Almost Every Pure State of Three Qubits Is Completely Determined by Its Two-Particle Reduced Density Matrices

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In a system of n quantum particles, we define a measure of the degree of irreducible n-way correlation, by which we mean the correlation that cannot be accounted for by looking at the states of $n-1$ particles. In the case of almost all pure states of three qubits, we show that there is no such correlation: almost every pure state of three qubits is completely determined by its two-particle reduced density matrices.

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A fundamental question in quantum information theory is to understand the different types of correlations that quantum states can exhibit. A particular issue for a quantum state shared among n parties is the extent to which the correlations between these parties is not attributable to correlations between groups of fewer than n parties. In this Letter, we introduce a way of characterizing this irreducible n-party correlation for general states of n parties. Our characterization is based on measuring the *information* in the given quantum state of n parties that is not already contained in the set of reduced states of $n-1$ parties.

These considerations lead us to consider the specific case of pure states of three qubits. We find the striking result that, for almost all such states, there is no more information in the full quantum state than is already contained in the three two-party reduced states. Expressed differently, the two-party correlations uniquely determine the three-party correlations.

In order to explain our construction, let us first treat the case of states of two parties; the local Hilbert spaces may have any dimension. Let the (generally mixed) state be ρ_{AB}. We ask how much more information there is in ρ_{AB} than is already contained in the two reduced states ρ_A and ρ_B. We address this question by finding another state $\tilde{\rho}_{AB}$ which is the most mixed state, i.e., the state of maximum entropy, consistent with the reduced states. Thus, $\tilde{\rho}_{AB}$ contains all the information in ρ_A and ρ_B but no more [1]. A simple calculation using Lagrange multipliers shows that $\tilde{\rho}_{AB}$ has the form

$$\tilde{\rho}_{AB} = \exp(\Lambda_A \otimes 1_B + 1_A \otimes \Lambda_B). \quad (1)$$

1_A and 1_B denote the identity operators on the Hilbert spaces of particles A and B, respectively. Λ_A and Λ_B come from the Lagrange multipliers and are to be determined by the condition that the reduced states of $\tilde{\rho}_{AB}$ are required to be ρ_A and ρ_B. We can now solve for the Lagrange multipliers and find that

$$\tilde{\rho}_{AB} = \rho_A \otimes \rho_B. \quad (2)$$

In the case that ρ_A and ρ_B do not have full rank, this calculation is a little delicate, since then the Lagrange multipliers as they appear in Eq. (1) are formally infinite. In that case, we can restrict the Lagrange multipliers to the ranges of ρ_A and ρ_B. Then Eq. (1) defines $\tilde{\rho}_{AB}$ only on the subspace in which it is nonzero, but Eq. (2) remains valid.

The difference $S(\tilde{\rho}_{AB}) - S(\rho_{AB})$, where S is the von Neumann entropy, can be interpreted as the amount of information in ρ_{AB} that is not contained in ρ_A and ρ_B. In fact, $S(\tilde{\rho}_{AB}) - S(\rho_{AB})$ is equal to the quantum mutual information $S(\rho_A) + S(\rho_B) - S(\rho_{AB})$, which measures the degree of correlation in ρ_{AB}. (Alternatively, we could use any measure of distance between $\tilde{\rho}_{AB}$ and ρ_{AB} to express the degree of correlation [2].) We use the word "correlation" rather than entanglement since, for mixed states, $\tilde{\rho}_{AB}$ will have greater entropy than ρ_{AB} if ρ_{AB} is separable but not of product form. For pure states, however, $S(\tilde{\rho}_{AB}) = S(\rho_{AB})$ if and only if ρ_{AB} is of product form, and in this case the difference $S(\tilde{\rho}_{AB}) - S(\rho_{AB})$ is, except for a factor of 2, the standard measure of bipartite entanglement [3]. We also note that, for a pure state with reduced states ρ_A and ρ_B, there are typically many states of two parties having the same reduced states. This is in contrast to the case for more parties, as we see below.

