PHY 4105: Quantum Information Theory
Lecture 10

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Mixed states

So far we have been talking about pure quantum states which are represented by rays in Hilbert space of the form

$$|\psi\rangle = \sum_i c_i|e_i\rangle = \sum_i \langle e_i|\psi\rangle|e_i\rangle, \qquad \sum_i |c_i|^2 = 1.$$

Measurement in the basis $|e_j\rangle$ gives

$$p_k = |\langle e_k|\psi\rangle|^2 = \langle\psi|P_k|\psi\rangle = \langle e_k|P_\psi|e_k\rangle.$$

In many situations we might have a collection (ensemble) of identical quantum systems for which we know that with a probability q_j the system is in the state $|\psi_j\rangle$. From measurements on the ensemble, the probability that we find the system in the state $|e_k\rangle$ is $p_k = \sum_j p_{k|j}q_j$, with

$$p_{k|j} = |\langle e_k|\psi_j\rangle|^2 = \langle e_k|\psi\rangle\langle\psi|e_k\rangle.$$

So we have

$$p_k = \sum_j q_j\langle e_k|\psi\rangle\langle\psi|e_k\rangle = \langle e_k|\Big(\sum_j q_j|\psi\rangle\langle\psi|\Big)|e_k\rangle.$$

We can represent the state of the system by a density operator,

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

The set $\{q_j, |\psi_j\rangle\}$ is an ensemble decomposition of the state ρ. In terms of the density operator,

$$p_k = \mathrm{tr}(\rho|e_k\rangle\langle e_k|).$$

For an observable $A = \sum_k \lambda_k|e_k\rangle\langle e_k|$, we have

$$\langle A\rangle = \sum_k \lambda_k p_k = \mathrm{tr}(\rho A).$$

A density operator is a Hermitian operator with non-negative eigenvalues that sum to 1 ($\mathrm{tr}\rho = 1$).

Before discussing the properties of density matrices, let us go back to a few things that we had left out when we discussed operators on D dimensional Hilbert spaces. The operators on a D dimensional Hilbert space $\mathcal{H}$ for a D^2 dimensional complex vector space $L_{\mathcal{H}}$, with inner product

$$(A,\, B) \equiv \mathrm{tr}(A^\dagger B).$$

An orthonormal basis for $L_{\mathcal{H}}$ is given by the operators $\tau_{jk} = |e_j\rangle\langle e_k$. We have

$$\mathrm{tr}(\tau_{lm}^{\dagger}\tau_{jk}) = \mathrm{tr}(|e_m\rangle\langle e_l|e_j\rangle\langle e_k|) = \delta_{jk}\delta_{km}.$$

An arbitrary operator can be expanded in this basis as

$$A = \sum_{jk} A_{jk}|e_j\rangle\langle e_k| = \sum_{jk} A_{jk}\tau_{jk}.$$

An alternate, non-orthogonal basis for $L_{\mathcal{H}}$ is given by the set of all 1D projectors (pure states) $|\psi\rangle$. A specific orthonormal set of 1D projectors can be chosen as the basis as follows:

$$|\phi_\alpha\rangle = \begin{cases} j = 1, \ldots, D & |e_j\rangle\langle e_j| = \tau_{jj} \\ j < k; & |\chi_{jk}\rangle\langle\chi_{jk}| = \frac{1}{2}(\tau_{jj} + \tau_{kk} + \tau_{jk} + \tau_{kj}) \\ & |\xi_{jk}\rangle\langle\xi_{jk}| = \frac{1}{2}(\tau_{jj} + \tau_{kk} - i\tau_{jk} + i\tau_{kj}), \end{cases}$$

where

$$\begin{aligned} |\chi_{jk}\rangle &= \frac{1}{\sqrt{2}}(|e_j\rangle + |e_k\rangle) \\ |\xi_{jk}\rangle &= \frac{1}{\sqrt{2}}(|e_j\rangle + i|e_k\rangle). \end{aligned}$$

So an operator A is specified by the inner products

$$(|\phi_\alpha\rangle\langle\phi_\alpha|,\, A) = \mathrm{tr}(|\phi_\alpha\rangle\langle\phi_\alpha|A) = \langle\phi_\alpha|A|\phi_\alpha\rangle.$$

An operator is over-specified if we give its sandwiches $\langle\psi|A|\psi\rangle$ with all the pure states. An operator is Hermitian if all $\langle\psi|A|\psi\rangle$ are real.

