Only n-Qubit Greenberger-Horne-Zeilinger States Are Undetermined by Their Reduced Density Matrices

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The generalized n-qubit Greenberger-Horne-Zeilinger (GHZ) states and their local unitary equivalents are the only states of n qubits that are not uniquely determined among pure states by their reduced density matrices of $n-1$ qubits. Thus, among pure states, the generalized GHZ states are the only ones containing information at the n-party level. We point out a connection between local unitary stabilizer subgroups and the property of being determined by reduced density matrices.

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Quantifying and characterizing multiparty quantum entanglement is a fundamental problem in the field of quantum information. Roughly speaking, one expects the states that are "most entangled" to be the most valuable resources for carrying out quantum information processing tasks such as quantum communication and quantum teleportation, and to give the most striking philosophical implications in terms of the rejection of local hidden variable theories [1].

Although no single definition of "most entangled" seems possible, since we know that multiparty entanglement occurs in many types that admit at best a partial order [2], it is still worthwhile to consider properties that carry some of the spirit of most entangled.

One such property is the failure of a state to be determined by its reduced density matrices. As reduced density matrices contain correlation information pertaining to fewer than the full number of parties in the system, states exhibiting entanglement involving all parties must possess information beyond that contained in their reduced density matrices. Linden, Popescu, and Wootters put forward this suggestion in [3,4] and proved the surprising result that almost all n-party pure states are determined by their reduced density matrices. In other words, the set of n-party pure states undetermined by their reduced density matrices is a set of measure zero. In [5], Diósi gave a constructive method that succeeds in almost all cases for determining a 3-qubit pure state from its reduced density matrices. Nevertheless, the question of precisely which states are determined by their reduced density matrices remained open.

In this Letter, we show that the only n-qubit states that are undetermined among pure states by their reduced density matrices are the generalized n-qubit Greenberger-Horne-Zeilinger (GHZ) states,

$$\alpha|00\cdots 0\rangle + \beta|11\cdots 1\rangle, \qquad \alpha, \beta \neq 0$$

and their local unitary (LU) equivalents. This means that, among pure states, the generalized GHZ states are the only ones containing information at the n-party level. For the case $n = 3$, this result was reported previously in [3]. Part of our argument employs the methods of [5] in an essential way.

Let D_n be the set of n-qubit density matrices. If $\rho \in D_n$ is an n-qubit density matrix, and $j \in \{1, \ldots, n\}$ is a qubit label, we may form an $(n-1)$-qubit reduced density matrix $\rho_{(j)} = \mathrm{tr}_j \rho$ by taking the partial trace of ρ over qubit j. Let

$$\mathrm{PTr}: D_n \rightarrow D_{n-1}^n$$

be the map $\rho \mapsto (\rho_{(1)}, \ldots, \rho_{(n)})$ that associates to ρ its n tuple of $(n-1)$-qubit reduced density matrices. The map PTr is neither injective (one-to-one) nor surjective (onto). Its failure to be surjective means that there are n tuples of $(n-1)$-qubit density matrices that cannot be produced from any n-qubit density matrix by the partial trace. The question of whether a collection of $(n-1)$-qubit reduced density matrices could have come from an n-qubit density matrix by the partial trace is the subject of recent and ongoing investigations [6,7]. The failure of PTr to be injective means that multiple n-qubit states can have the same reduced density matrices. States $\rho_1 \neq \rho_2$ with $\mathrm{PTr}(\rho_1) = \mathrm{PTr}(\rho_2)$ require more information for their determination than is contained in their $(n-1)$-qubit reduced density matrices.

Let

$$P_n = \{\rho \in D_n | \rho^2 = \rho\}$$

be the set of pure n-qubit states. If we are interested primarily in pure states, we can restrict the partial trace map to pure n-qubit states.

$$\mathrm{ptr} = \mathrm{PTr}|_{P_n}: P_n \rightarrow D_{n-1}^n.$$

Given a pure state ψ with $|\psi\rangle\langle\psi| \in P_n$, the set $\mathrm{ptr}^{-1}[\mathrm{ptr}(\psi)]$ contains all pure states with the same reduced density matrices as ψ. [We abbreviate $\mathrm{ptr}(\psi) = \mathrm{ptr}(|\psi\rangle \times \langle\psi|)$.]