We now turn to the more interesting case of quantum states of more than two parties; the local Hilbert spaces may again have any dimension. For ease of exposition, we treat the three-party case explicitly; the extension to more parties follows straightforwardly. Consider, then, a general three-party state ρ_{ABC}. We ask how much more information there is in ρ_{ABC} than is already contained in the three reduced states ρ_{AB}, ρ_{BC}, ρ_{AC}.

Before we analyze this situation, we point out that there are a number of new issues in the three-party case that do not arise in the two-party case. Consider a set of states ρ_{AB}, ρ_{BC}, ρ_{AC} which are supposed to be the reduced states of some (possibly mixed) state of three parties. These three must certainly satisfy some consistency conditions: the reduced state ρ_A can arise from both ρ_{AB} and ρ_{AC}, and this puts constraints on these two reduced bipartite states. However, a set of states satisfying this condition (and the analogous ones for each of the other parties) may still not correspond to a legitimate state of three parties. Consider the following set of reduced states which are supposed to be the reduced states of some state of three qubits: ρ_{AB}, ρ_{BC}, ρ_{AC} are all singlets held between the given pairs, e.g.,

$$\rho_{AB} = \frac{1}{\sqrt{2}}(|0\rangle_A|1\rangle_B - |1\rangle_A|0\rangle_B). \tag{3}$$

The reduced states of the individual parties are all the maximally mixed state of a qubit and so are consistent with each other; however, it is easy to convince oneself that these putative reduced states are not the reduced state of any three-party state of three qubits.

We now return to the main theme of our discussion. We are given a general three-party state ρ_{ABC}. We argue that a measure of the irreducible three-party correlations in the state is the entropy difference between the state itself and the three-party state $\tilde{\rho}_{ABC}$ that contains no more information than the reduced states. As in the two-party case, we may use Lagrange multipliers to find $\tilde{\rho}_{ABC}$. If ρ_{ABC} has maximal rank, then $\tilde{\rho}_{ABC}$ is of the form

$$\tilde{\rho}_{ABC} = \exp(\Lambda_{AB} \otimes 1_C + \Lambda_{AC} \otimes 1_B + \Lambda_{BC} \otimes 1_A). \tag{4}$$

Here Λ_{AB}, Λ_{BC}, and Λ_{AC} come from the Lagrange multipliers and are to be determined by the condition that the reduced states of $\tilde{\rho}_{ABC}$ be those of ρ_{ABC}. Unlike the case of two parties, we have not been able to calculate these Lagrange multipliers in closed form, in general. Nonetheless, the form of $\tilde{\rho}_{ABC}$ is illuminating. Consider a completely general state of three parties. It can be expanded using a basis of operators composed of tensor products of operators spanning each individual Hilbert space. For example, for three qubits, a general mixed state may be written as

$$\rho_{ABC} = \frac{1}{8}(1 \otimes 1 \otimes 1 + \alpha_i \sigma_i \otimes 1 \otimes 1 + \beta_i 1 \otimes \sigma_i \otimes 1 + \gamma_i 1 \otimes 1 \otimes \sigma_i + R_{ij}\sigma_i \otimes \sigma_j \otimes 1 + S_{ij}\sigma_i \otimes 1 \otimes \sigma_j + T_{ij} 1 \otimes \sigma_i \otimes \sigma_j + Q_{ijk}\sigma_i \otimes \sigma_j \otimes \sigma_k), \tag{5}$$

since the set of matrices $(1, \sigma_x, \sigma_y, \sigma_z)$ is a basis for the operators on $\mathbb{C}^2$. It is not the case that the tensor Q describes the three-party correlations (consider a density matrix which is of the form $\rho_A \otimes \rho_B \otimes \rho_C$—it has nonzero Q). However, the discussion above shows that, for generic density matrices, a state which has all its information contained in its reduced states has the property that its logarithm has no term of the form $q_{ijk}\sigma_i \otimes \sigma_j \otimes \sigma_k$.

