Density Matrix

Given a pure state $|\psi\rangle$, the expectation value of any observable $\hat{O}$ w.r.t. $|\psi\rangle$ is

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle$$

$$= tr[|\psi\rangle\langle\psi| \hat{O}] \quad \text{where } tr \equiv \text{trace}$$

To show this, recall that trace of an operator is $tr\,\hat{\Omega} = \sum_i \langle \phi_i | \hat{\Omega} | \phi_i \rangle$ where $\{|\phi_i\rangle\}$ is <u>any</u> orthonormal basis. It is important to note that it doesn't matter what basis one uses. To calculate $tr[|\psi\rangle\langle\psi| \hat{O}]$ let's choose a basis where one of the elements of the basis is $|\psi\rangle$ itself. By construction, all the other elements in the basis set are orthogonal to $|\psi\rangle$. Lets call $|\psi\rangle = |\phi_1\rangle$ and the other basis elements are $|\phi_2\rangle, |\phi_3\rangle, \ldots$ etc.

$$\Rightarrow \quad \mathrm{tr}\,[|\psi\rangle\langle\psi|\hat{O}]$$

$$= \sum_i \langle\phi_i|\psi\rangle\langle\psi|\hat{O}|\phi_i\rangle$$

$$= \langle\phi_1|\psi\rangle\langle\psi|\hat{O}|\phi_1\rangle + \sum_{i>1}\langle\phi_i|\psi\rangle\langle\psi|\hat{O}|\phi_i\rangle$$

$$= \langle\psi|\psi\rangle\langle\psi|\hat{O}|\psi\rangle = \langle\psi|\hat{O}|\psi\rangle$$

where we have used that $|\phi_1\rangle = |\psi\rangle$ and $\langle\phi_i|\psi\rangle = 0$ for $i>1$ since the basis is orthonormal.

The operator $|\psi\rangle\langle\psi|$ is called "density matrix" and often denoted as $\hat{\rho}$.

Therefore $\langle\psi|\hat{\Omega}|\psi\rangle = \mathrm{tr}(\hat{\rho}\,\hat{\Omega})$ where $\hat{\rho} = |\psi\rangle\langle\psi|$. $\hat{\rho}$ is the quantum analog of a probability distribution f^n (p.d.f.) since given a classical p.d.f. $\rho(x_1, x_2, \ldots x_n)$ over n variables

$x_1, x_2, \ldots x_n$, the expectation value of an arbitrary f^n $f(x_1, x_2 \ldots x_n)$ is given by,

$$\langle f \rangle = \int dx_1 \ldots dx_n \; \rho(x_1, x_2 \ldots x_n) f(x_1, \ldots x_n)$$

$$= \mathrm{tr}[\rho f] \quad \text{if we think of}$$

ρ as a diagonal 'matrix'. Of course, the (quantum) density matrix $\hat{\rho} = |\psi\rangle\langle\psi|$ when written in a generic basis will have off-diagonal elements, and has many non-intuitive properties (e.g. quantum entanglement), so this analogy with a classical p.d.f. only goes so far.

Quantum Entanglement

Consider a composite system whose Hilbert space is $\mathcal{H}_A \otimes \mathcal{H}_B$. We say that a state $|\psi\rangle$ in this Hilbert space is unentangled (or "separable") if and only if $|\psi\rangle$ <u>can</u> be written as

$$|\psi\rangle = |\phi\rangle_A \otimes |\phi\rangle_B$$

where $|\phi\rangle_A$ and $|\phi\rangle_B$ live in Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively.

Let's consider a few examples:

(a) $|0\rangle \otimes |0\rangle$ and $|1\rangle \otimes |1\rangle$ are clearly unentangled.

(b) $(|0\rangle \otimes |1\rangle \pm |1\rangle \otimes |0\rangle)$ and $(|0\rangle \otimes |0\rangle \pm |1\rangle \otimes |1\rangle)$ are <u>entangled</u> i.e. can not be written as $|\phi\rangle_A \otimes |\phi\rangle_B$.

(c) $|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle + |0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle$

is unentangled / separable because it can be written as $(|0\rangle + |1\rangle) \otimes (|0\rangle + |1\rangle)$.

These examples illustrate that it can sometimes be difficult to tell if a state is entangled or not by a quick inspection. Fortunately, there is a number one can calculate that is zero if and only if the state is unentangled. This quantity, called von Neumann entanglement (or entanglement entropy) is given by

$$S_A = - \mathrm{tr}_A [\rho_A \log \rho_A]$$

where $\rho_A = \mathrm{tr}_B (|\psi\rangle\langle\psi|)$

where tr_A, tr_B denote partial traces over $\mathcal{H}_A$, $\mathcal{H}_B$ respectively.

Specifically, for any operator $\hat{O}$ that acts on $\mathcal{H}_A \otimes \mathcal{H}_B$,

$$\mathrm{tr}_A \, \hat{O} = \sum_i \langle A_i | \hat{O} | A_i \rangle \quad \text{where}$$

$|A_i\rangle$ is a complete basis for $\mathcal{H}_A$.

One similarly defines tr_B. Note that $\mathrm{tr}_A \hat{O}$ is an <u>operator</u> that acts on the $\mathcal{H}_B$ = the Hilbert space that was not traced out.

