8.1. Definitions

Recall $|\psi\rangle$ ket : $\begin{bmatrix}\psi_1 \\ \psi_2 \\ \vdots \\ \psi_n\end{bmatrix}$ $\langle\psi|$ bra : $[\psi_1, \psi_2, \ldots, \psi_n]$

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Define density operator ρ on Hilbert space H as having the following:

Hermitian : $\rho = \rho^\dagger$ aka its conjugate transpose, so $\rho_{ij} = \overline{\rho_{ji}}$ for ρ_{ij} entries of ρ

Non-negative : $\langle v|\rho|v\rangle \geq 0$ for all $|v\rangle$

Trace $\mathrm{tr}\,\rho = 1$, meaning ρ's diagonals sum to 1

Properties of density operators that follow:

- always diagonalizable
- real, non-negative eigenvalues summing to 1
- to construct a convex sum:

$$\rho = p_1\rho_1 + p_2\rho_2, \quad p_1 + p_2 = 1, \; p_1, p_2 \geq 0$$

These operators form a convex set: any convex sum like the one above is also itself another density operator

Pure states: for a quantum state $|\psi\rangle$, this is given by the density operator $\rho = |\psi\rangle\langle\psi|$

It is an extremal point in a convex set of density operators that cannot be expressed as a convex set of other states than $|\psi\rangle$.

Mixed states: all other states that are not pure states can be written as a convex sum of pure states : $\sum_i p_i |\psi_i\rangle\langle\psi_i|$ for $p_i \geq 0$ w/ $\sum_i p_i = 1$.

Note: $|\psi_i\rangle\langle\psi_i|$ is often described as a rank-one projector,

8.2 Statistical mixtures

Mixed state (aka mixture of states): — say, $|\psi_i\rangle$ w/ probability p_i —

Example: Say Alice prepares a quantum system in one state from the normalized but not necessarily orthogonal states $|\psi_1\rangle, |\psi_2\rangle, \ldots |\psi_m\rangle$.
If she gives the system to Bob without telling him, then his best "description" of the system, since it must account for all possible states with their respective probabilities, is the mixed state:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

Note: this is not the same as a preparation of the system in a defined state vector that is the superposition $\sum_i p_i |\psi_i\rangle$. Alice knows which $|\psi_i\rangle$ state vector the system is described by, and Bob's $\sum_i p_i |\psi_i\rangle\langle\psi_i|$ comes from his personal uncertainty. But he only knows the possible states $|\psi_1\rangle, |\psi_2\rangle, \ldots |\psi_m\rangle$ and their probability distribution $p_1 \ldots p_m$.
The mixed state describes Bob's ignorance about the state preparation and can be used to make statistical predictions in the absence of a defined state vector.

Say observable M describes the measurement. For preparation in state vector $|\psi_i\rangle$:
the average expected value of M, $\langle M\rangle = \langle\psi|M|\psi\rangle =$ trace (tr) $M|\psi\rangle\langle\psi|$
(This is what Alice expects)
For a mixed state, this is given by $\langle M\rangle = \mathrm{tr}\, M\left(\sum_i p_i |\psi_i\rangle\langle\psi_i|\right) = \underline{\mathrm{tr}\, M\rho}$
(This is what Bob expects)
Let's call ρ the density operator :(it is a convex sum of rank-one projectors, depends on constituent states $|\psi_i\rangle$ and their probabilities, and describes the uncertain state preparation.
(And call the set $\{(p_i, |\psi_i\rangle\langle\psi_i|\}$ a convex decomposition of ρ, but we won't use this much)

Note that the exact composition of states and associated probabilities is not present in the computation of observable statistics, only the derived density operator.

Different mixtures of pure states can yield an identical density operator and will be indistinguishable statistically. Put another way, preparations can only be distinguished if they yield distinct density operators.

8.2 addendum - mixed state indistinguishability example scenarios:

Alice:

1. Flips a coin

Heads: Prepare state $|0\rangle$

Tails: Prepare state $|1\rangle$

and gives the system to Bob...