In a number of places in the above discussion, we have noted that the case when the states have nonmaximal rank may need careful treatment. For example, one clearly cannot take the logarithm of such a state to determine whether its information is contained in its reduced states. A particularly important class of states of nonmaximal rank is the set of pure states. As we now see, this set has surprising properties.

Let us consider the particular case of a system of three qubits. All pure states of this system are equivalent under local unitary transformations to states of the following form [4]:

$$|\eta\rangle = a|000\rangle + b|001\rangle + c|010\rangle + d|100\rangle + e|111\rangle. \tag{6}$$

The labels within each ket refer to qubits A, B, and C in that order. We now show that almost all of these states have no irreducible three-party correlation in the sense developed in this Letter. That is, we show the following: except when the parameters a, b, c, d, e have certain special values, the state $|\eta\rangle$ is the *only* state (pure or mixed) consistent with its two-party reduced states.

Let ω be a three-qubit density matrix whose two-particle reduced states are the same as those of $|\eta\rangle$. We can think of ω as obtained from a pure state $|\psi\rangle$ of a larger system, consisting of the three qubits and an environment E: thus, $\omega = \mathrm{Tr}_E|\psi\rangle\langle\psi|$. To get a constraint on the form of $|\psi\rangle$, consider the state ρ_{AB} of qubits A and B as obtained from $|\eta\rangle$:

$$\rho_{AB} = |\phi_0\rangle\langle\phi_0| + |\phi_1\rangle\langle\phi_1|, \tag{7}$$

where the unnormalized vectors $|\phi_0\rangle$ and $|\phi_1\rangle$ are

$$|\phi_0\rangle = a|00\rangle + c|01\rangle + d|10\rangle; \qquad |\phi_1\rangle = b|00\rangle + e|11\rangle. \tag{8}$$

We insist that $|\psi\rangle$ give this same ρ_{AB} when restricted to the pair AB. Because ρ_{AB} is confined to the two-dimensional space spanned by $|\phi_0\rangle$ and $|\phi_1\rangle$, $|\psi\rangle$ must have the form

$$|\psi\rangle = |\phi_0\rangle|E_0\rangle + |\phi_1\rangle|E_1\rangle, \tag{9}$$

where $|E_0\rangle$ and $|E_1\rangle$ are vectors in the state space of the composite system consisting of qubit C and the environment E. Computing the density matrix of AB from Eq. (9) and comparing it with Eq. (7), we see that $|E_0\rangle$ and $|E_1\rangle$ must be orthonormal. It is helpful to expand $|E_0\rangle$ and $|E_1\rangle$ in terms of states of C and states of E:

$$|E_0\rangle = |0\rangle|e_{00}\rangle + |1\rangle|e_{01}\rangle; \qquad |E_1\rangle = |0\rangle|e_{10}\rangle + |1\rangle|e_{11}\rangle. \tag{10}$$

Here the environment states $|e_{ij}\rangle$ are *a priori* not necessarily either normalized or orthogonal. Combining Eqs. (8)–(10), we can write

$$|\psi\rangle = (a|00\rangle + c|01\rangle + d|10\rangle)(|0\rangle|e_{00}\rangle + |1\rangle|e_{01}\rangle) + (b|00\rangle + e|11\rangle)(|0\rangle|e_{10}\rangle + |1\rangle|e_{11}\rangle). \quad (11)$$

In order to see what further constraints are imposed on $|\psi\rangle$ by the requirement that the reduced states agree with $|\eta\rangle$ for the other pairs, let us consider three specific elements of the two-party density matrices.

$\langle 11|\rho_{BC}|11\rangle$: As computed from the state $|\eta\rangle$, this matrix element has the value $|e|^2$. As computed from Eq. (11), it has the value $|c|^2\langle e_{01} \mid e_{01}\rangle + |e|^2\langle e_{11} \mid e_{11}\rangle$.

