Statistical mechanics of multipartite entanglement

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Entanglement is one of the most intriguing features of quantum mechanics. It is widely used in quantum communication and information processing and plays a key role in quantum computation.

At the same time, entanglement is not fully understood and has many puzzling features. It is deeply rooted into the linearity of quantum theory and in the superposition principle and (for pure states) is essentially and intuitively related to the impossibility of factorizing the state of the total system in terms of states of its constituents.

Let us make an example: consider an ensemble of \( n \) spin-1/2 particles (qubits), whose Hilbert space \( \mathcal{H} = (\mathbb{C}^2)^\otimes n \) has dimension \( N = 2^n \), and divide this set in two balanced parts, \( A \) and \( \bar{A} \), made up of \( n_A \) and \( n_{\bar{A}} \) qubits respectively (\( n = n_A + n_{\bar{A}} \), \( n_A = \lfloor n/2 \rfloor \leq n_{\bar{A}} \) with no loss of generality). The total Hilbert space factorizes in the tensor product \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_{\bar{A}} \), with dimensions \( N_A = 2^{n_A} \) and \( N_{\bar{A}} = 2^{n_{\bar{A}}} \) respectively (\( N = N_A N_{\bar{A}} \)). A pure state

\[
\mathcal{H} \ni |\psi\rangle = \sum_{j=0}^{N-1} z_j |j\rangle, \quad z_j \in \mathbb{C}, \quad \sum_{j=0}^{N-1} |z_j|^2 = 1
\]

(1)
can be conveniently written in terms of the so-called computational basis \( \{|j\rangle\}_{j=0,\ldots,N-1} \), that in turn can be naturally expressed in terms of binary sequences belonging to \( \{0,1\}^n \) (whose decimal representation are the indices \( j \)). Each binary sequence is essentially the collection of the eigenvalues of third Pauli matrices \( \sigma_3 = \text{diag}(1,-1) \), each acting on a single qubit.

We shall say that the state is separable if it can be factorized:

\[
|\psi\rangle = |\psi_A\rangle \otimes |\psi_{\bar{A}}\rangle, \quad \text{with} \quad |\psi_A\rangle \in \mathcal{H}_A, \quad |\psi_{\bar{A}}\rangle \in \mathcal{H}_{\bar{A}}.
\]

(2)
Otherwise \( |\psi\rangle \) is entangled.

The characterization and quantification of entanglement is an open and challenging problem. It is possible to give a good definition of bipartite entanglement, namely when the original ensemble of qubits is divided in two parts, \( A \) and \( \bar{A} \), like before. The problem of
defining *multipartite* entanglement (whatever we mean by this expression) is more difficult and no unique definition exists.

A good bipartite entanglement measure is the so-called *purity* of subsystem $A$, which is defined in terms of the reduced density operator of $A$, $\rho_A = \text{Tr}_{\bar{A}} \rho$ ($\rho = |\psi\rangle\langle\psi|$ being the total density operator):

$$\pi_A = \text{Tr}_A \rho_A^2.$$  \hfill (3)

It is easy to see that $\pi_A = \text{Tr}_A \rho_A^2$ and that

$$\frac{1}{N_A} \leq \pi_A \leq 1.$$  \hfill (4)

Purity $\pi_A = 1$ if and only if $\rho_A$ and $\rho_{\bar{A}}$ are projectors, that is, if the state is separable as in (2). Otherwise, if $\pi_A < 1$, $|\psi\rangle$ is entangled. Moreover, $\pi_A$ saturates its minimum $N_A^{-1} = 2^{-n_A} = 2^{-\lfloor n/2 \rfloor}$ if and only if the reduced density operator of the (smaller) balanced partition $A$ is proportional to the identity matrix $\rho_A = 1/N_A$. In such a case $|\psi\rangle$ is said to be endowed with *maximal bipartite entanglement* [at fixed bipartition $(A, \bar{A})$].

After a preceptive summary of the idea of entanglement, we introduce the notion of *maximally multipartite entangled* (pure) states (MMES) of $n$ qubits as a generalization of the bipartite case. Their bipartite entanglement does not depend on the bipartition and is maximal for all possible bipartitions. In other words, we require

$$\pi_A = \frac{1}{N_A}, \quad \forall \text{ balanced bipartitions } (A, \bar{A}).$$  \hfill (5)

Some examples of MMES for small $n$ are investigated, both analytically and numerically. These states are the solutions of an optimization problem, that can be recast in terms of statistical mechanics.