Maximally multipartite entangled states

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We introduce the notion of maximally multipartite entangled states of n qubits as a generalization of the bipartite case. These pure states have a bipartite entanglement that does not depend on the bipartition and is maximal for all possible bipartitions. They are solutions of a minimization problem. Examples for small n are investigated, both analytically and numerically.

The characterization of multipartite entanglement is no simple matter. The *bipartite* entanglement of a composed quantum system [1] can be consistently defined and quantified in terms of the entropy of entanglement or some physically equivalent quantity. On the other hand, there is no unique way of characterizing the *multipartite* entanglement. Different definitions often do not agree with each other, because they adopt different strategies, focus on different aspects, and capture different features of this quantum phenomenon [2–4]. There is a profound reason behind this problem: the number of measures (i.e., real numbers) needed to quantify multipartite entanglement grows exponentially with the size of the system (e.g., the number of qubits). Therefore, the definition of appropriate entanglement measures, able to summarize the most salient global features of entanglement, can be very difficult and their evaluation bears serious computational difficulties. This difficulty is a characteristic trait of complexity [6], and entanglement is no exception in this respect [7,8]; we shall introduce here multipartite entangled states that bear the symptoms of frustration.

The aim of this Rapid Communication is to explore "maximally" multipartite entangled states of n qubits. These states, to be precisely defined later, are maximally (bipartite) entangled for *all* possible bipartitions. The focus is therefore on the global, partition-independent features of entanglement. We will consider only *pure* states, the extension to mixed states being not straightforward, due to well-known phenomena such as bound entanglement [9].

We consider an ensemble $S=\{1,2,\dots,n\}$ of n qubits in the Hilbert space $\mathcal{H}=(\mathbb{C}^2)^{\otimes n}$, whose state is

$$|\psi\rangle = \sum_{k \in Z_2^n} z_k |k\rangle, \quad z_k \in \mathbb{C}, \quad \sum_{k \in Z_2^n} |z_k|^2 = 1, \quad (1)$$

where $k=(k_i)_{i \in S}$, with $k_i \in Z_2=\{0,1\}$, and

$$|k\rangle = \underset{i \in S}{\otimes} |k_i\rangle, \quad |k_i\rangle \in \mathbb{C}_i^2. \quad (2)$$

In order to analyze the multipartite features of the entanglement shared by the qubits, we proceed as follows. Consider a bipartition $(A,\bar{A})$ of the system, made up of n_A and $n_{\bar{A}}$ qubits, respectively, where $A \subset S$ is a subset of n_A elements, $\bar{A}$

$=S\backslash A$ is its complement, $n_A+n_{\bar{A}}=n$, and we will stipulate $n_A \leq n_{\bar{A}}$ with no loss of generality. The total Hilbert space is accordingly factorized into $\mathcal{H}=\mathcal{H}_A \otimes \mathcal{H}_{\bar{A}}$, with $\mathcal{H}_A=\otimes_{i \in A}\mathbb{C}_i^2$, of dimensions $N_A=2^{n_A}$ and $N_{\bar{A}}=2^{n_{\bar{A}}}$, respectively ($N_A N_{\bar{A}}=N$). As a measure of the *bipartite* entanglement between the two subsets, we consider the purity of subsystem A,

$$\pi_A = \text{Tr}_A \, \rho_A^2, \quad \rho_A = \text{Tr}_{\bar{A}} |\psi\rangle\langle\psi|, \quad (3)$$

Tr_X being the partial trace over subsystem X. We notice that $\pi_A = \pi_{\bar{A}}$ and

$$1/N_A \leq \pi_A \leq 1. \quad (4)$$

State (1) can be written according to the bipartition $(A,\bar{A})$ as

$$|\psi\rangle = \sum_{k \in Z_2^n} z_k |k^A\rangle \otimes |k^{\bar{A}}\rangle, \quad (5)$$

where $|k^A\rangle = \otimes_{i \in A} |k_i\rangle \in \mathcal{H}_A$. By plugging Eq. (5) into Eq. (3), we obtain

$$\pi_A = \sum_{k_i \in Z_2^n} z_{k_1} \bar{z}_{k_2} z_{k_3} \bar{z}_{k_4} \delta_{k_1^A,k_4^A} \delta_{k_2^A,k_3^A} \delta_{k_1^{\bar{A}},k_2^{\bar{A}}} \delta_{k_3^{\bar{A}},k_4^{\bar{A}}}. \quad (6)$$

