Physics 305, Fall 2008
Entanglement and the Density Matrix

Definition of a Qubit

A qubit is the simplest quantum mechanical system, namely one with only two states. Two ways to realize a qubit experimentally are to use the spin states of a spin 1/2 particle or the polarizations of a photon. We could write spin states using the kets $|\uparrow\rangle$ and $|\downarrow\rangle$ or the polarization states using $|\updownarrow\rangle$ and $|\leftrightarrow\rangle$. The most general state of such a system, which we will label A, is

$$\begin{aligned} |\psi\rangle_A &= a_0|\uparrow\rangle_A + a_1|\downarrow\rangle_A \\ &= a_0|\updownarrow\rangle_A + a_1|\leftrightarrow\rangle_A \ , \end{aligned}$$

where a_0 and a_1 are complex numbers such that $|a_0|^2 + |a_1|^2 = 1$. In analogy with the two possible values of a classical bit in an ordinary computer, we will henceforth label the kets $|0\rangle$ and $|1\rangle$:

$$|\psi\rangle_A = a_0|0\rangle_A + a_1|1\rangle_A \ . \tag{1}$$

More information is needed to specify the state of a qubit than to specify the state of a classical bit. A classical bit can be on or off, while a qubit can be in a linear superposition of states specified by two complex numbers with a normalization constraint. Much of the promise of quantum computing lies in this crucial difference in the underlying mechanism for storing information.

We can measure the state of a qubit by measuring the eigenvalue of some Hermitian operator $\mathcal{O}$ that acts on the Hilbert space of the qubit. The most general Hermitian operator $\mathcal{O}$ that can act on our state $|\psi\rangle_A$ takes the form

$$\mathcal{O} = v_0 \mathrm{Id} + \sum_{j=1}^{3} v_j \sigma_j \tag{2}$$

where the coefficients v_0 and the v_j must be real numbers. The σ_j are the Pauli spin matrices. The σ_j themselves measure (up to a prefactor $\hbar/2$) the coefficient of spin in the j direction. Measuring σ_3 is called *reading* the qubit. The outcome of the measurement is a classical bit. The numbers $|a_0|^2$ and $|a_1|^2$ give the probabilities that the measurement yields as outcome the corresponding classical bit.

Two Qubit States

Consider now a system consisting of two qubits A and B. One possible state of such a system is a *product* state

$$\begin{aligned} |\Psi_{\text{product}}\rangle &= |\psi\rangle_A|\phi\rangle_B \\ &= \big(a_0|0\rangle_A + a_1|1\rangle_A\big)\big(b_0|0\rangle_B + b_1|1\rangle_B\big) \ . \end{aligned}$$

It must be emphasized that a product state is *not* the most general state of such a system. For example, the EPR state, made famous by Einstein, Podolsky, and Rosen,

$$|\Psi_{\mathrm{EPR}}\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle_A|1\rangle_B - |1\rangle_A|0\rangle_B\big) \ ,$$

cannot be written in such a factorized form. States that do not factorize into a product form we call *entangled*. Entangled states have the property that the outcome of a measurement of system B affects the state of system A. A more general definition of entanglement will be given below.

N Qubit States

Now consider a system of N qubits, $\vec{x} = \{s_0, s_1, \ldots, s_N\}$ where s_i can be zero or one. The number of possible states has risen exponentially to 2^N. The most general linear superposition of these states $|\vec{x}\rangle$ takes the form

$$|\Psi\rangle = \sum_{\vec{x}} c_{\vec{x}}|\vec{x}\rangle \qquad \text{subject to} \qquad \sum_{\vec{x}} |c_{\vec{x}}|^2 = 1 \ . \tag{3}$$

To specify such a superposition, we need 2^N complex numbers $c_{\vec{x}}$ subject to a single normalization constraint. In contrast, to specify a product state, of the form

$$|\Psi_{\mathrm{product}}\rangle = \prod_{j=1}^{N}\big(a_{0j}|0\rangle_j + a_{1j}|1\rangle_j\big)$$

we would only need $2N$ complex numbers subject to a single normalization constraint. This vast amount of extra information in a general state $|\Psi\rangle$ is encoded in the entanglement between the different qubits.

