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Entanglement and mixed states

A qubit is a two-state quantum system, or a state of one. A general "pure" state has the form

$$|\psi\rangle = a|0\rangle + b|1\rangle \tag{1}$$

where $|0\rangle$ and $|1\rangle$ form an orthonormal basis for the (two dimensional) qubit Hilbert space. (We'll discuss "mixed" states below. From here on, a pure state will be referred to simply as a "state," and a mixed state will be referred to as such.) Normalization $\langle\psi|\psi\rangle = 1$ implies $|a|^2 + |b|^2 = a_R^2 + a_I^2 + b_R^2 + b_I^2 = 1$, which is the equation for a 3-sphere S^3 in four Euclidean dimensions. But states related by a phase factor are physically equivalent, so the manifold of *physically distinct* states has one dimension less. We'll see below that it forms a 2-sphere S^2, called the **Bloch sphere**. Every point on the Bloch sphere corresponds to a circle in the S^3.[1]

The Hilbert space of a pair of qubits is the tensor product of two single qubit Hilbert spaces, so is four dimensional. A basis for this space is $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, where $|00\rangle \equiv |0\rangle|0\rangle$, etc. A general pure state in the two qubit Hilbert space has the form

$$|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle, \tag{2}$$

wtih $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$. The manifold of these states is thus a 7-sphere in eight Euclidean dimensions, and the manifold of physically distinct states is thus *six* dimensional.

Entanglement

Two qubit states that have the product form $|\alpha\rangle|\beta\rangle$ for some pair of single qubit states $|\alpha\rangle$ and $|\beta\rangle$ are called **separable**, **unentangled**, or **product states**. When a state is written out as a sum of basis vectors, it isn't always obvious whether or not it is separable. For example, the state (2) with $a = b = c = d$ is actually separable: it's equal to $a(|0\rangle + |1\rangle)(|0\rangle + |1\rangle)$. A nonseparable basis for the Hilbert space is the basis of **Bell states**,

$$|\phi^\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}, \qquad |\psi^\pm\rangle = (|01\rangle \pm |10\rangle)/\sqrt{2}. \tag{3}$$

Most states are nonseparable. In fact, (2) is separable if and only if $ad - bc = 0$. This is one complex condition, hence the separable states lie in a 4-dimensional submanifold of the 6-dimensional space of states.[2]

Mixed states and density matrices

Suppose a two qubit system is in the state $|\psi\rangle = a|00\rangle + b|11\rangle$, and consider the expectation value of any observable $A \otimes I$ that is nontrivial only on the first factor:

$$\langle\psi|A \otimes I|\psi\rangle = |a|^2\langle 00|A \otimes I|00\rangle + |b|^2\langle 11|A \otimes I|11\rangle + a^*b\langle 00|A \otimes I|11\rangle + b^*a\langle 11|A \otimes I|00\rangle \tag{4}$$

$$= |a|^2\langle 0|A|0\rangle + |b|^2\langle 1|A|1\rangle. \tag{5}$$

[1] This map $S^3 \to S^2$ is called the *Hofp fibration*. The two circles in the S^3 corresponding to any two states are linked. A group theoretic description of this map is $SU(2) \to SU(2)/U(1)$, where the group quotient is the space of cosets.

[2] The manifold of product states has topology $S^2 \times S^2$, corresponding to the product of Bloch spheres of the factors.

The expectation value is a sum of expectation values in the two possible states for the first qubit, weighted by the probability $|a|^2$ of being $|0\rangle$ and probability $|b|^2$ of being $|1\rangle$. The first qubit isn't by itself in a definite pure state, but rather is described by a statistical mixture, called a **mixed state**. That is, a mixed state is a ensemble of pure states, weighted with some probabilities. In the example just given, these are "quantum probabilities," since they originate from the amplitudes in a pure quantum state. However, one could also consider mixed states whose probability has a different origin.

A convenient way to describe a mixed state is via a **density matrix** ρ. To introduce this notion, first notice that the expectation value of an observable A in a state $|\psi\rangle$ can be expressed as[3]

$$\langle\psi|A|\psi\rangle = \mathrm{Tr}(|\psi\rangle\langle\psi|A), \tag{6}$$

that is, as the trace of the projection of A into the $|\psi\rangle$ subspace. In the case of a mixed state, this is replaced by a weighted sum,

$$\langle A\rangle := \sum_i p_i\,\mathrm{Tr}(|\psi_i\rangle\langle\psi_i|A) =: \mathrm{Tr}\rho A, \tag{7}$$

where in the last step the density matrix is defined,

$$\rho := \sum_i p_i\,|\psi_i\rangle\langle\psi_i|. \tag{8}$$

The density matrix is a probability weighted sum of projection operators. The defining properties of a general density matrix are thus $\rho^\dagger = \rho$, $\mathrm{Tr}\rho = 1$, and $\rho \geq 0$, where the last condition means that the eigenvalues of ρ are nonnegative. Equivalently, it means that $\langle\psi|\rho|\psi\rangle \geq 0$ for all states $|\psi\rangle$.