We define a state ψ to be determined among pure states if $\mathrm{ptr}^{-1}[\mathrm{ptr}(\psi)]$ contains only $|\psi\rangle\langle\psi|$, and undetermined among pure states if $\mathrm{ptr}^{-1}[\mathrm{ptr}(\psi)]$ contains more than one state. Similarly, we define a state $\rho \in D_n$ to be determined among arbitrary states if $\mathrm{PTr}^{-1}[\mathrm{PTr}(\rho)]$ contains only ρ, and undetermined among arbitrary states if $\mathrm{PTr}^{-1}[\mathrm{PTr}(\rho)]$ contains more than one state.

The surprising result of Linden and Wootters [4] is that almost all n-qubit pure states are determined among arbitrary states.

Nevertheless, there are pure states that are undetermined among pure states (and consequently undetermined among arbitrary states). For example, consider the one-parameter family of n-qubit states

$$|\eta\rangle = \frac{1}{\sqrt{2}}|00\cdots 0\rangle + \frac{\eta}{\sqrt{2}}|11\cdots 1\rangle,$$

where η is a complex number with magnitude 1. If $\eta_1 \neq \eta_2$, then $|\eta_1\rangle$ and $|\eta_2\rangle$ are different states with different density matrices $|\eta_1\rangle\langle\eta_1| \neq |\eta_2\rangle\langle\eta_2|$, yet they share the same reduced density matrices; that is, $\mathrm{ptr}(|\eta_1\rangle \times \langle\eta_1|) = \mathrm{ptr}(|\eta_2\rangle\langle\eta_2|)$.

We see that almost all pure n-qubit states are determined among pure states, yet n-qubit GHZ states are undetermined among pure states. The question then becomes, precisely which states ψ are undetermined among pure states?

Main result.—An n-qubit state ψ is undetermined among pure states if and only if ψ is LU equivalent to a generalized n-qubit GHZ state.

Proof.—Let ψ be an n-qubit pure state.

Suppose that ψ is LU equivalent to a generalized n-qubit GHZ state, so we have

$$U|\psi\rangle = \alpha|00\cdots 0\rangle + \beta|11\cdots 1\rangle,$$

where U is a local unitary transformation. Define $U|\psi'\rangle = \alpha|00\cdots 0\rangle - \beta|11\cdots 1\rangle$. Then $|\psi\rangle\langle\psi| \neq |\psi'\rangle\langle\psi'|$, since $\alpha\beta \neq 0$, but $\mathrm{ptr}(\psi) = \mathrm{ptr}(\psi')$. Hence, ψ is undetermined among pure states.

Conversely, suppose that $|\psi\rangle$ is undetermined among pure states. Then there is an n-qubit state vector $|\psi'\rangle \neq e^{i\alpha}|\psi\rangle$ that has the same reduced density matrices as $|\psi\rangle$.

Claim: If $|\psi\rangle$ and $|\psi'\rangle$ have the same reduced density matrices, then for each qubit $j \in \{1, \ldots, n\}$, there is a one-qubit local unitary transformation L_j such that $|\psi'\rangle = L_j|\psi\rangle$.

To prove this, let $j \in \{1, \ldots, n\}$ be a qubit label. Let ρ_j denote the one-qubit reduced density matrix of $|\psi\rangle$ for qubit j. We write ρ_j as a spectral decomposition,

$$\rho_j = \sum_{i_j=0}^{1} p_j^{i_j}|i_j\rangle\langle i_j|,$$

for some orthonormal basis $|i_j\rangle$, where p_j^0 and p_j^1 are the eigenvalues of ρ_j. If $p_j^0 \neq p_j^1$, then the orthonormal basis $|i_j\rangle$ is uniquely determined up to a phase. If $p_j^0 = p_j^1$, then any one-qubit orthonormal basis can be used.

