Local Hamiltonians for Maximally Multipartite Entangled States

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We study the conditions for obtaining maximally multipartite entangled states (MMES) as non-degenerate eigenstates of Hamiltonians that involve only short-range interactions. We investigate small-size systems (with a number of qubits ranging from 3 to 5) and show some example Hamiltonians with MMES as eigenstates.

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I. INTRODUCTION

The elusive features of multipartite entanglement are attracting increasing attention lately. While in the bipartite case different mathematical definitions are physically equivalent [1–5], a unique characterization of multipartite quantum correlations does not exist, and interesting alternative proposals are possible [4–8], that highlight different features of this inherently quantum phenomenon, including links with complexity and frustration [9]. The interest in multipartite entanglement is motivated by possible applications in quantum enhanced tasks, but also by genuine foundational aspects.

We proposed that the multipartite entanglement of a system of qubits can be characterized in terms of the distribution function of bipartite entanglement (e.g., purity) over all possible bipartitions of the qubits [10]. This led us to formulate the notion of “maximally multipartite entangled states” (MMES), as those states for which average purity (over all balanced bipartitions) is minimal. This notion can be extended to continuous variable systems [11,12] and unveils novel applications, such as quantum teamwork [11] and controlled qubit teleportation [13].

By their very definition, MMES exhibit very strong and distributed non-local correlations. This naturally leads to the following question: can MMES be obtained by making use of Hamiltonians that only involve local interactions? In the context of spin systems (that mostly concerns us here), “local” means both few-body and nearest-neighbors. For example, it would be remarkable if one could find Hamiltonians containing up to 2-body interaction terms, whose ground state is a MMES. If this were impossible, one could soften the requirement and ask whether can one find Hamiltonians containing up to 2-body interaction terms, whose eigenstate is a MMES. This is the problem we intend to tackle in the present paper. A similar problem was analyzed in the context of GHZ states [14,16].

This article is organized as follows. In Section II we review the notion of maximally multipartite entangled state. In Section III we sketch out our general strategy for the search of MMES as eigenstates of Hamiltonians with short range interactions. In Section IV we explicitly construct Hamiltonians having a MMES as an eigenstate for a number of qubits ranging from 3 to 5. This is of interest in few-qubit applications. We conclude with a discussion on possible perspectives and applications.

II. MAXIMALLY Multipartite Entangled States

Let a system of \( n \) qubits be in a pure state \( |\psi\rangle \in \mathcal{H} \), which is the only case we will consider henceforth. We consider a partition \((A,\bar{A})\) of the system \( S = \{1,2,\ldots,n\} \), made up of \( n_A \) and \( n_{\bar{A}} \) qubit, respectively, with \( n_A + n_{\bar{A}} = n \) and \( n_A < n_{\bar{A}} \) with no loss of generality. Purity reads

\[
\pi_A = \text{Tr}(\rho_A^2),
\]

where

\[
\rho_A = \text{Tr}_{\bar{A}}(|\psi\rangle\langle\psi|)
\]

is the reduced density matrix of party \( A \). Purity ranges between

\[
\frac{1}{2^{n_A}} \leq \pi_A \leq 1,
\]

where the upper bound 1 is reached by unentangled, factorized states with respect to the bipartition \((A,\bar{A})\). On the other hand, the lower bound is obtained for maximally bipartite entangled states, whose reduced density matrix is completely mixed:

\[
\rho_A = \frac{1}{2^{n_A}} \mathbb{I}_A,
\]

where \( \mathbb{I}_A \) is the identity operator on the Hilbert space of subsystem \( A \).