Notice that for a *given* bipartition, it is very easy to saturate the lower bound $1/N_A$ of Eq. (6): one looks for those maximally *bipartite* entangled states that yield a totally mixed state $\rho_A = \mathbb{1}/N_A$. We will generalize the above property by requiring maximal possible mixedness for *each* subsystem $A \subset S$, given the constraint that the total system be in a pure state. A state endowed with this property will be called a *maximally multipartite entangled state* (MMES).

In the most favorable case, this means that every subsystem A composed of $n_A \leq n/2$ qubits is in a totally mixed state $\rho_A = \mathbb{1}/N_A$ and thus $\pi_A = 1/N_A$ (recall that $\pi_A = \pi_{\bar{A}}$, thus when $n_A > n/2$ the above requirement applies to $\bar{A}$). In fact, it is sufficient to look at maximal subsystems of size $n_A = [n/2]$ ([x]=integer part of x), because the density matrix of every smaller part $B \subset A$ would automatically be of the sought form, $\rho_B = \text{Tr}_{\bar{B} \cap A} \rho_A = \mathbb{1}/N_B$. Therefore, a *perfect* MMES would be maximally entangled for *every* bipartition $(A,\bar{A})$ and would be characterized by $\pi_A = 1/N_A$ for all *balanced* bipartitions. Observe that the requirement of maximal

mixedness for $(A,\bar{A})$, $\pi_A = 1/N_A$, *and the analogous require-ment for a different balanced bipartition $(B,\bar{B})$, with $B \neq A$, might not be compatible with each other, so that, at variance with the bipartite case, perfect MMESs do not necessarily exist.

We define a MMES as a minimizer of what we shall call the *potential of multipartite entanglement*,

$$\pi_{\mathrm{ME}} = \binom{n}{n_A}^{-1} \sum_{|A|=n_A} \pi_A, \qquad (7)$$

where $n_A = [n/2]$. The above quantity is related to the (aver-age) linear entropy $S_L = (1 - \pi_{\mathrm{ME}})N_A/(N_A - 1)$ introduced in [4], which extends ideas put forward in [3]. See also [5]. The quantity π_{ME} measures the average bipartite entanglement over all possible balanced bipartition and thus inherits prop-erty (4), i.e.,

$$1/N_A \leq \pi_{\mathrm{ME}} \leq 1. \qquad (8)$$

The upper bound $\pi_{\mathrm{ME}} = 1$ is attained by the fully factorized states, $z_k = \Pi_{i \in S}\alpha^i_{k_i}$, with $|\alpha^i_0|^2 + |\alpha^i_1|^2 = 1$. On the other hand, the lower bound $\pi_{\mathrm{ME}} = 1/N_A$, if attained, would correspond to a perfect MMES, maximally entangled for every biparti-tion. However, it can happen that the requirements of maxi-mal mixedness for different bipartitions compete with each other. In such a case, the system is frustrated and the mini-mum of the potential (7) is strictly larger than the lower bound in (8), i.e., min $\pi_{\mathrm{ME}} > 1/N_A$. Since in such a situation it may happen that different bipartitions yield different val-ues of π_A, our strategy will be to seek those states among the minimizers that have the smallest variance.