$\langle 11|\rho_{AC}|11\rangle$: As computed from $|\eta\rangle$, this matrix element has the value $|e|^2$. As computed from Eq. (11), it has the value $|e|^2\langle e_{11} \mid e_{11}\rangle + |d|^2\langle e_{01} \mid e_{01}\rangle$. Hence, for generic values of c, d, and e, $|e_{01}\rangle = 0$ and $\langle e_{11} \mid e_{11}\rangle = 1$, from which it follows that $|e_{10}\rangle = 0$ and $\langle e_{00} \mid e_{00}\rangle = 1$.

$\langle 01|\rho_{BC}|10\rangle$: As computed from $|\eta\rangle$, this matrix element has the value bc^*. As computed from Eq. (11) (with $|e_{01}\rangle = |e_{10}\rangle = 0$), it has the value $bc^*\langle e_{00} \mid e_{11}\rangle$. We conclude, again for generic values of the parameters, that $|e_{00}\rangle = |e_{11}\rangle$.

Inserting these inferences into Eq. (11), we find that

$$|\psi\rangle = (a|000\rangle + b|001\rangle + c|010\rangle + d|100\rangle + e|111\rangle)|e_{00}\rangle. \quad (12)$$

When we trace out the environment to get the state ω, we see that we must have $\omega = |\eta\rangle\langle\eta|$. That is, the only state (*pure or mixed*) consistent with the two-particle reduced states of $|\eta\rangle$ is $|\eta\rangle$ itself.

The above treatment deals simply with the generic pure state of three qubits. We have found it necessary to use a slightly more involved analysis, to be found in the Appendix, to identify those special states for which the two-party reduced states do not uniquely determine the full three-party state. The results in the Appendix show that the only states that do not have this generic property are those which are equivalent under local rotations to states of the form

$$a|000\rangle + b|111\rangle. \quad (13)$$

The results of this Letter clearly raise many questions. For example, whether the properties that we have found for generic pure states of three qubits extend to systems of more parties and in higher dimensional Hilbert spaces [5]; we intend to return to this in a future publication. Also, it is interesting to find nontrivial classes of n-party states that are determined by their reduced states of *fewer* than $n - 1$ parties and to characterize their entanglement properties. An example is the family of states

$$a|0001\rangle + b|0010\rangle + c|0100\rangle + d|1000\rangle. \quad (14)$$

These states are uniquely determined by their two-party reduced states.

Finally, we note that many of the ideas we have put forward here also shed light on classical probability distributions [6]. For example, the idea of characterizing the n-party correlations using the information in the $(n - 1)$-party marginal distributions. In light of our results on pure states of three qubits, it is intriguing to consider the case of probability distributions $P(X, Y, Z)$ of three random variables, each of which has two values; such a distribution arises from local von Neumann measurements on states of three qubits. In this case, it is not difficult to see that generic distributions are by no means determined by their marginal distributions. Consider a given set of probabilities p_{ijk} where p_{000} is the probability that $X = 0$, $Y = 0$, $Z = 0$, etc. The set of probabilities $q_{ijk} = p_{ijk} + \delta(-1)^{\epsilon(ijk)}$ has the same two-party marginal distributions, where δ is a constant and $\epsilon(ijk)$ is the parity of the bit string ijk.

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Appendix.—Consider an arbitrary pure state $|\eta\rangle = \sum_{ijk} a_{ijk}|ijk\rangle$ of three qubits A, B, and C. We give an alternative derivation that, for generic a_{ijk}, $|\eta\rangle$ is uniquely determined by its two-party reduced states and find those states for which this is not true.

We can quickly dispose of the case in which $|\eta\rangle$ is the product of a single-qubit state and a two-qubit state. In that case, the two-party reduced states determine both factors in the product and, therefore, determine $|\eta\rangle$ uniquely. In what follows, we assume that $|\eta\rangle$ does not have this product form.