The extension of this treatment to the multipartite scenario is based on the average purity (“potential of multipartite entanglement”) [10,17]

\[
\pi_{\text{ME}}(|\psi\rangle) = \frac{1}{C_{n_A}} \sum_{|A|=n_A} \pi_A,
\]
where $C_n^m$ is the binomial coefficient, $|A|$ is the cardinality of the set $A$ and the sum is over balanced bipartitions $n_A = [n/2]$, $[\cdot]$ denoting the integer part. The quantity $\pi_{\text{ME}}$ in Eq. (5) measures the average bipartite entanglement over all possible balanced bipartitions and inherits the bounds (3) (with $n_A = [n/2]$)

$$\frac{1}{2^{[n/2]}} \leq \pi_{\text{ME}}(\psi) \leq 1.$$  

A maximally multipartite entangled state (MMES) [10] $|\varphi\rangle$ is a minimizer of $\pi_{\text{ME}}$,

$$\pi_{\text{ME}}(|\varphi\rangle) = \pi_0^{(n)},$$

$$\pi_0^{(n)} = \min\{\pi_{\text{ME}}(\psi) \mid |\psi\rangle \in \mathcal{H}_S, (\psi|\psi) = 1\}.$$  

Given a quantum system whose (pure) state is a MMES, the density matrix of each one of its subsystems $A \subset S$ is as mixed as possible (given the constraint that the total system is in a pure state), so that the information contained in a MMES is as distributed as possible. The average purity (5) is related to the average linear entropy (7) and inherits the property (8).

We notice that a necessary and sufficient condition for a state to be a perfect MMES is to be maximally entangled with respect to balanced bipartitions. On the other hand, this requirement can be too strong: it can be shown that perfect MMES do not exist for $n > 8$ [17].

### III. GENERAL STRATEGY

The problem of finding a Hamiltonian involving local (two-body and nearest-neighbor) interactions and on-site external magnetic fields, one of whose eigenstates is a MMES is non-trivial. As a matter of fact, as we explained in the Introduction, MMES exhibit strongly non-local correlations, which, in principle, could be impossible to obtain by using only local terms. On the other hand, it is trivial to find Hamiltonians involving non-local interaction terms, whose ground state is an $n$-qubit MMES: consider $n$ qubits on a circle and the Hamiltonian

$$H(\epsilon, \mathcal{K}) = \epsilon \mathcal{P} + H^\perp(\mathcal{K}),$$

where $\mathcal{P} = |\varphi\rangle\langle\varphi|$ is the projection on the MMES $|\varphi\rangle$ and $H^\perp$ is a Hermitian operator depending on the set of parameters $\mathcal{K}$ and satisfying

$$\mathcal{P} H^\perp \mathcal{P} = 0.$$  

If $H^\perp = 0$ and $\epsilon < 0$, the MMES $|\varphi\rangle$ is by construction the non-degenerate ground state for $H$. This simple observation enables us to define our problem more precisely. The Hamiltonian (9) can be separated into a local part, in the sense defined above, and a nonlocal part, that contains all other interaction terms:

$$H(\epsilon, \mathcal{K}) = H_{\text{loc}}(\epsilon, \mathcal{K}) + H_{\text{nonloc}}(\epsilon, \mathcal{K}).$$  

Our desideratum is to find a set of parameters $(\bar{\epsilon}, \bar{\mathcal{K}})$ such that $H_{\text{nonloc}}(\bar{\epsilon}, \bar{\mathcal{K}}) = 0$, so that the MMES $|\varphi\rangle$ is a non-degenerate eigenstate (possibly the ground state). Clearly, this requirement might be impossible to satisfy. In the following we will consider some explicit examples for systems of 3, 4, and 5 qubits.

### IV. ENCODING A MMES INTO THE EIGENSTATE OF A HAMILTONIAN

#### A. Three qubits

For a system of three qubits, MMES are equivalent by local unitaries to the GHZ states:

$$|G^\perp_1\rangle = \frac{1}{\sqrt{2}}(|000\rangle \pm |111\rangle),$$

$$|G^\perp_2\rangle = \frac{1}{\sqrt{2}}(|001\rangle \pm |110\rangle),$$

$$|G^\perp_3\rangle = \frac{1}{\sqrt{2}}(|010\rangle \pm |101\rangle),$$

$$|G^\perp_4\rangle = \frac{1}{\sqrt{2}}(|011\rangle \pm |100\rangle),$$

where we have used the conventions $\sigma^z|0\rangle = |0\rangle$ and $\sigma^z|1\rangle = -|1\rangle$, $\sigma^z$ being the third Pauli matrix. Since these states form a basis of the Hilbert space of the system, the most generic Hamiltonian can be written as