Entanglement with the Environment

The notion of entanglement is important in any realistic description of a quantum system A that is in contact with some other quantum system B. This other system B is in fact always present, since any finite quantum system A will not be completely isolated from its environment. For example, the environment may include the measuring apparatus with which we plan to measure the quantum system A. Let us call the system B the environment of system A.

Up to now, we have considered situations where the state of the quantum system and its environment factorizes into a product state

$$|\Psi_{\mathrm{product}}\rangle = |\psi\rangle_A|\phi\rangle_B \ . \tag{4}$$

In this situation, we can ignore the environment. Given an operator $\mathcal{O}_A$ that acts just on the quantum system A (and not on B), we have

$$\langle\Psi_{\mathrm{product}}|\mathcal{O}_A|\Psi_{\mathrm{product}}\rangle = {}_A\langle\psi|\mathcal{O}_A|\psi\rangle_A \ .$$

In such a situation, the quantum system A is said to be in a *pure state*.

Now let $|i\rangle_A$ be a basis of the Hilbert space for system A and $|j\rangle_B$ be a basis for the environment. We can decompose

$$|\psi\rangle_A = \sum_i a_i |i\rangle_A , \qquad\qquad |\phi\rangle_B = \sum_j b_j |j\rangle_B ,$$

$$|\Psi_{\text{product}}\rangle = \sum_{i,j} a_i b_j |i\rangle_A |j\rangle_B \tag{5}$$

for some set of amplitudes a_i and b_j. As we indicated before, product states of this form are special and live in a small corner of the product Hilbert space of the two systems.

The most general quantum state of systems A and B has the form

$$|\Psi\rangle = \sum_{i,j} c_{ij} |i\rangle_A |j\rangle_B \tag{6}$$

where c_{ij} are arbitrary complex amplitudes. For the product state, $c_{ij} = a_i b_j$, but in general, c_{ij} can not be factorized in this way. If c_{ij} cannot be factorized, we say that the system A and its environment B are *entangled*. In this case, the quantum system A is said to be in a *mixed state*. We would like to find a way of describing a mixed state without having to include the environment in our description.

The Density Matrix

We will see that the density matrix can be used to give a complete characterization of a system in a mixed state. Let $|i\rangle$ label some basis of the Hilbert space of system A. We write the matrix as

$$\rho = \sum_{ij} |i\rangle \rho_{ij} \langle j| , \tag{7}$$

with complex entries ρ_{ij}. We require the matrix satisfy three properties:

1. The matrix is Hermitian:
$$\rho^\dagger = \rho$$
   or equivalently $\rho_{ij} = \rho_{ji}^*$.

2. The matrix has trace one:
$$\operatorname{tr}\rho = 1 ,$$
   or equivalently $\sum_i \rho_{ii} = 1$.

3. The matrix is positive semi-definite. In other words, all of its eigenvalues are non-negative.

The expectation value of an operator for a system described by ρ is defined to be

$$\langle \mathcal{O} \rangle = \sum_{ij} \rho_{ij} \langle j|\mathcal{O}|i\rangle = \operatorname{tr}(\rho\mathcal{O}) . \tag{8}$$

3

Given that the density matrix is Hermitian, we can find a special basis $|n\rangle$ such that ρ is diagonal:

$$\rho = \sum_n |n\rangle \rho_{nn} \langle n| \ . \tag{9}$$

The non-negativity of the eigenvalues ρ_{nn} and the condition that $\operatorname{tr}\rho = 1$ then imply that $0 \leq \rho_{nn} \leq 1$. We define

$$p_n \equiv \rho_{nn}$$

to be the probability for the system to be in the state $|n\rangle$. A density matrix thus describes a statistical mixture — in sharp distinction to a quantum superposition — of quantum states where $\sum p_n = 1$. In this diagonal basis, the expectation value of $\mathcal{O}$ takes the form of a statistical average

$$\langle \mathcal{O} \rangle = \sum_n p_n \langle n|\mathcal{O}|n\rangle \ .$$

Pure States and Mixed States

A quantum system in a pure state is described by a wave function

$$|\psi\rangle = \sum_i a_i |i\rangle \ . \tag{10}$$

The expectation value of an operator $\mathcal{O}$ then reads

$$\langle \mathcal{O} \rangle = \langle \psi|\mathcal{O}|\psi\rangle = \sum_{ij} a_i a_j^* \langle j|\mathcal{O}|i\rangle \ .$$

