Basics about Entanglement

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Theorem 1. Let $|\psi\rangle$ be a pure quantum state of a lattice Hamiltonian. For an operator O that is supported on one part of the bipartited of lattice the following holds:

$$\langle \psi | O | \psi \rangle = \operatorname{Tr}(\rho_i O) \tag{1}$$

where ρ_i is the (reduced) density matrix of the selected part of lattice, and the trace is taken over either states thereof or of the full system (they give the same result).

Proof. The full wavefunction can be decomposed into

$$\left|\psi\right\rangle = \sum_{i,o} \omega_{i,o} \left|\phi_{i}\right\rangle \left|\phi_{o}\right\rangle \tag{2}$$

and ρ_i is

$$\rho_{i} = \operatorname{Tr}_{o}(|\psi\rangle \langle \psi|) = \sum_{o} \langle \phi_{o}|\psi\rangle \langle \psi|\phi_{o}\rangle$$

$$= \sum_{i,i'} \left(\sum_{o} \omega_{i,o} \,\omega_{o,i'}^{*}\right) |\phi_{i}\rangle \langle \phi_{i'}|$$
(3)

Measurement tracing density matrix over all $|\psi_i\rangle$ is

$$\operatorname{Tr}(\rho_i O) = \sum_i \langle \phi_i | \rho_i O | \phi_i \rangle$$

=
$$\sum_{i,i'} \left(\sum_o \omega_{i,o} \, \omega_{o,i'}^* \right) \, \langle \phi_{i'} | O | \phi_i \rangle$$
(4)

Note that one can also do a trace over states of the full lattice as long as $|\phi_o\rangle$ is normalized, which doesn't matter since O acting only on $|\phi_i\rangle$. On the other hand, a direct measure by $\langle \psi | O | \psi \rangle$ is

$$\langle \psi | O | \psi \rangle = \sum_{i',o'} \sum_{i,o} \omega_{o'i'}^* \omega_{i,o} \langle \phi_{o'} \phi_{i'} | O | \phi_i \phi_o \rangle$$

$$= \sum_{i,i'} \left(\sum_o \omega_{i,o} \omega_{o,i'}^* \right) \langle \phi_{i'} | O | \phi_i \rangle$$
(5)

where in the last contraction we used the fact that O is supported on part i of Hilbert space. \Box

Theorem 2. If ρ and ρ' act on disjoint Hilbert spaces, then the von-Neumann entanglement entropy satisfies

$$S(\rho \otimes \rho') = S(\rho) + S(\rho')$$

Proof. Since entanglement is invariant under change of basis, we can diagonalize ρ and ρ' and calculate EE using their diagonal elements:

$$\tilde{\rho} = \sum_{i} a_{i} |a_{i}\rangle \langle a_{i}|, \ \tilde{\rho}' = \sum_{j} b_{j} |b_{j}\rangle \langle b_{j}|$$

so the compoiste matrix used in $S(\rho \otimes \rho')$ is

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ho}\otimes ilde{
ho}'=\sum_{ij}a_ib_j\ket{a_ib_j}raket{b_ja_i}$$

$$\log(\tilde{\rho}\otimes\tilde{\rho}') = \sum_{ij} (\log a_i + \log b_j) |a_i b_j\rangle \langle b_j a_i|$$

the total entanglement entropy is thus

$$S(\tilde{\rho} \otimes \tilde{\rho}') = -\sum_{ij} a_i b_j \log(a_i) + a_i b_j \log(b_i)$$

= $-\sum_i a_i \log(a_i) \sum_j b_j - \sum_j b_j \log(b_j) \sum_i a_i$
= $-\sum_i a_i \log(a_i) - b_i \log(b_i)$
= $S(\tilde{\rho}) + S(\tilde{\rho}')$

where we used $Tr(\rho) = 1$ in the 2nd step.

Theorem 3. von-Neumann entanglement entropy is maximal iff there exists a basis in which its (reduced) density matrix is an equally weighted diagonal matrix.

Proof. In a diagonalized reduced density matrix $diag(\epsilon_1, \ldots, \epsilon_n)$, the von-Neumann entropy is

$$S = -\sum_{i} \epsilon_i \log \epsilon_i \quad S.t. \ \sum_{i} \epsilon_i = 1$$

To see its maximum apply Lagrangian multiplier

$$L(\vec{\epsilon}, \lambda) = \sum_{i} -\epsilon_{i} \log \epsilon_{i} - \lambda \left(\sum_{i} \epsilon_{i} - 1\right)$$

by derivative wrt ϵ_j we have

$$\forall \epsilon_i, \quad \log \epsilon_i + 1 + \lambda = 0$$

there's only one constraint characterized by λ , so all ϵ_i must have the same value.

Definition 0.1 (Maximally entangled state). For a bipartite system $A \cup B$, the wavefunction of a maximally entangled state is given by

$$|\psi\rangle = \frac{1}{\sqrt{D}} \sum_{i=1}^{D} |i_A\rangle \otimes |i_B\rangle \tag{6}$$

with $D = \min(\dim \mathcal{H}_A, \dim \mathcal{H}_B), \langle i | i' \rangle = \delta_{i,i'}$.

The interpretation as maximally entangled comes from the fact that

$$\rho_A = \frac{1}{D_A} \mathbb{1}_A$$

where we assumed $D = D_A$ WLOG. As a result, we must have

$$S(\rho_A) = \sum_i \frac{1}{D_A} \log D_A = \log D_A \sim \text{vol } A$$

where $\log D_A \sim \text{vol } A$ is because (assuming 1 qubit per site)

$$\log D_A = \log \left(2^{\text{number of sites in A}}\right) \propto \text{number of sites in A}$$

which is proptional to the volumn of A in a system where dofs are uniformly distributed. This is the famous bound on EE:

$$0 \le S(\rho_A) \le \log D_A \propto \text{vol } A \tag{7}$$