$$H = \sum_{i=1}^{4} (\epsilon_i^+ \mathcal{P}_i^+ + \epsilon_i^- \mathcal{P}_i^-) + H_M,$$

where

$$\mathcal{P}_i^\pm = |G^\perp_i\rangle\langle G^\perp_i|$$

are the projections on the GHZ basis states and $H_M$ is a Hermitian operator containing terms of the form

$$|G^\perp_i\rangle\langle G^\perp_j| + \text{H.c. with } i \neq j.$$  

We notice that each projection can be decomposed in two terms

$$\mathcal{P}_i^\pm = \mathcal{Q}_i \pm \mathcal{C}_i,$$

where $\mathcal{Q}_i$ contains products of two Pauli matrices, while $\mathcal{C}_i$ includes cubic terms. For example, $\mathcal{P}_1^-$ can be decom-
posed in the following operators:

\[
Q_1 = \frac{1}{2} \left( |000\rangle\langle000| + |111\rangle\langle111| \right),
\]
\[
= \frac{1}{8} \left( \mathds{1} + \sigma^+_1 \sigma^+_2 + \sigma^+_2 \sigma^+_3 + \sigma^+_1 \sigma^+_3 \right)
\]
\[
C_1 = \frac{1}{2} \left( |000\rangle\langle111| + |111\rangle\langle000| \right)
\]
\[
= \frac{1}{8} \left( \sigma^+_1 \sigma^+_2 \sigma^+_3 - \sigma^-_1 \sigma^-_2 \sigma^-_3 - \sigma^+_1 \sigma^-_2 \sigma^-_3 - \sigma^-_1 \sigma^+_2 \sigma^-_3 \right)
\]

(20)

The decomposition in Eq. (19) enables us to rewrite the Hamiltonian [16]:

\[
H = \sum_{i=1}^{4} (\epsilon^+_i + \epsilon^-_i) Q_i + \sum_{i=1}^{4} (\epsilon^+_i - \epsilon^-_i) C_i + H_M.
\]

(22)

We notice that cubic terms in the operators \(C_i\) are absent in \(H_M\), and the \(C_i\)'s are orthogonal to each other

\[
C_i C_j = 0 \quad \forall i \neq j.
\]

(23)

Thus, the only way to cancel such cubic terms is to impose

\[
\epsilon^+_i = \epsilon^-_i \quad \forall i.
\]

(24)

This equality immediately implies that

\[
\langle G^+_i | H_2 | G^+_i \rangle = \langle G^-_i | H_2 | G^-_i \rangle, \quad \forall i,
\]

(25)

where

\[
H_2 = \sum_{i,j,\alpha,\beta} C_{ij}^{\alpha \beta} \sigma_i^\alpha \sigma_j^\beta
\]

(26)

denotes a local Hamiltonian (cubic couplings are absent). As a consequence, the state \(|G^+_1\rangle\) (and any equivalent state by local unitaries) can never be the non-degenerate ground state of \(H_2\). Indeed, let us suppose that \(|G^+_1\rangle\) is the ground state of \(H_2\), whose spectrum ranges from \(E_0\) to \(E_{\text{max}}\). If \(|G^+_1\rangle\) is also an eigenstate, then \(E_0\) is degenerate, since condition (25) must hold; if \(|G^+_1\rangle\) is not an eigenstate, then we must have

\[
E_0 < \langle G^-_1 | H_2 | G^-_1 \rangle < E_{\text{max}}
\]

(27)

and thus, as a consequence of Eq. (25), \(|G^+_1\rangle\) cannot be the ground state.

