Entanglement

Our lecture today shall be concerned with one of the most fundamental concepts in the field of quantum information theory – entanglement. To get our discussion of the ground let us start with the most elementary building block of quantum information – the qubit.

Definition of a qubit

A qubit is the simplest quantum mechanical system, namely one with only two states (or levels). Experimentally, such a qubit might be realized by the two spin states of a spin-½ particle or the polarization of a photon (amongst many other possible realizations). We write for such a system, which we label A

$$|\psi\rangle_A = a_0 |\uparrow\rangle_A + a_1 |\downarrow\rangle_A \qquad \text{(spins)}$$

$$= a_0 |\updownarrow\rangle_A + a_1 |\leftrightarrow\rangle_A \qquad \text{(polarization)}$$

$$= a_0 |0\rangle_A + a_1 |1\rangle_A \qquad \text{(general notation)}$$

where a_0 and a_1 are complex numbers such that $|a_0|^2 + |a_1|^2 = 1$.

Note that 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.

Two-qubit states

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

$$|\psi_{\text{product}}\rangle = |\psi\rangle_A |\phi\rangle_B$$

$$= (a_0 |0\rangle_A + a_1 |1\rangle_A) \cdot (b_0 |0\rangle_B + b_1 |1\rangle_B).$$

It must be emphasized that a product state is not the most general state of such a system. A more interesting example is the so-called EPR state made famous by Einstein, Podolsky, and Rosen

$$|\psi_{EPR}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A |1\rangle_B - |1\rangle_A |0\rangle_B \right)$$

which 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.

Reflecting on the latter, one might think that this is somewhat puzzling, or in the words of Einstein, Podolsky, and Rosen somewhat "spooky" – a statement which at the time was so newsworthy that it made the front page of the New York Times.

A more general definition of entanglement will follow shortly.

N-qubit states

Now consider a system of N qubits, $\vec{x} = \{s_0, s_1, s_2, \dots, s_N\}$ 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

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

To specify such a superposition we need 2^N complex numbers subject to a single normalization constraint. In contrast, to specify a product state of the form

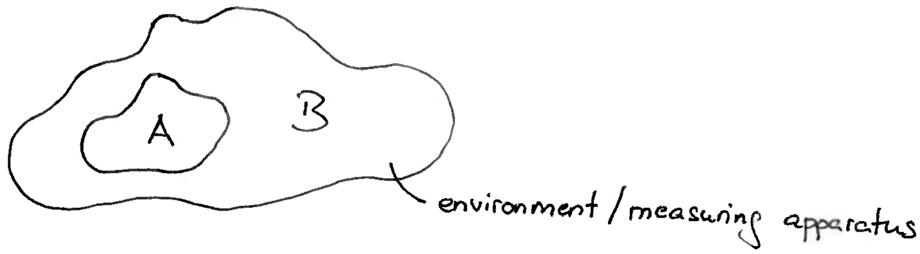
$$|\psi_{\text{product}}\rangle = \prod_{j=1}^{N} \left(a_{0j} |0\rangle_j + a_{1j} |1\rangle_j \right)$$

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 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.



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

$$|\psi_{product}\rangle = |\psi\rangle_A \cdot |\phi\rangle_B$$

For such a situation, we can ignore the environment. Given an operator O_A that acts on the quantum system A only (and not on B) we have

$$\langle \psi_{product} | O_A | \psi_{product} \rangle = \langle \psi|_A \, O_A \, |\psi\rangle_A \cdot \underbrace{{}_B\langle \phi | \phi \rangle_B}_{=1}$$

We say that the quantum system A is in a pure state.
Now let $|i\rangle_A$ be a basis of the Hilbert space of A and $|j\rangle_B$ be a basis of the Hilbert space of B. We can decompose

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

$$|\psi_{product}\rangle = \sum_{ij} a_i b_j |i\rangle_A |j\rangle_B$$

for some set of amplitudes a_i and b_j.

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

$$|\psi\rangle = \sum_{ij} c_{ij} \, |i\rangle_A \, |j\rangle_B$$

where c_{ij} are arbitrary complex amplitudes (subject to a normalization constraint).
For the product state we have

$$c_{ij} = a_i b_j$$

but, in general, c_{ij} cannot be factorized in this way.

If c_{ij} cannot be factorized, we say system A and environment B are entangled. In this case, the quantum system A is said to be in a mixed state.