In the basis that diagonalizes a density matrix, the eigenvalues are the probabilities for the corresponding basis states in the ensemble. A pure state density matrix is a projection operator, which has one eigenvalue equal to 1 and all others equal to 0, and satisfies $\rho^2 = \rho$. A **maximally mixed state** is one for which all probabilities are equal, so the density matrix is proportional to the identity. A weighted linear combination of density matrices is another density matrix,

$$\rho_3 = \lambda\rho_1 + (1-\lambda)\rho_2, \tag{9}$$

provided λ is any real number between 0 and 1. Any mixed state density matrix can be expressed as a weighted sum of other density matrices, in an infinite number of different ways. Pure states can only be expressed in one way, by a unique projection operator.

Density matrix for a qubit: the Bloch ball

A general density matrix for a qubit has the form

$$\rho = \tfrac{1}{2}(I + \vec{b}\cdot\vec{\sigma}), \tag{10}$$

since this is the most general 2×2 hermitian matrix with unit trace. The eigenvalues of (10) are $\frac{1}{2}(1\pm|\vec{b}|)$, so the positivity condition implies that $|\vec{b}|$ is less than or equal to unity. The collection of all density matrices for a qubit thus forms a unit ball in three-dimensional space, sometimes called the **Bloch ball**. If $|\vec{b}| = 1$, then one eigenvalue is 1 and the other is 0, so ρ is a pure state projection operator. The pure states therefore correspond to the surface of the unit ball, called the Bloch sphere. All the other density matrices describe mixed states. The maximally mixed state $\frac{1}{2}I$ sits at the center of the Bloch ball.

[3]The trace moves the leading ket to the end of the expression: $\mathrm{Tr}(|\psi\rangle\langle\psi|A) = \sum_n\langle n|\psi\rangle\langle\psi|A|n\rangle = \sum_n\langle\psi|A|n\rangle\langle n|\psi\rangle = \langle\psi|A|\psi\rangle$, where the $|n\rangle$ comprise a complete orthonormal set of vectors.

Reduced density matrix

The density matrix ρ_A for the A subsystem of a tensor product of Hilbert spaces $\mathcal{H}_A \otimes \mathcal{H}_B$ is called the **reduced density matrix**, and is given by the **partial trace**, $\mathrm{Tr}_B\rho$, where ρ is the density matrix of the full system. To see this, consider the expectation value of any observable that acts only on the A factor:

$$\mathrm{Tr}\rho(O \otimes I) = \sum_{a,b} \langle ab|\rho(O \otimes I)|ab\rangle = \sum_a \langle a|\Big(\sum_b \langle b|\rho|b\rangle\Big) O|a\rangle =: \mathrm{Tr}(Tr_B\rho)O \tag{11}$$

Here $\{|a\rangle\}$ and $\{|b\rangle\}$ are orthonormal bases for $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively, and the final step defines the partial trace over the B factor. If the reduced density matrix for a pure bipartite state is maximally mixed, the state is said to be **maximally entangled**. For example, the Bell states (3) are maximally entangled. If the composite state is pure, the von Neumann entropy $S_A = -\mathrm{Tr}\rho_A \ln \rho_A$ of the reduced density matrix is called **entanglement entropy**.

Schmidt decomposition

There is a very convenient way to write a general entangled state, called the **Schmidt decomposition**: any **bipartite** pure state $|\psi\rangle$, i.e. a state in the tensor product of two Hilbert spaces $\mathcal{H}_A \otimes \mathcal{H}_{\tilde{A}}$, can be written in the Schmidt form

$$|\psi\rangle = \sum_a \sqrt{p_a}\, |a\rangle|\tilde{a}\rangle, \tag{12}$$

where the vectors $|a\rangle$ are orthonormal in $\mathcal{H}_A$, the vectors $|\tilde{a}\rangle$ are orthonormal in $\mathcal{H}_{\tilde{A}}$, and the p_a are probabilities, with $0 < p_a \leq 1$, and $\sum_a p_a = 1$. In fact, these are nothing but the probability eigenvalues of the reduced density matrix on subsystem A or on subsystem $\tilde{A}$. If the p_a are all distinct, this decomposition of $|\psi\rangle$ is unique except for the freedom to multiply $|a\rangle$ and $|\tilde{a}\rangle$ by opposite phases. When two or more p_a are equal, there is ambiguity.