This result shows that it is impossible for a three-qubits MMES to be the non-degenerate ground state of a local Hamiltonian. On the other hand, we now try to understand whether there exists a condition such that \(|G^+_1\rangle\) is a non-degenerate (excited) eigenstate. The most general two-body (local) Hamiltonian is

\[
H_2 = \sum_{i<j} \left( J^{xy}_{ij} \sigma^x_i \sigma^y_j + J^{y}_{ij} \sigma^y_i \sigma^y_j + J^{z}_{ij} \sigma^z_i \sigma^z_j \right)
\]
\[
+ \sum_{i \neq j} \left( K_{ij} \sigma^x_i \sigma^y_j + X_{ij} \sigma^z_i \sigma^z_j + Y_{ij} \sigma^y_i \sigma^x_j \right)
\]
\[
+ \sum_{i} \left( h^x_i \sigma^x_i + h^y_i \sigma^y_i + h^z_i \sigma^z_i \right).
\]

(28)

By explicit calculation, it is possible to see that \(|G^+_1\rangle\) is an eigenstate of \(H_2\) if and only if the parameters satisfy the following conditions:

\[
\sum_{i=1}^{3} h^x_i = 0
\]
\[
\sum_{j \neq i} X_{ij} = 0 \quad \text{for} \quad i = 1, 2, 3,
\]
\[
\sum_{j \neq i} Y_{ij} = 0 \quad \text{for} \quad i = 1, 2, 3,
\]
\[
h^x_1 = J^{xy}_{12} - J^{xy}_{13}, \quad h^x_2 = J^{xy}_{21} - J^{xy}_{23}, \quad h^x_3 = J^{xy}_{31} - J^{xy}_{32},
\]
\[
h^y_1 = K_{12} + K_{13}, \quad h^y_2 = K_{23} + K_{32}, \quad h^y_3 = K_{13} + K_{21}.
\]

(29-34)

Thus, the Hamiltonian \(H_2\) has 23 free parameters.

It is important to notice that the requirement that \(|G^+_1\rangle\) be an eigenstate does not have any influence on the coupling between two qubits along the \(z\)-axis; actually, terms of the form \(\sigma^x_1 \sigma^x_2\) are the only ones that leave the GHZ state invariant.

To understand whether \(|G^+_1\rangle\) is degenerate is not straightforward. The task can be simplified by reducing the number of free parameters satisfying Eqs. (29)-(34). We consider a model in which the qubits are coupled along the \(x\) and \(z\) axes in a uniform external field acting along \(x\):

\[
H_{Jk} = J \sum_{i=1}^{3} \sigma^x_i \sigma^x_{i+1} + k \sum_{i=1}^{3} \left( \sigma^y_i \sigma^x_{i+1} - \sigma^x_i \sigma^y_{i+1} \right),
\]

(35)

with periodic boundary conditions. The state \(|G^+_1\rangle\) corresponds to the eigenvalue 3\(J\), which is non-degenerate if and only if

\[
J \neq 0, \quad k \neq 0, \quad J \neq -\frac{k}{2}.
\]

(36)

As has been argued, the GHZ cannot be the ground state of \(H_{Jk}\); it corresponds to the first non-degenerate excited state if the system is completely ferromagnetic \((J < 0\) and \(k < 0\)) or if \(k > 0\) and \(J < -k/2\). In the latter case, the ground state \(|\text{GS}\rangle\) is not a MMES but has a large value of entanglement, with \(\pi_{\text{ME}} \lesssim 0.556\). [Recall that in Eq. (48) \(\sigma_0^{(3)} = 1/2\)]. Thus, we have found a range of values for the parameters of the local Hamiltonian such that the two lowest energy states contain a large amount of multipartite entanglement. Figure 11 shows the dependence on the parameters \(J\) and \(k\) of the potential of multipartite entanglement \(\pi_{\text{ME}}\) for the ground state of the Hamiltonian (35).

### B. Four qubits

In the case of four qubits it is known that perfect MMESs do not exist [10,17,21,23]. Numerical and analytical analyses show that the minimum of the potential...
In fact, it can be verified that the three- and four-qubits be a non-degenerate ground state of a local Hamiltonian.