We would now like to find a way of describing a mixed state without having to include the environment in our description.

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. The density matrix with entries ρ_{ij} is defined as the operator

$$\hat{\rho} = \sum_{ij} |i\rangle \rho_{ij} \langle j|$$

where the entries ρ_{ij} are complex numbers.

We will require the following three properties:

1) $\underbrace{\rho_{ij} = \rho_{ji}^*}_{\text{density matrix is hermitian } \hat{\rho} = \hat{\rho}^+}$

2) $\underbrace{\sum_i \rho_{ii} = 1}_{\text{trace of density matrix is 1: } \mathrm{Tr}(\hat{\rho}) = 1}$

3) $\underbrace{\rho_{ii} \geq 0}_{\text{density matrix is positive semi-definite}}$ in diag. form

One main use of the density matrix is to define the expectation values of operators $\hat{O}$ that act on the Hilbert space (of system A)

$$\langle \hat{O} \rangle = \sum_{ij} \rho_{ij} \langle j | \hat{O} | i \rangle = \mathrm{Tr}(\hat{\rho}\hat{O})$$

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

$$\rho = \sum_n |n\rangle \rho_{nn} \langle n| \qquad \text{(Schmidt decomposition)}$$

with the non-negativity of the eigenvalues ρ_{nn} and the condition that $\mathrm{Tr}(\rho) = 1$ then implying that

$$0 \leq \rho_{nn} \leq 1.$$

We therefore 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 of quantum states where

$$\sum_n p_n = 1 .$$

Such a statistical mixture should be sharply distinguished to a (coherent) superposition of quantum states.

In this diagonal basis the expectation value of the operator $\hat{O}$ takes the form of a statistical average

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

Pure states and mixed states

A quantum system in a pure state is described by a wavefunction

$$|\psi\rangle = \sum_i a_i |i\rangle$$

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

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle = \sum_{ij} \underbrace{a_i a_j^*}_{= \rho_{ij}} \langle j | \hat{O} | i \rangle$$

According to its definition the density matrix associated with this pure state is

$$\hat{\rho} = \sum_{ij} |i\rangle \underbrace{a_i a_j^*}_{\rho_{ij}} \langle j| = |\psi\rangle\langle\psi|$$

Comparing this with the diagonal form of the density matrix, we see that the density matrix of a pure state $|\psi\rangle$, when diagonalized, has one single eigenvalue

$$p_n = 1 \qquad \text{for } |n\rangle = |\psi\rangle$$

$$\text{and} \qquad p_m = 0 \qquad \text{for all } m \neq n$$

In consequence, the density matrix of a pure state has the special property

$$\rho^2 = \rho$$

In general we have

$$\mathrm{Tr}(\rho^2) = 1 \quad \text{for a pure state}$$

$$\mathrm{Tr}(\rho^2) < 1 \quad \text{for a mixed state.}$$

We thus see that the density matrix of a given state can readily distinguish a pure state from a mixed state and as such a product state from an entangled state. The density matrix thus serves as an indicator of entanglement.

Entanglement entropy

While we have seen above that the density matrix can serve as a qualitative measure of entanglement (differentiating mixed states from pure ones) one can actually go a step further and use the (reduced density matrix) density matrix to define a quantitative measure of entanglement. One often studied family of such quantitative measures are the so-called entanglement entropies. The most prominent example of this family is the so-called van Neumann entropy defined as

$$\rho = |\psi\rangle\langle\psi|$$

$$\rho_A = \sum_j \langle j|_B \, |\psi\rangle\langle\psi| \, |j\rangle_B = \mathrm{Tr}_B\, \rho$$

$$S(\rho_A) = -\mathrm{Tr}(\underbrace{\rho_A}_{\text{reduced density matrix}} \cdot \log \rho_A)$$

where the subindex A again indicates that we are looking at the reduced density matrix of system A after tracing out the environment B.
The van Neumann entropy is the first representative of the family of Renyi entropies defined as

$$S_n(\rho_A) = \frac{1}{1-n} \log\left(\mathrm{Tr}(\rho_A^n)\right)$$

of which one often considers the second Renyi entropy ($n=2$) in field theory / numerics

$$S_2(\rho_A) = -\log\left(\mathrm{Tr}(\rho_A^2)\right).$$