This quest can be recast as an optimization problem: search for the minimum of the cost function

$$\tilde{\pi}_{\mathrm{ME}}(\lambda) = \pi_{\mathrm{ME}} + \lambda\sigma_{\mathrm{ME}}, \qquad (9)$$

where $\lambda \geq 0$ is a Lagrange multiplier and

$$\sigma^2_{\mathrm{ME}} = \binom{n}{n_A}^{-1} \sum_{|A|=n_A} (\pi_A - \pi_{\mathrm{ME}})^2 \qquad (10)$$

is the variance of π_A over all balanced bipartitions. Notice that the introduction of λ enables one to look for a compro-mise between the minimal purity π_{ME} (maximal average en-tanglement) and the minimal standard deviation σ_{ME} of the distribution (maximally distributed entanglement). In gen-eral, the solution of this optimization problem completely defines a class of states with the maximal possible entangle-ment (minimum purity), that is also well distributed, being as insensitive as possible to the particular choice of the biparti-tion.

If $\lambda \gg 1$, the minimization process will yield a very well peaked distribution of π_A around its average: entanglement will be uniformly distributed, but this does not necessarily provide a MMES; for example, a completely separable state has a (vanishing) entanglement that is insensitive to the change of the bipartition ($\pi_A = 1$ for all bipartitions). More interesting is the case $\lambda = 0$; indeed, a solution that minimizes the cost function $\tilde{\pi}_{\mathrm{ME}}(0)$ will have an entanglement distribu-tion centered on the minimum of the potential π_{ME}. There-

fore, if this minimum saturates the lower bound in (8), the width σ_{ME} must vanish. This would be our desideratum. However, it is known that, for $n \geq 8$, perfect MMESs do not exist [4]. The general problem is therefore complicated. As a first step we set $\lambda = 0$ in Eq. (9), and focus on the minimiza-tion of the potential $\pi_{\mathrm{ME}} \equiv \tilde{\pi}_{\mathrm{ME}}(0)$. We shall tackle this prob-lem both analytically and numerically. By plugging Eq. (6) into Eq. (7), one gets after some combinatorics

$$\pi_{\mathrm{ME}} = \sum_{k_i \in Z^n_2} \Delta(k_1,k_2;k_3,k_4)z_{k_1}z_{k_2}\bar{z}_{k_3}\bar{z}_{k_4}, \qquad (11)$$

with

$$\Delta(k_1,k_2;l_1,l_2) = \binom{n}{n_A}^{-1} \sum_{|A|=n_A} \delta_{k^A_1,l^A_1}\delta_{k^A_2,l^A_2}\delta_{k^{\bar{A}}_1,l^{\bar{A}}_2}\delta_{k^{\bar{A}}_2,l^{\bar{A}}_1}$$

$$= g(k_1 \oplus l_1 \vee k_2 \oplus l_2, k_1 \oplus l_2 \vee k_2 \oplus l_1),$$

$$g(a,b) = \binom{n}{n_A}^{-1} \delta_{a \wedge b, 0}\binom{n - |a| - |b|}{n_A - |a|}, \qquad (12)$$

where $a \oplus b = (a_i + b_i \bmod 2)_{i \in S}$ is the XOR operation, $a \vee b = (a_i + b_i - a_i b_i)_{i \in S}$ the OR operation, $a \wedge b = (a_i b_i)_{i \in S}$ the AND operation, and $|a| = \Sigma_{i \in S}a_i$. Equations (11) and (12) yield a closed expression for the average purity that is amenable to analytic and numerical investigation.

In order to further simplify the problem, in the following discussion we will replace $r_k = |z_k|$ in Eq. (1) with its mean value $1/\sqrt{N}$, and focus on the states

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{k \in Z^n_2} e^{i\varphi_k}|k\rangle. \qquad (13)$$