Four qubit, it can be shown that the MMES (37) cannot mixed tensor products of the basis. Also in the case of states and $H \epsilon$ By definition, $M$ is a (Hermitian) linear combination of the $|M_4^1\rangle$ corresponds to the constant value $J \epsilon 2\sqrt{J^2 - 2Jk + 4k^2}.$

of multipartite entanglement is $E^{(4)} = 1/3 > 1/4$. In this section we will search for local Hamiltonians having a non-degenerate eigenstate (possibly the ground state), corresponding to the uniform real state $|\psi\rangle$ determined by the coefficients

$$
\zeta^{(4)} = \{1, 1, 1, 1, 1, 1, -1, -1, -1, 1, -1, 1, -1, 1, 1, 1, -1\}.
$$

This case can be treated in the same way as the three-qubit system: we can construct a basis formed by 16 MMES, which will be labelled as $|M_4^1\rangle$, all equivalent by local unitaries. The generic Hamiltonian acting on the Hilbert space of the system can be written as

$$
H = \sum_{i=1}^{16} \epsilon_i M_4^1 + H_M
$$

where $M_4^1$ is the projection on the basis state $|M_4^1\rangle$. In particular we have

$$
M_4^1 = \frac{1}{16}(\sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2 + \sigma_z^1 \sigma_z^2 + \sigma_x^1 \sigma_y^2 + \sigma_x^2 \sigma_y^1 + \sigma_y^1 \sigma_y^2 + \sigma_z^1 \sigma_z^2 + \sigma_z^2 \sigma_z^1 + \sigma_x^2 \sigma_z^1 + \sigma_y^2 \sigma_z^1 - \sigma_z^1 \sigma_z^2 - \sigma_z^2 \sigma_z^1 + \sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2 + \sigma_z^1 \sigma_z^2 + \sigma_z^2 \sigma_z^1).
$$

By definition, $\epsilon_i$ are the expectation values on the basis states and $H_M$ is a (Hermitian) linear combination of the mixed tensor products of the basis. Also in the case of four qubit, it can be shown that the MMES (37) cannot be a non-degenerate ground state of a local Hamiltonian. In fact, it can be verified that the three- and four-qubits couplings present in (40) and in the other projections $M_4^2$ are absent in $H_M$. As a consequence, the expectation value of the residual Hamiltonian on a basis state must be equal to that of the other three states. By an argument similar to that used in the case of three qubits, we find that, if the state (37) is the ground state of a two-body (not necessarily local) Hamiltonian, it is at least four-fold degenerate. The search for the most general local Hamiltonian having $|M_4^1\rangle$ as an eigenstate has led to 24 independent terms which leave the state $|M_4^1\rangle$ invariant, except for an overall constant. They are graphically illustrated in Fig. 2. For the meaning of the symbols, see the caption.

The most evident characteristic of these terms is the abundance of interactions coupling Pauli matrices along different axis. The presence of these interactions is necessary if we want the eigenstate $|M_4^1\rangle$ to be non-degenerate. General conditions for non-degeneracy are very difficult to find if the coupling parameters are generic. Such conditions can be obtained more easily in a simplified Hamiltonian, which depends only on a small number of param-
The purity of the state where \(\psi_{\text{MMES}}\) is a perfect MMES. The most general Hamiltonian acting on the Hilbert space of the system which is formed only of the basis vectors. We again choose to consider a uniform open chain rather than on a ring. The eigenstate \(|M^1_4\rangle\), corresponding to the eigenvalue \(2J\), is non-degenerate if the following conditions hold

\[
J \neq 0, \quad k \neq 0, \quad J \neq \pm \sqrt{\frac{3}{2}}k, \quad J \neq \pm \sqrt{3}k. \tag{42}
\]

Despite the model dependence on a small number of parameters, it is not easy to analytically determine the position of the excited eigenstate \(|M^1_4\rangle\) in the spectrum. Thus, we turned to a numerical analysis: after generating \(4 \cdot 10^4\) random coupling parameters (uniformly distributed in \([-1, 1]^2\)], we found that the average position of the eigenvalue \(2J\) is in the centre of the energetic band; in the best case \(|M^1_4\rangle\) is the second excited state (as it cannot be the ground state).