The $(n-1)$-qubit reduced density matrix

$$\rho_{(j)} = \mathrm{tr}_j|\psi\rangle\langle\psi|,$$

obtained by taking the partial trace of $|\psi\rangle\langle\psi|$ over qubit j, has the same nonzero eigenvalues as ρ_j,

$$\rho_{(j)} = \sum_{i_j=0}^{1} p_j^{i_j}|i_j;(j)\rangle\langle i_j;(j)|.$$

If $p_j^0 \neq p_j^1$, then the $(n-1)$-qubit eigenvectors $|0;(j)\rangle$ and $|1;(j)\rangle$ are unique up to a phase. If $p_j^0 = p_j^1$, then the eigenvectors of $\rho_{(j)}$ with eigenvalue $p_j^0 = p_j^1 = 1/2$ constitute a two-dimensional subspace of the 2^{n-1}-dimensional vector space of $(n-1)$-qubit vectors, and any orthonormal pair of vectors in this subspace may be chosen as a basis.

We choose the one-qubit orthonormal basis $|i_j\rangle$ and the $(n-1)$-qubit orthonormal basis $|i_j;(j)\rangle$ so that $|\psi\rangle$ can be written

$$|\psi\rangle = \sqrt{p_j^0}|0\rangle \otimes_j |0;(j)\rangle + \sqrt{p_j^1}|1\rangle \otimes_j |1;(j)\rangle,$$

where $\otimes_j$ is the tensor product that inserts a one-qubit ket just before the jth factor in the $(n-1)$-qubit ket $|i_j;(j)\rangle$.

Now $|\psi'\rangle$ can be regarded as the state of a bipartite system composed of qubit j and all qubits but j, and it has a Schmidt decomposition with respect to those subsystems,

$$|\psi'\rangle = \sqrt{q_j^0}|0'\rangle \otimes_j |0';(j)\rangle + \sqrt{q_j^1}|1'\rangle \otimes_j |1';(j)\rangle,$$

where $|0'\rangle, |1'\rangle$ are orthonormal one-qubit vectors and $|0';(j)\rangle, |1';(j)\rangle$ are orthonormal $(n-1)$-qubit vectors. Taking the partial trace over qubit j, we have

$$\mathrm{tr}_j|\psi'\rangle\langle\psi'| = q_j^0|0';(j)\rangle\langle 0';(j)| + q_j^1|1';(j)\rangle\langle 1';(j)|.$$

Since this must be equal to $\rho_{(j)}$, it must have the eigenvalues of $\rho_{(j)}$, $q_j^0 = p_j^0$, and $q_j^1 = p_j^1$. We consider two cases, depending on whether $\rho_{(j)}$ has distinct eigenvalues or not. Let us treat first the case of distinct eigenvalues, $p_j^0 \neq p_j^1$. In this case, the eigenvector $|0';(j)\rangle$ can be off by at most a phase from the eigenvector $|0;(j)\rangle$, and similarly for $|1';(j)\rangle$. The same argument applied to the one-qubit reduced density matrix ρ_j shows that $|0'\rangle$ can be off by at most a phase from $|0\rangle$, and similarly for $|1'\rangle$. In this case, then, we can write

$$|\psi'\rangle = \sqrt{p_j^0}(L_j|0\rangle) \otimes_j |0;(j)\rangle + \sqrt{p_j^1}(L_j|1\rangle) \otimes_j |1;(j)\rangle, \quad (1)$$

with L_j a 2×2 diagonal unitary matrix.