Plugging Eq. (13) into Eq. (6), we find

$$\pi_A = \frac{N_A + N_{\bar{A}} - 1}{N}$$

$$+ \frac{2}{N^2} \sum_{l \neq l', m \neq m'} \cos(\varphi^p_{lm} - \varphi^p_{l'm} + \varphi^p_{l'm'} - \varphi^p_{lm'}), \quad (14)$$

where $\varphi^p_{lm} = \varphi_{p^{-1}(l,m)}$, p being a permutation such that $A = \{p(1), p(2), \ldots, p(n_A)\}$. This is an interesting formula that is worth discussing in detail: (i) first of all, if $\varphi_k = \Sigma_{i \in S}\varphi^i_{k_i}$ in Eq. (13), one obtains separable states, which yield the maximum possible value $\pi_A = 1$ for all bipartitions: indeed the $N(N_A - 1)(N_{\bar{A}} - 1)/4$ cosines in the summation in Eq. (14) are all 1; (ii) the first addendum on the right-hand side corresponds to the average entanglement of typical states [8,10]. Thus, the combination of phases in the summation can increase or re-duce the value of the purity with respect to the typical one (at fixed bipartition); (iii) in order to get a lower value of purity, one should look for combinations of angles that tend to yield negative cosines. On the other hand, it is also clear that for $n > 2$, not all cosines can be -1, as this would yield a purity smaller than $1/N_A$; (iv) at fixed bipartition $(A,\bar{A})$, it is always possible to find combinations of cosines that saturate the lower bound $\pi_A = 1/N_A$. However, when plugged into Eq. (11), the requirement that this lower bound be saturated for

every A might not be satisfiable. This problem is in general n-dependent.

We now explicitly look at the simplest examples. For two qubits, we only have one bipartition and the potential of multipartite entanglement reduces to

$$\pi_{ME}^{(2)} = \frac{3}{4} + \frac{1}{4}\cos(\varphi_0 - \varphi_1 - \varphi_2 + \varphi_3), \qquad (15)$$

where the indices of the phases are expressed in terms of k, in decimal notation. The minimization of the potential consists in solving the equation $\pi_{ME}^{(2)} = \frac{1}{2}$ (remember that $N_A = N_{\bar{A}} = 2$). It is straightforward to obtain $\varphi_0 - \varphi_1 - \varphi_2 + \varphi_3 = \pi$, which yields the MMES

$$|\psi_2\rangle = \frac{1}{2}(e^{i\varphi_0}|0\rangle + e^{i\varphi_1}|1\rangle + e^{i\varphi_2}|2\rangle - e^{i(-\varphi_0+\varphi_1+\varphi_2)}|3\rangle). \qquad (16)$$

In this degenerate case, multipartite entanglement coincides with bipartite entanglement, and this state is obviously equivalent, up to local operations, to a Bell state.

For three qubits, one must look for the solutions of $\pi_{ME}^{(3)} = \frac{1}{2}$, where

$$\pi_{ME}^{(3)} = \frac{5}{8} + \frac{1}{48}\sum_p \left[\cos(\varphi_{p(0)} + \varphi_{p(7)} - \varphi_{p(1)} - \varphi_{p(6)}) + \cos(\varphi_{p(2)}\right.$$
$$+ \varphi_{p(5)} - \varphi_{p(4)} - \varphi_{p(3)}) + 2\cos(\varphi_{p(0)} + \varphi_{p(3)} - \varphi_{p(1)}$$
$$\left. - \varphi_{p(2)}) + 2\cos(\varphi_{p(7)} + \varphi_{p(4)} - \varphi_{p(6)} - \varphi_{p(5)})\right], \qquad (17)$$

where the sum is over the three cyclic permutations (of the qubits). A class of solutions is

$$|\psi_3\rangle = \frac{1}{8}(e^{i\varphi_0}|0\rangle + e^{i\varphi_1}|1\rangle + e^{i\varphi_2}|2\rangle - e^{i(-\varphi_0+\varphi_1+\varphi_2)}|3\rangle + e^{i\varphi_4}|4\rangle$$
$$- e^{i(-\varphi_0+\varphi_1+\varphi_4)}|5\rangle + e^{-i\varphi_6}|6\rangle + e^{i(-\varphi_0+\varphi_1+\varphi_6)}|7\rangle) \qquad (18)$$

and form a five-dimensional submanifold. These states are equivalent, up to local unitaries, to the GHZ state [11] and share the same properties of the GHZ state for what concerns concurrence and one-tangle. Note that $\pi_{ME}^{(3)}$ contains 12 cosines with different arguments, 6 of which are counted twice.