C. Five qubits

For a system of five qubits, where perfect MMESs do exist \([10]\), we proceed in the same way as in the case of four qubits. We again choose to consider a uniform MMES

\[
|M^1_5\rangle = \frac{1}{4\sqrt{\pi}} \sum_{i=0}^{31} \zeta^{(5)}_i |k\rangle, \tag{43}
\]

with

\[
\zeta^{(5)} = \{1, 1, 1, 1, 1, -1, -1, 1, 1, -1, -1, 1, 1, 1, 1, 1, -1, -1, 1, -1, 1, -1, 1, -1, -1, 1, 1\}. \tag{44}
\]

The purity of the state \(|M^1_4\rangle\) is minimal for any bipartition and such a state is, therefore, a perfect MMES. As in the case of four qubits, we can construct a basis of the Hilbert space of the system which is formed only by MMES. The most general Hamiltonian acting on the Hilbert space of the system is

\[
H = \sum_{i=1}^{32} \epsilon_i |M^1_5\rangle \langle M^1_5| + H_M, \tag{45}
\]

where \(M^1_5 = |M^1_5\rangle \langle M^1_5|\) is a projection and \(H_M\) is an Hermitian linear combination of the mixed tensor products of the basis vectors.

\[
H_{jk} = J(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + k(\sigma_i^z \sigma_j^z + \sigma_i^x \sigma_j^x - \sum_{i=1}^4 \sigma_i^z). \tag{41}
\]

The Hamiltonian \((41)\) contains interactions of the form \(\sigma_i^x \sigma_j^x\) and the coupling to an external field along the \(z\)-axis. We notice that it does not couple qubits 3 and 4 to each other and, therefore, it can be implemented on an open chain rather than on a ring. The eigenstate \(|M^1_4\rangle\), corresponding to the eigenvalue \(2J\), is non-degenerate.

We have investigated whether it is possible to obtain \(n\)-qubit MMES (for \(2 \leq n \leq 5\)) as eigenstates of

\[
\begin{align*}
\text{FIG. 3: (Color online) Graphic representation of all the elementary local Hamiltonians having } |M^1_5\rangle \text{ as an eigenstate. The meaning of the symbols is analogous to that in Fig. 2.}
\end{align*}
\]
Hamiltonians involving only local (few-body and nearest-neighbors) interactions and fields. Since MMES exhibit very distributed non-local correlations, the answer to this problem is nontrivial. We found that MMES are the non-degenerate ground state only for $n = 2$. Already for $n = 3$ the requirement that a MMES be the non-degenerate ground state must be relaxed, and one finds that MMES can at most be the first non-degenerate excited state. This can be interpreted as a manifestation of entanglement frustration [9, 25, 26]. For $n = 4$ we found, in a restricted family of Hamiltonians, a MMES only as the second non-degenerate excited eigenstate.

Besides its foundational interest, the present work is also motivated by few-qubit applications. Most, if not all, practically realizable quantum tasks involve only a very small number of qubits. The most advanced quantum applications require that these qubits be prepared in highly entangled states with high fidelity. One expects that more performing applications would become possible by making use of MMES: some examples were proposed in [11–13]. This clearly calls for efficient methods to prepare/generate MMES with large yield and efficiency. For example, if a MMES were the ground state of some Hamiltonian $H$, then clearly one could engineer it by constructing $H$ and letting the system relax toward its ground state. However, since this is not the case, one must consider a partial relaxation combined with control techniques or devise alternative strategies. Another possible mechanism for generating MMES is dynamical rather than static. This is obviously related to the degree of complexity of a quantum circuit that generates MMES using, for instance, two-qubit gates. Future investigations will be surely devoted to this subject.

From the above mentioned point of view, due to the small number of qubits considered, it would be interesting to study the possibility of using presently realizable quantum systems with a proper engineering of the interaction terms for generating MMES. Finally, the physical conditions and strategies that would enable one to efficiently prepare states with large entanglement, such as MMES, can be clearly generalized to other classes of entangled states. Work is in progress in this direction.

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