A positive operator G is one for which $\langle\psi|G|\psi\rangle$ is real and non-negative for all $|\psi\rangle$. The positivity condition is denoted as $G \geq 0$. An operator G is positive if an only if it is Hermitian with non-negative eigenvalues. Two positive operators G_1 and G_2 are orthogonal ($\mathrm{tr}(G_1G_2) = 0$) if an only if $G_1G_2 = 0$.

Positive operators have square roots:

$$\sqrt{G} = \sum_j \sqrt{\lambda}|e_j\rangle\langle e_j|.$$

An operator is positive definite ($G > 0$) if $\langle\psi|G|\psi\rangle > 0$ for all $|\psi\rangle$. Positive definite operators are Hermitian with positive eigenvalues and they are invertible.

An operator ρ is a density operator if and only if $\rho \geq 0$ and $\mathrm{tr}(\rho) = 1$. A pure state density operator is a rank 1 projector, $\rho = |\psi\rangle\langle\psi|$. A unit trace Hermitian operator is ρ is a pure state density matrix if and only if $\rho^2 = \rho$ (A projector has to be Hermitian but not necessarily unit trace). Alternatively, a density operator ρ represents a pure state if and only if $\mathrm{tr}(\rho^2) = 1$.

Now let us turn our attention from the vector space of operators $L_{\mathcal{H}}$ to the set (not vector space) of density operators. To do that we have to look at what a convex set is. A set S is convex if for any $v_1, v_2 \in S$,

$$\lambda v_1 + (1 - \lambda)v_2 \in S.$$

Or in general,

$$\sum_j \lambda_j v_j \in S, \qquad \sum_j \lambda_j = 1 \quad \text{and} \quad \lambda_j \geq 0.$$

An extreme point of a convex set S is a point that cannot be written as a proper $(0 < \lambda < 1)$ convex combination of any other points. If S is closed and bounded then every point in S can be written as a convex combination of the extreme points. A simplex is a special type of convex set for which every point can be written uniquely in terms of the extreme points of the set. The set of probability distributions on a random variable form a simplex.

The density operators are a closed and bounded convex set whose extreme points are the pure states.

For qubit density operators, we start with the general decomposition,

$$\rho = A_0 \mathbb{1} + \vec{A} \cdot \vec{(\sigma)} = (A_0 + |\vec{A}|)|\vec{n}\rangle\langle\vec{n}| + (A_0 - |\vec{A}|)|-\vec{n}\rangle\langle-\vec{n}|.$$

The second equality above follows from the fact that ρ has to be Hermitian and hence A_0 and $\vec{A}$ are real. We also have $A_0 = 1/2$ from the trace condition on ρ since $\mathrm{tr}(\rho) = 2A_0$ from the equation above. Finally positivity of ρ means that $|\vec{A}| \leq 1$ because otherwise the second eigenvalue of ρ, $A_0 - |\vec{A}|$ will be negative. So we have

$$\rho = \frac{1}{2}(\mathbb{1} + \vec{S} \cdot \vec{\sigma}), \quad |\vec{S}| \leq 1.$$

The vector $\vec{S}$ is the Bloch vector describing the state. Now its length can be less than one also. Which means that if we consider all the states of a qubit, including mixed state, we find that they are represented by points on the surface and within the Bloch sphere (Bloch ball).

In the Bloch sphere, pure states are on the surface while mixed states are represented by points inside. In higher dimensions, mixed states form a $(d^2 - 1)$ dimensional manifold while pure states are a $2(d-1)$ dimensional surface.

Consider a mixed state with Bloch vector $\vec{S}$. We have seen ensemble decomposition of mixed states as

$$\rho = \sum_j q_j |\psi_j\rangle\langle\psi_j|, \qquad |\psi_j\rangle = \frac{1}{2}(\mathbb{1} + \vec{n}_j \cdot \vec{\sigma}).$$

Any set of states $|\psi_j\rangle$ such that $\vec{S} = \sum_j q_j \vec{n}_j$ will furnish an ensemble decomposition of the mixed state. This means that the decomposition of a mixed state into an ensemble of pure states is not unique. This means that the space of density operators is not a simplex.