To verify these properties, let's first check the converse: if $|\psi\rangle$ has the the form (12), then the reduced density matrix on $\mathcal{H}_A$ is

$$\rho_A = \mathrm{Tr}_{\tilde{A}}|\psi\rangle\langle\psi| = \mathrm{Tr}_{\tilde{A}} \sum_{a,a'} \sqrt{p_a p_{a'}}\, |a\rangle\langle a'| \otimes |\tilde{a}\rangle\langle\tilde{a}'| = \sum_{a,a'} \sqrt{p_a p_{a'}}\, \langle\tilde{a}'|\tilde{a}\rangle\; |a\rangle\langle a'| = \sum_a p_a\, |a\rangle\langle a|. \tag{13}$$

That is, the $|a\rangle$ come from the eigenbasis of ρ_A, and the p_a are the corresponding eigenvalues. Conversely, let $|\psi\rangle$ be any bipartite state, and let $|a\rangle$ be an orthonormal basis of eigenvectors of the reduced density matrix for the A factor, $\rho_A = \mathrm{Tr}_{\tilde{A}}|\psi\rangle\langle\psi|$. Any state $|\psi\rangle$ in the Hilbert space can of course be written as $|\psi\rangle = \sum_a |a\rangle|\bar{a}\rangle$ for *some* set of vectors $|\bar{a}\rangle$ in $\mathcal{H}_{\tilde{A}}$. Now let's evaluate the partial trace of the projector:

$$\mathrm{Tr}_{\tilde{A}}|\psi\rangle\langle\psi| = \mathrm{Tr}_{\tilde{A}} \sum_{a,a'} |a\rangle|\bar{a}\rangle\langle\bar{a}'|\langle a'| = \sum_{a,a'} \langle\bar{a}'|\bar{a}\rangle\; |a\rangle\langle a'| \tag{14}$$

Since we chose $|a\rangle$ to be the eigenbasis of ρ_A, it must evidently be the case that $\langle\bar{a}'|\bar{a}\rangle = p_a\delta_{aa'}$. The vectors $|\bar{a}\rangle$ are thus orthogonal, but not normalized. Defining normalized vectors by $|\bar{a}\rangle =: \sqrt{p_a}\,|\tilde{a}\rangle$, we have thus arrived at the Schmidt decomposition (12) for any bipartite state.

Note that local unitary transformations $U_A \otimes U_{\tilde{A}}$ acting on $|\psi\rangle$ change each of the reduced density matrices, without changing the probabilities p_a. Such transformations thus don't change the degree of entanglement between the two factors. In fact, any two states with the same set of nonzero p_a's are related by such a transformation. Note also that the entanglement entropies for ρ_A and $\rho_{\tilde{A}}$ are equal, since these density matrices have the same nonzero probability eigenvalues.

Maximally entangled states

For two qubits, the Bell states (3) provide an example of maximally entangled states. To construct the most general maximally entangled two-qubit state we can choose any pair of states $|a\rangle$, $|\tilde{a}\rangle$, and define the state $(|a\rangle|\tilde{a}\rangle + e^{i\phi}|a^{\perp}\rangle|\tilde{a}^{\perp}\rangle)/\sqrt{2}$, where the $\perp$ superscript denotes an orthogonal state. The freedom in choosing this state appears to be parametrized by the five dimensional manifold $S_2 \times S_2 \times S_1$, because each of the two states comes from a Bloch sphere, and the relative phase between the two terms is significant. However, some of these choices give the same state. For example, a spin singlet $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ of two spin-1/2 systems is maximally entangled, and is unchanged by any common rotation of the two spins. Rotations about the z-axis would not change the presentation of this state, since they just multiply the two spin states by opposite phases, so the distinct presentations are parametrized by $SU(2)/U(1)$, which is a 2-sphere. A similar statement applies to any maximally entangled state, albeit with a different identification of the equivalence transformations. Thus the dimension of the manifold of maximally entangled states is $5 - 2 = 3$. I've read that the actual manifold is $SU(2)/Z_2$ (which is the same as $SO(3)$ and RP^3), but I don't know at present how to deduce this.