A general state that agrees with $|\eta\rangle$ in its reduced states can always be obtained from a pure state $|\psi\rangle$ of the three qubits plus an environment E. Let us first ask what form $|\psi\rangle$ must take in order to be consistent with the (generally mixed) state of the pair AB derived from $|\eta\rangle$. By an argument essentially identical to the one leading to Eq. (11), we find that $|\psi\rangle$ must be of the form

$$|\psi\rangle = \sum_{ijkl} a_{ijl}|ijk\rangle|e_{lk}\rangle. \quad (15)$$

Here l takes the values 0 and 1, and the states $|e_{lk}\rangle$, which are states of E alone, satisfy the orthonormality condition

$$\sum_k \langle e_{lk} \mid e_{l'k}\rangle = \delta_{ll'}. \quad (16)$$

Similarly, by considering AC and BC, we see that

$$|\psi\rangle = \sum_{ijkl} a_{ilk}|ijk\rangle|f_{lj}\rangle = \sum_{ijkl} a_{ljk}|ijk\rangle|g_{li}\rangle, \quad (17)$$

with $\sum_j\langle f_{lj} \mid f_{l'j}\rangle = \delta_{ll'}$ and $\sum_i\langle g_{li} \mid g_{l'i}\rangle = \delta_{ll'}$. Here we regard the coefficients a_{ijk} as fixed—that is, the state $|\eta\rangle$ is fixed—and we are looking for environment vectors $|e_{lk}\rangle$, $|f_{lj}\rangle$, and $|g_{li}\rangle$ that satisfy the various linear equations arising from the fact that the three expressions for $|\psi\rangle$ in Eqs. (15) and (17) must all be equal.

It is instructive to write down explicitly, as an example, the two equations arising from (15) and (17) that involve only the vectors $|e_{00}\rangle$, $|e_{10}\rangle$, $|f_{00}\rangle$, and $|f_{10}\rangle$:

$$a_{000}|e_{00}\rangle + a_{001}|e_{10}\rangle = a_{000}|f_{00}\rangle + a_{010}|f_{10}\rangle, \tag{18}$$

$$a_{100}|e_{00}\rangle + a_{101}|e_{10}\rangle = a_{100}|f_{00}\rangle + a_{110}|f_{10}\rangle. \tag{19}$$

Notice that these two equations are linearly independent: if they were not, then the state $|\eta\rangle$ would be factorable into a single-qubit state and a two-qubit state, contrary to our current assumptions.

These equations and analogous ones relating $|e_{lk}\rangle$ to $|g_{li}\rangle$ and $|f_{lj}\rangle$ to $|g_{li}\rangle$ can be solved fully, and one finds that the general solution for the vectors $|e_{lk}\rangle$ is

$$\begin{aligned} |e_{01}\rangle &= (a_{011}a_{101} - a_{111}a_{001})|v\rangle, \\ |e_{10}\rangle &= (a_{000}a_{110} - a_{100}a_{010})|v\rangle, \\ |e_{00}\rangle &= (a_{100}a_{011} + a_{101}a_{010})|v\rangle + |w\rangle, \\ |e_{11}\rangle &= (a_{000}a_{111} + a_{001}a_{110})|v\rangle + |w\rangle, \end{aligned} \tag{20}$$

the vectors $|v\rangle$ and $|w\rangle$ being arbitrary. The corresponding expressions for the f and g vectors can be obtained from Eq. (20) by permuting indices; for example, the expression for each f vector is obtained from the expression for the corresponding e vector by permuting the last two indices of every a_{ijk} (without changing the vectors $|v\rangle$ and $|w\rangle$). Thus, once the two vectors $|v\rangle$ and $|w\rangle$ have been chosen, the solution is determined. The form of the solution shows that at most two dimensions of the environment can ever be used.