A special ensemble decomposition of the density matrix is one that makes it diagonal. This is furnished by the eigenvectors of ρ as

$$\rho = \sum_j \lambda_j |e_j\rangle\langle e_j|.$$

The support of ρ is subspace of Hilbert space spanned by the eigenvectors of ρ corresponding to the non-zero eigenvalues of ρ. The null-space of ρ is the subspace spanned by the eigenvectors corresponding to zero eigenvalues. These subspaces are orthogonal to each other. A subspace that is orthogonal to another subspace S is called the orthocomplement of S. The projectors on to the support and null-space of ρ are respectively

$$P_S = \sum_{\lambda_j \neq 0} |e_j\rangle\langle e_j|, \qquad P_N = \sum_{\lambda_j = 0} |e_j\rangle\langle e_j|.$$

The number of non-zero eigenvalues of ρ is called the rank of the density matrix. If we consider an ensemble decomposition of ρ given by $\{q_j, |\psi_j\rangle$ then it is clear that all $|\psi_j\rangle$ must be Hilbert space vectors that lie in the support of ρ.

1. *The Hughston, Jozsa, and Wootters (HJW) theorem originally discovered by Schrödinger*

For the purposes of stating and proving the theorem we will denote an ensemble decomposition $\{q_j, |\psi_j\rangle\}$ of a density operator ρ as $\{|\bar{\psi}_j\rangle\}$ by absorbing $\sqrt{q_j}$ into $|\psi_j\rangle$ so that

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

Theorem: Two ensemble decomposition $\{|\bar{\psi}_\alpha\rangle\}$ and $\{|\bar{\phi}_\alpha\rangle\}$ correspond to the same density operator if and only if there exists a unitary operator $U_{\alpha\beta}$ such that

$$|\bar{\phi}_\alpha\rangle = U_{\alpha\beta}|\bar{\psi}_\beta\rangle.$$

Note that if one ensemble decomposition has fewer elements than the other, one can always pad the shorter one with zero vectors so that $U_{\alpha\beta}$ is well defined.
Proof:

$$\begin{aligned}\sum_\alpha |\bar{\phi}_\alpha\rangle\langle\bar{\phi}_\alpha| &= \sum_{\alpha,\beta\gamma} U_{\alpha\beta}|\bar{\psi}_\beta\rangle\langle\bar{\psi}_\gamma|U^*_{\alpha\gamma} = \sum_{\beta,\gamma}|\bar{\psi}_\beta\rangle\langle\bar{\psi}_\gamma| \sum_\alpha U_{\alpha\beta}U^*_{\alpha\gamma} \\ &= \sum_{\beta,\gamma}|\bar{\psi}_\beta\rangle\langle\bar{\psi}_\gamma|\,\delta_{\beta\gamma} = \sum_\alpha |\bar{\psi}_\alpha\rangle\langle\bar{\psi}_\alpha|.\end{aligned}$$

To prove the reverse let us consider, without loss of generality, one of the two ensemble decompositions to be the eigen-decomposition of ρ. So we have

$$\rho = \sum_\alpha |\bar{\psi}_\alpha\rangle\langle\bar{\psi}_\alpha| = \sum_{|e_j\rangle\in S} |\bar{e}_j\rangle\langle\bar{e}_j|.$$

Since $|\bar{\psi}_\alpha\rangle$ has support only in S as mentioned earlier, we can expand it as

$$|\bar{\psi}_\alpha\rangle = \sum_{|e_j\rangle\in S}|e_j\rangle\langle e_j|\bar{\psi}_\alpha\rangle = \sum_{|e_j\rangle\in S}|\bar{e}_j\rangle\frac{\langle e_j|\bar{\psi}_\alpha\rangle}{\sqrt{\lambda_j}}, \qquad \text{define} \qquad M_{\alpha j} = \frac{\langle e_j|\bar{\psi}_\alpha\rangle}{\sqrt{\lambda_j}}$$

Now we have to show that $M_{\alpha j}$ is unitary. So

$$\sum_\alpha M_{\alpha j}M^*_{\alpha k} = \langle e_j|\frac{\sum_\alpha |\bar{\psi}_\alpha\rangle\langle\bar{\psi}_\alpha|}{\sqrt{\lambda_j\lambda_k}}|e_k\rangle = \frac{1}{\sqrt{\lambda_j\lambda_k}}\langle e_j|\rho|e_k\rangle = \frac{1}{\sqrt{\lambda_j\lambda_k}}\lambda_k\delta_{jk} = \delta_{jk}.$$

Note that $M_{\alpha j}$ is an $N\times R$ matrix where N is the number of elements in the ensemble decomposition and R is rank of ρ but M can be extended to be an unitary by adding zeros.