The solution proposed corresponds to 2 cosines=1, 4 cosines=$-\beta$, 4×2 cosines=-1, and 2×2 cosines=β, with $\beta = \cos(\varphi_0 - \varphi_2 - \varphi_4 + \varphi_6)$, that sum up to $2 - 4\beta - 8 + 4\beta = -6$. In fact, there are three families of solutions of the form (13), corresponding to the three submanifolds $M_p = \{\varphi_i | \varphi_{p(0)} + \varphi_{p(7)} - \varphi_{p(1)} - \varphi_{p(6)} = 0$, $\varphi_{p(2)} + \varphi_{p(5)} - \varphi_{p(4)} - \varphi_{p(3)} = 0$, $\varphi_{p(0)} + \varphi_{p(3)} - \varphi_{p(1)} - \varphi_{p(2)} = \pi\}$ with p a cyclic permutation. All three classes yield the same pattern of cosines in $\pi_{ME}^{(3)}$ (β being given by the corresponding permutation).

For a number of qubits larger than 3, we turned to a numerical approach: we generated a typical state of the form (13) and numerically tackled the minimization problem through different kinds of iterative algorithms (for a review of numerical techniques and their implementation, see [12]). We first used deterministic algorithms. In general, we found that minimization is strongly dependent on the initial conditions. Therefore, we sampled a large number of initial states in order to test the reliability of the solutions obtained. Among others, the truncated Newton method gave us the best results in terms of both reliability and speed. The use of stochastic algorithms gave us comparable results. In both cases, the existence of a large number of degenerate (local and global) minima required an accurate analysis.

For $n=4$ qubits, we numerically obtained $\min \pi_{ME}^{(4)} \simeq 0.333 > \frac{1}{4}$ with $\sigma_{ME} \simeq 10^{-4}$. If the requirement $|z_k| = 1/\sqrt{N}$ in Eq. (1) [and Eq. (13)] is relaxed, one can make σ_{ME} vanish. This is a first example of frustration among the bipartitions, which prevents the existence of a perfect MMES. It is curious that the requirement that purity be minimal for all balanced bipartitions generate conflicts already for $n=4$ qubits. This is consistent with results obtained by other authors [13,14].

For $n=5$ and 6, the landscape of the manifold on which the minimization is performed becomes complicated. Nonetheless, we found perfect MMES, namely, solutions for $\pi_{ME}^{(5)} = \frac{1}{4}$ and $\pi_{ME}^{(6)} = \frac{1}{8}$, respectively. Therefore, and curiously, frustration is present for $n=4$ qubits while it is absent for $n=5$ and 6. For example, a 5-qubit perfect MMES is defined by Eq. (13) with the following set of phases:

$$(\varphi_k) = (0,0,0,0,0,\pi,\pi,0,0,\pi,\pi,0,0,0,0,0,0,0,\pi,\pi,0,\pi,0,\pi,\pi,0,\pi,0,\pi,\pi,0,0) \qquad (19)$$

and lives on a seven-dimensional manifold. The distribution of the angles $x = \varphi_{jl}^p - \varphi_{jl'}^p + \varphi_{j'l'}^p - \varphi_{j'l}^p$, for a given 6-qubit MMES is displayed in Fig. 1. We observe interesting features, shared by all the MMESs we investigated and for all values of n: first of all, the distribution is symmetric around $x = \pi$; second, there is a large number of instances such that $\cos x = -1$, partially compensated by the contribution of $\cos x = 1$; third, the distribution of the remaining angles is symmetric around $x = \pi/2$ and yields a vanishing contribution to π_{ME}.