Note that one may also write the entanglement $S_A = -\sum_i \lambda_{iA} \log \lambda_{iA}$

where λ_{iA} are eigenvalues of ρ_A.

Let's consider a few examples.

(a) Let's first consider any separable state : $|\psi\rangle = |\phi_A\rangle \otimes |\phi_B\rangle$ so that

$$\rho = |\psi\rangle\langle\psi|$$
$$= |\phi_A\rangle \otimes |\phi_B\rangle \langle\phi_A| \otimes \langle\phi_B|$$

$$Tr_B \rho = \sum_i \langle B_i | \rho | B_i \rangle$$ where

$|B_i\rangle$ is an orthonormal basis for $\mathcal{H}_B$.

One may choose $|\phi_B\rangle$ as one the basis elements and the rest are therefore orthogonal to $|\phi_B\rangle \Rightarrow \rho_A =$

$$Tr_B \rho = \langle\phi_B| \, |\phi_A\rangle \otimes |\phi_B\rangle \langle\phi_A| \otimes \langle\phi_B| \phi_B\rangle$$
$$= |\phi_A\rangle\langle\phi_A|$$

Since this is a projector onto $|\phi_A\rangle$, this operator has only one non-zero eigenvalue, namely, one.

$\Rightarrow \quad S_A = 1 \times \log(1) = 0$

(b) $|\psi\rangle = \frac{1}{\sqrt{2}}\left[|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B \right]$

$$\rho_A = \mathrm{Tr}_B \, |\psi\rangle\langle\psi|$$

$$= {}_B\langle 0|\psi\rangle\langle\psi|0\rangle_B + {}_B\langle 1|\psi\rangle\langle\psi|1\rangle_B$$

$$|\psi\rangle\langle\psi| = \frac{1}{2}\Big[|0\rangle_A |0\rangle_B \, {}_A\langle 0| \, {}_B\langle 0|$$

$$+ |1\rangle_A |1\rangle_B \, {}_A\langle 1| \, {}_B\langle 1| + |0\rangle_A |0\rangle_B \, {}_A\langle 1| \, {}_B\langle 1|$$

$$+ |1\rangle_A |1\rangle_B \, {}_A\langle 0| \, {}_B\langle 0| \Big]$$

In the tr_B, only the first two terms yield non-vanishing contribution:

$$\rho_A = \frac{1}{2}\left[|0\rangle_A \, {}_A\langle 0| + |1\rangle_A \, {}_A\langle 1| \right]$$

$$\equiv \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

$$\Rightarrow S_A = -\frac{1}{2}\log\left(\frac{1}{2}\right) - \frac{1}{2}\log\left(\frac{1}{2}\right) = \log(2)$$

Pure States Vs Mixed States

A single quantum state $|\psi\rangle$ is called a 'pure state'. The corresponding density matrix $\rho = |\psi\rangle\langle\psi|$ is projector i.e. it satisfies $\rho^2 = \rho$.

Next consider an ensemble of such pure states $\{|\psi_i\rangle\}$. Let's say the pure state $|\psi_i\rangle$ is prepared with probability p_i. The expectation value of any observable $\hat{O}$ is then

$$\langle \hat{O} \rangle = \sum_i p_i \langle \psi_i | \hat{O} | \psi_i \rangle$$

$$= \sum_i p_i \, \mathrm{Tr} \, \hat{O} (|\psi_i\rangle\langle\psi_i|)$$

$$= \mathrm{Tr} [\hat{O} (\sum_i p_i |\psi_i\rangle\langle\psi_i|)]$$

$$= \mathrm{Tr}[\hat{O} \hat{\rho}]$$

where $\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ is the mixed-state (or mixed density matrix) corresponding to the ensemble $\{|\varphi_i\rangle\}$.

As discussed above, a pure state $|\varphi\rangle$ defined over the tensor-product Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ is considered unentangled (or separable) if $|\varphi\rangle$ can be written as $|\varphi\rangle = |\phi_A\rangle \otimes |\phi_B\rangle$. In a similar spirit, a mixed state ρ is considered unentangled/separable if it can be written as $\rho = \sum_i p_i |\phi_{iA}\rangle \otimes |\phi_{iB}\rangle \langle\phi_{iA}| \otimes \langle\phi_{iB}|$ where $p_i > 0$ are some numbers. Let's consider an example.

Consider a mixed state that is an equal mixture of the following to entangled pure states

$$|\varphi_1\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \quad |\varphi_2\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$

That is,

$$\rho = \frac{1}{2}\left[|\varphi_1\rangle\langle\varphi_1| + |\varphi_2\rangle\langle\varphi_2|\right]$$

One may naively think that ρ is entangled since both $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are entangled. However, this is an incorrect guess. After substituting the expressions for $|\varphi_1\rangle, |\varphi_2\rangle$, one finds

$$\rho = \frac{1}{2}\left[|00\rangle\langle 00| + |11\rangle\langle 11|\right]$$

which is clearly of the form

$$\rho = \sum_i p_i \, |\phi_{iA}\rangle \otimes |\phi_{iB}\rangle \langle\phi_{iA}| \otimes \langle\phi_{iB}| .$$

and hence not entangled. Compared to pure states, it is a much harder to determine if a given mixed state is unentangled.