\rangle\langle\psi_i| (\text{Tr}_B |b_j\rangle\langle b_i|) = \sum_{ij} |\psi_j\rangle\langle\psi_i| \langle b_i | b_j \rangle \\ &= \sum_j |\psi_j\rangle\langle\psi_j|, \end{aligned}$$

where we have used $\text{Tr} |b_i\rangle\langle b_j| = \langle b_j | b_i \rangle = \delta_{ij}$. It is easy to check that the partial trace maps density operators on AB to density operators on A (or B), i.e. it preserves positivity and trace. In fact it is the only function f such that

$$\text{Tr} [Pf(\rho_{AB})] = \text{Tr} [(P \otimes \mathbb{1})\rho_{AB}],$$

for any projector P on A. So, you have no choice, get used to the partial trace.

III. QUANTUM OPERATIONS

Physical operations that transform quantum states are described by *completely* positive trace preserving maps, \mathcal{E} . They are linear operators that act on (density) operators, and are often referred to as superoperators. The adjective *completely* requires some explanation, but let us start with the following three specific examples.

Embedding. Given any physical system, described by ρ we can add any other quantum system, in some pure state state, here labelled as $|0\rangle$. This is the isometric (preserving the inner product) embedding in the space of a larger dimension, $|\psi\rangle \mapsto |\psi\rangle|0\rangle$, also written as

$$\rho \mapsto \rho \otimes |0\rangle\langle 0|.$$

Unitary evolution. For consistency with the state vector description any unitary evolution U must be an admissible quantum operation

$$\rho \mapsto U\rho U^\dagger$$

Partial trace. The act of disregarding a part of the composite system is also an admissible quantum operation, it is described by the partial trace

$$\rho \mapsto \rho_A = \text{Tr}_B \rho.$$

We now postulate that any quantum operation \mathcal{E} is a composition of an arbitrary number of these three transformations. For example,

$$\rho \mapsto \rho_A = \text{Tr}_B [(U(\rho \otimes |0\rangle\langle 0|)U^\dagger)].$$

Quantum operations are more subtle than maps which just preserve trace and positivity. Take, for example, the transpose operation on a single qubit,

$$\begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \xrightarrow{T} \begin{pmatrix} a & c^* \\ c & b \end{pmatrix}.$$

It certainly preserves both trace and positivity, and the result is a density matrix. However, if this qubit is part of a two qubit system initially in the entangled state $|0\rangle|0\rangle + |1\rangle|1\rangle$, and the transpose is applied only to one the two qubits, say, the first one, then, under the action of partial transposition $T \otimes \mathbb{1}$, the density matrix of the two qubits evolves as

$$\frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \xrightarrow{T \otimes \mathbb{1}} \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The resulting matrix has a negative eigenvalue and hence does not represent a quantum state. The transpose is an example of a positive map which is not completely positive. A completely positive map is a map which preserves positivity of the density operator not only of the principal system but also of any extension of this system.