For $n=7$, we numerically found configurations with

$\min \pi_{ME}^{(7)} \simeq 0.134 > \frac{1}{8}$ and $\sigma_{ME} \simeq 10^{-2}$, which improves previous bounds [4,14]. By minimizing the cost function (9) with a nonvanishing λ, one can reduce σ_{ME} to $\simeq 10^{-3}$ at the expense of a higher $\pi_{ME} \simeq 0.136$. It is not clear at present if the impossibility of reaching the absolute minimum for $n=7$ is to be ascribed to the numerical procedure. For $n=8$ and 9, where perfect MMESs do not exist [4], the convergence of the numerical simulations becomes very slow. This is a typical signature of frustration. The numerical results show that, in order to obtain a vanishing width of the distribution for frustrated systems, it is necessary to increase the value of the
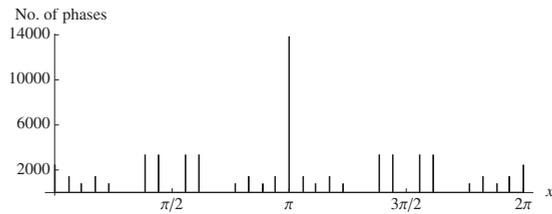
FIG. 1. Distribution of the arguments x of the cosines in $\pi_{\mathrm{ME}}^{(6)}$, for a given 6-qubit MMES. Notice the symmetries around π and $\pi/2$. The total number of phases is 62 720. Different phases are fully resolved by the binning.

TABLE I. Perfect MMESs for different n.

n	Perfect MMESs
2,3,5,6	exist
4	do not exist
7	?
≥ 8	do not exist

average of the purity. These conclusions are summarized in Table I.

A comment is now in order. Although in this Rapid Communication perfect MMESs are exhibited as minimizers of the potential of entanglement, they are, by their very nature, independent of the method used to find them. In fact, by virtue of their maximal mixedness, they saturate all measures of multipartite entanglement. This is the case, for example, of the global entanglement measure of Meyer and Wallach [3], as well as its generalizations. Indeed, any entanglement monotones, being functions of the partial density matrices of subsystems of qubits, attain their maximal values on perfect MMESs. The minimization procedure we propose is just a convenient way to construct them. For nonperfect MMESs, due to a possible finite value of σ_{ME}, different measures of entanglement can resolve a part of the degeneracy of the manifold of minimizers.

It is interesting to briefly discuss one straightforward potential application. Consider the 5-qubit perfect MMES $|\psi_5\rangle$ defined by Eqs. (13) and (19). One can easily prove that

$$\langle \psi_5 | \sigma_1^z \sigma_2^z \sigma_3^y \sigma_4^y \sigma_5^z | \psi_5 \rangle = 1, \tag{20}$$

where σ_i^y and σ_i^z are Pauli matrices. Therefore, the single- and two-qubit statistics are always "flat," but the measurements of the observables in Eq. (20) are always strictly cor-

related. *Any* two parties, which can be far apart, can therefore share a cryptographic key only if the other three parties agree on measuring their respective observables in Eq. (20) and making their results public. Notice that the key is shared by the two parties but is unknown to the other three. We call this phenomenon majority-agreed key distribution.

In conclusion, we introduced a class of multipartite entangled states that maximize the amount and distribution of entanglement. The features of these states depend strongly on the number of qubits involved. In our numerical search, we noticed that already for a relatively small number of qubits ($n \geq 7$), the landscape of the parameter space where the optimization procedure is performed has a complex structure with a large number of local minima and a very slow convergence. The presence of frustration, due to the competition among different partitions (observed already for $n=4$), appears to be a general feature of many-body systems. It prevents the possibility to find perfect MMESs but introduces interesting perspectives. In this sense, the minimization task is a problem that requires a careful analysis and the use of numerical and analytical strategies from different research fields. In this paper, we just started to explore these connections. Thus, the study of maximally multipartite entangled states paves the way toward a deeper comprehension of the complex structure of quantum correlations arising in many-body systems.

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