Let us treat next the case of repeated eigenvalues, $p_j^0 = p_j^1$. In this case, the eigenvectors $|0';(j)\rangle$ and $|1';(j)\rangle$ must merely span the same two-dimensional complex space that is spanned by $|0;(j)\rangle$ and $|1;(j)\rangle$. In this case, the primed eigenvectors must be related to the unprimed eigenvectors by a two-dimensional unitary transformation,

$$|0';(j)\rangle = u_{00}|0;(j)\rangle + u_{01}|1;(j)\rangle$$
$$|1';(j)\rangle = u_{10}|0;(j)\rangle + u_{11}|1;(j)\rangle$$

with

$$\begin{bmatrix} u_{00} & u_{01} \\ u_{10} & u_{11} \end{bmatrix} \in U(2).$$

The same argument applied to the one-qubit reduced density matrix ρ_j shows that there must be some 2×2 unitary matrix v_{lm} with

$$|0'\rangle = v_{00}|0\rangle + v_{01}|1\rangle \qquad |1'\rangle = v_{10}|0\rangle + v_{11}|1\rangle.$$

In this case, then, we can write Eq. (1) with L_j the 2×2 unitary matrix equal to the product of the transpose of v_{lm} with u_{lm}. (We have abused notation by using the symbol L_j to represent both the 2×2 unitary matrix and also the local unitary transformation on n-qubit state vectors

$$I \otimes \cdots \otimes I \otimes L_j \otimes I \otimes \cdots \otimes I,$$

with the 2×2 matrix L_j in the jth slot of this tensor product, and one-qubit (2×2) identity operators in all other slots.) This completes the proof of the Claim.

For each pair of qubit labels j, k, we have

$$|\psi\rangle = L_k^{-1} L_j |\psi\rangle.$$

Next, spectrally decompose each L_j with unitary matrices U_j so that

$$D_j = U_j L_j U_j^{-1}$$

are diagonal. We have

$$D_k^{-1} D_j U_1 \cdots U_n |\psi\rangle = U_1 \cdots U_n U_k^{-1} D_k^{-1} U_k U_j^{-1} D_j U_j |\psi\rangle$$
$$= U_1 \cdots U_n |\psi\rangle.$$

Using the multi-index $I = (i_1 i_2 \cdots i_n)$, where each i_j is zero or 1, and the basis

$$|I\rangle = |i_1 i_2 \cdots i_n\rangle = |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle,$$

expand

$$U_1 \cdots U_n |\psi\rangle = \sum_I c_I |I\rangle$$

and write

$$D_j = e^{i\alpha_j} \begin{bmatrix} e^{i\beta_j} & 0 \\ 0 & e^{-i\beta_j} \end{bmatrix},$$

where $e^{i\beta_j} \neq e^{-i\beta_j}$, since $|\psi'\rangle$ is a different state from $|\psi\rangle$. Now we have

$$c_I = c_I \exp\{i[\alpha_j - \alpha_k + (-1)^{i_j}\beta_j - (-1)^{i_k}\beta_k]\}$$

for all multi-indices I and all $j, k \in \{1, \ldots, n\}$. We see that for each multi-index I, either $c_I = 0$ or

$$\exp\{i[\alpha_j - \alpha_k + (-1)^{i_j}\beta_j - (-1)^{i_k}\beta_k]\} = 1$$

for all $j, k \in \{1, \ldots, n\}$. Let J be a multi-index with $c_J \neq 0$. If I is any multi-index that agrees with J in at least one entry (say the jth qubit entry), and disagrees with J in at least one entry (say the kth qubit entry), then $c_I = 0$. We conclude that c_J and $c_{\bar{J}}$, where $\bar{J}$ is the multi-index consisting of the complements of each of the n bits in multi-index J, are the only nonzero coefficients in $U_1 \cdots U_n |\psi\rangle$. Consequently, $|\psi\rangle$ is LU equivalent to a generalized n-qubit GHZ state. □

Much of this argument carries over to the more general situation of a system of n parties in which party j has dimension d_j (party j is a qubit if and only if $d_j = 2$). In particular, the Claim carries over. Suppose that $|\psi\rangle$ and $|\psi'\rangle$ are states of a system of n parties in which party j has dimension d_j. If $|\psi\rangle$ and $|\psi'\rangle$ have the same reduced density matrices, then for each party $j \in \{1, \ldots, n\}$, there is a one-party local unitary transformation L_j such that $|\psi'\rangle = L_j|\psi\rangle$. The second part of the argument is complicated by the possibility of repeated eigenvalues in the transformations D_j. We leave this as a question for future work.