From the definition (8), the density matrix associated to this pure state is

$$\rho = \sum_{ij} |i\rangle a_i a_j^* \langle j| = |\psi\rangle\langle\psi| \ .$$

Comparing with (9), we see that the density matrix of a pure state $|\psi\rangle$, when diagonalized, has one single eigenvalue $p_n = 1$ (for $|n\rangle = |\psi\rangle$) while $p_m = 0$ for all other $m \neq n$. In consequence, the density matrix of a pure state has the special property that $\rho^2 = \rho$. In general,

$$\operatorname{tr}(\rho^2) = 1 \qquad \text{for a pure state,}$$
$$\operatorname{tr}(\rho^2) < 1 \qquad \text{for a mixed state.}$$

Mixed States from Entanglement

Let us return to the general entangled state (6) for the two quantum systems A and B. We want to compute the density matrix that describes the mixed state of system A. Consider

an operator $\mathcal{O}_A$ that acts within the Hilbert space of A only. Its expectation value can be evaluated as

$$
\begin{aligned}
\langle \mathcal{O} \rangle &= \langle \Psi | \mathcal{O} | \Psi \rangle \\
&= \sum_{ijkl} c_{ij} c_{kl}^* {}_B\langle l | j \rangle_B {}_A\langle k | \mathcal{O} | i \rangle_A \\
&= \sum_{ik} \left(\sum_j c_{ij} c_{kj}^* \right) {}_A\langle k | \mathcal{O} | i \rangle_A \ .
\end{aligned}
$$

From here, we read off that the density matrix for the quantum system A is

$$
\rho_{ik}^A = \sum_j c_{ij} c_{kj}^* \ . \tag{11}
$$

For the product state (5), the entries of the density matrix can be factored $\rho_{ik} = a_i a_k^*$, which describes a pure state. However for general c_{ij}, the density matrix (11) cannot be written in this pure state form. In this more general case, A is said to be in a mixed state.

Measurement and Decoherence

The notion of pure states and mixed states plays an important role in the description of a quantum mechanical measurement. Again, consider a quantum system A. To do a measurement on A, we must put it in contact with a measuring device B. Let us assume that, initially, system A is in a pure state (10). The measuring apparatus is in some other state $|\phi\rangle_B$ that initially is uncorrelated with the state of A. So before the measurement starts, the combined system is in a product state of the form (4), or when written out in some eigenbasis, as in Eq. (5).

To perform the measurement, we assume that the measuring device has a basis of states that correlates with the basis of states of system A. This correlation is such that, when system A is in the eigenstate $|i\rangle_A$, then the measuring apparatus will go in a measurement state that says: "I have just measured the system A is in the state $|i\rangle_A$." We denote such a state of the measuring apparatus by $|i\rangle_B$.

The measurement process is described by the Schrödinger equation of system A together with the measuring device B. The total Hamiltonian will have an interaction term that acts on the combined Hilbert space of A and B. For a well designed measuring apparatus, this Hamiltonian is such that after a while, the combined state looks as follows

$$
|\Psi_{\text{after}}\rangle = \sum_i a_i |i\rangle_A |i\rangle_B \ . \tag{12}
$$

In other words, the combined system is in a maximally entangled state where there is a one-to-one correlation between the state of the quantum system A and that of the measuring device B. For an ideal measurement, the amplitudes a_i of $|\Psi_{\text{after}}\rangle$ are identical to the amplitudes a_i of the initial pure state (10). After the measurement, however, system A is no longer in a pure state, but in a mixed state with a diagonal density matrix

$$
\rho_{\text{after}}^A = \sum_i |i\rangle_A\, p_i\, {}_A\langle i| \qquad \text{such that} \qquad p_i = |a_i|^2 \ . \tag{13}
$$

In complete accord with the familiar description of quantum mechanical measurement, the probability that system A ends up in state $|i\rangle$ is $p_i = |a_i|^2$. What has happened, however, is that after the interaction with the measurement device, the different states $|i\rangle$ and amplitudes a_i are no longer added up coherently as in the pure state (10), but they are added as in a statistical ensemble with classical probabilities p_i. The time-evolution from the initial product state (4) to the final entangled state (12), or equivalently, from the initial pure state (10) to the final mixed state (13), is known as decoherence.