2. Flip a coin

Heads: Prep state $|+\rangle$

Tails: Prep state $|-\rangle$

$|+\rangle := 1/\sqrt{2}(|0\rangle + |1\rangle) = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$

$|-\rangle := 1/\sqrt{2}(|0\rangle - |1\rangle) = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$

superposition states of $|0\rangle$ and $|1\rangle$

3. Flip a coin

Heads: Prep state $|u_1\rangle$

Tails: Prep state $|u_2\rangle$

where u_1 & u_2 are orthonormal

Bob's density matrix ρ:

1. $= \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$

2. $= \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| = \frac{1}{4}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \frac{1}{4}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$

3. Since any 2 orthonormal states of a qubit form a complete basis, this $= \frac{1}{2}|u_1\rangle\langle u_1| + \frac{1}{2}|u_2\rangle\langle u_2| = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ $(\frac{1}{2}\,Id)$ $= \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$

All three scenarios yield the same density operators despite having different states.

8.3 Instructive examples

We know density matrix for $|\psi\rangle$ is $|\psi\rangle\langle\psi|$. This is well-defined (distinct $|\psi\rangle \to$ distinct $|\psi\rangle\langle\psi|$) and global phases do not affect the density matrix.

Let's look closer at this matrix form.

Generally, the diagonal entries of a density matrix describe the probability distributions on the set of basis vectors. They must add to $\hat{1}$ (per our def'n. in 8.1). The non-diagonal entries are called <u>coherences</u>.

<u>Coherences</u>: quantify the degree to which a quantum system can witness <u>interference</u>.

So, a classical system will have 0 values for coherences. Moreover, <u>decoherence</u> is the process by which off-diagonal entries go to 0. Example:

$$\begin{bmatrix}|\alpha|^2 & \alpha\beta^* \\ \beta\alpha^* & |\beta|^2\end{bmatrix} \longmapsto \begin{bmatrix}|\alpha|^2 & 0 \\ 0 & |\beta|^2\end{bmatrix}$$

$$= \begin{bmatrix}|\alpha|^2 & \varepsilon \\ \varepsilon^* & |\beta|^2\end{bmatrix}, \qquad = \begin{bmatrix}|\alpha|^2 & \varepsilon \\ \varepsilon & |\beta|^2\end{bmatrix},$$

$\varepsilon = \alpha\beta^*$; full interference capability, pure quantum state

$\varepsilon = 0$; no interference capability, pure classical state

<u>Spectral decomposition</u>: for any density matrix ρ, the spectral decomposition is the most natural mixture that yields ρ. We've seen different mixtures yield the same ρ already. The most natural one is given by the pairs of eigenvectors $|u_i\rangle$ and eigenvalues p_i of ρ:

$$\rho = \sum_i p_i |u_i\rangle\langle u_i|$$

<u>Maximally mixed state</u>: state s.t. outcomes of <u>any</u> measurement are <u>completely random</u>; this will typically mean that the outcome of any state is equally likely, so usually this implies that all diagonals will have uniform values. For a system without interference, the maximally mixed state will thus be proportional to the identity. Example:

For $|u_1\rangle, |u_2\rangle, \ldots |u_n\rangle$ forming an orthonormal basis and with equal probabilities $1/n$, $\frac{1}{n}\sum_{i=1}^{n}|\psi_i\rangle\langle\psi_i| = \frac{1}{n}\mathrm{Id}$ (aka $\frac{1}{n}\mathbf{1}$)

<u>Non-normalized states projectors</u>: For states like $|\tilde{\psi}_i\rangle = \sqrt{p_i}|\psi_i\rangle$, where ψ_i is normalized, p_i is its probability, we use this $|\tilde{\psi}_i\rangle$ to incorporate the probability into the length of the state vector in order to more compactly write density operators. In this case, the density operator would look like:

$$\rho = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|.$$