It is worthwhile to point out the significance of stabilizer subgroups of the local unitary group in this work. The local unitary group for n-qubit density matrices is the group $G = \mathrm{SU}(2)^n$, consisting of a special unitary transformation on each qubit. Each (pure or mixed) state ρ has a stabilizer subgroup I_ρ consisting of elements of G that leave ρ fixed under the action $g\rho g^{-1}$ for $g \in G$. We have seen that a state that is undetermined among pure states has a special type of enlarged stabilizer subgroup.

There are two alternative formulations of the main result that may suggest promising avenues for the classification of entanglement types. One can precisely characterize the pure n-qubit states that are undetermined among pure states in terms of the stabilizer subalgebra of the state, that is the Lie algebra of the stabilizer subgroup of the state. It is shown in [8] that the generalized n-qubit GHZ state has (for $n \geq 3$) stabilizer subalgebra

$$K_\rho = \left\{ \sum_{j=1}^{n} i t_j Z_j \,\middle|\, \sum_{j=1}^{n} t_j = 0 \right\},$$

where Z_j is the Pauli matrix σ_z applied to qubit j. States of n qubits undetermined among pure states are precisely those which are LU equivalent to states with this subalgebra.

A second alternative formulation of the main result is in terms of the dimension of the stabilizer subgroup. For $n = 3$ and $n \geq 5$, an n-qubit state is undetermined among pure states if and only if it is not a product state and its stabilizer subgroup has dimension $n - 1$ [9].

We have shown that all n-qubit states other than generalized n-qubit GHZ states and their LU equivalents are completely determined by their reduced density matrices. Is it necessary to specify all of the reduced density matrices? Which states are undetermined by specifying only $n-1$ (rather than all n) of the $(n-1)$-qubit reduced density matrices? Is it a larger set than the generalized GHZs? The answer is yes, and stabilizers can help us understand this. For example, the state

$$|\chi\rangle = \frac{1}{\sqrt{3}}(|0000\rangle + |0001\rangle + |1111\rangle)$$

is undetermined by its 3-qubit reduced density matrices obtained by taking the partial trace over qubit 1, the partial trace over qubit 2, and the partial trace over qubit 3. It is not LU equivalent to a generalized 4-qubit GHZ state (it has a different stabilizer subalgebra structure, and a stabilizer subalgebra structure is an LU invariant). Note that $Z_1|\chi\rangle = Z_2|\chi\rangle = Z_3|\chi\rangle \neq e^{i\alpha}|\chi\rangle$. The state $Z_1|\chi\rangle$ has the same 3-qubit reduced density matrices as $|\chi\rangle$ when taking the partial trace over qubit 1, 2, or 3. These two states have a different 3-qubit reduced density matrix when taking the partial trace over qubit 4.

A pure state's LU-equivalence class is often considered to contain all of the information about the entanglement of the state. An interesting question is, are there n-qubit pure states with entanglement information that is not contained in their reduced density matrices? We might interpret this question as equivalent to the question, are there n-qubit pure states for which the LU-equivalence class of the state is undetermined by its reduced density matrices? The answer to this question is no. Every n-qubit pure state can be determined (among pure states) up to a local unitary transformation by its reduced density matrices. This can be seen directly from the Claim at the beginning of our proof. Two pure states that have the same reduced density matrices must be LU equivalent.

We have not answered the question of which n-qubit pure states are undetermined among arbitrary states by their reduced density matrices. The set of n-qubit states undetermined among arbitrary states must contain the generalized GHZ states, but it could be strictly larger than the set that is undetermined among pure states. This remains an open question.

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