We have not yet taken into account the orthonormality conditions for the environment states. Let us now consider just Eq. (16) which constrains the e vectors. It is helpful to rewrite Eq. (20) in terms of a new arbitrary vector $|z\rangle$ that replaces $|w\rangle$:

$$\begin{aligned} |e_{01}\rangle &= \alpha|v\rangle, \qquad |e_{10}\rangle = \beta|v\rangle, \\ |e_{00}\rangle &= |z\rangle, \qquad |e_{11}\rangle = |z\rangle + \gamma|v\rangle, \end{aligned} \tag{21}$$

where $\alpha = a_{011}a_{101} - a_{111}a_{001}$, $\beta = a_{000}a_{110} - a_{100}a_{010}$, and $\gamma = a_{000}a_{111} + a_{001}a_{110} - a_{100}a_{011} - a_{101}a_{010}$. In terms of these parameters, the orthonormality condition of Eq. (16) is expressed by the following three equations:

$$\begin{aligned} \langle z \mid z\rangle + |\alpha|^2\langle v \mid v\rangle &= 1, \\ \langle z \mid z\rangle + (|\beta|^2 + |\gamma|^2)\langle v \mid v\rangle + \gamma\langle z \mid v\rangle + \bar{\gamma}\langle v \mid z\rangle &= 1, \\ \bar{\alpha}\gamma\langle v \mid v\rangle + \beta\langle z \mid v\rangle + \bar{\alpha}\langle v \mid z\rangle &= 0. \end{aligned} \tag{22}$$

Taking the difference between the first two of these equations, and treating separately the real and imaginary parts of the third, we obtain three homogeneous linear equations for the three real variables $\langle v \mid v\rangle$, $\mathrm{Re}\langle z \mid v\rangle$, and $\mathrm{Im}\langle z \mid v\rangle$. For generic values of α, β, and γ, these three equations are linearly independent, so that the only solution is $|v\rangle = 0$. This in turn implies, by Eq. (20), that $|e_{01}\rangle = |e_{10}\rangle = 0$ and $|e_{00}\rangle = |e_{11}\rangle$. Thus, in this generic case only a single dimension of the environment is used — that is, the environment is in a pure state — and the qubits ABC *must* be in the given state $|\eta\rangle$.

This conclusion can be avoided only if the determinant D of the 3×3 matrix associated with the three homogeneous linear equations vanishes, and the corresponding determinants computed from the two other orthonormality conditions (for the vectors f and g) are also zero. Computing D explicitly, we find that $D = 0$ if and only if (i) $|\alpha| = |\beta|$ and (ii) $\bar{\gamma}^2\alpha\beta$ is real and non-negative.

Suppose now that $|\eta\rangle$ is *not* determined by its two-party reduced states, so that the above conditions (i) and (ii) must be satisfied. These conditions imply that there exists a local rotation on qubit C that will bring both α and β to zero, thus bringing $|\eta\rangle$ to the form

$$|p_A\rangle|p_B\rangle|0\rangle + |q_A\rangle|q_B\rangle|1\rangle. \tag{23}$$

Here $|p_A\rangle$ and $|q_A\rangle$ are (unnormalized) vectors in the space of qubit A, and $|p_B\rangle$ and $|q_B\rangle$ belong to qubit B. We now use in a similar way the conditions analogous to (i) and (ii) but derived from the orthonormality relations for the f vectors. These imply that we can apply to the form (23) a local rotation on qubit B to bring it to the form $|p_A\rangle|0\rangle|0\rangle + |q_A\rangle|1\rangle|1\rangle$. Finally, from the conditions derived from the g vectors, it follows that we can rotate qubit A and arrive at the form $a|000\rangle + b|111\rangle$.

We conclude, then, that the only pure three-qubit states that might *not* be uniquely determined by their two-particle reduced states are those that are equivalent under local rotations to the form given in Eq. (13). In fact, it is easy to see that for any state of this form with $a \neq 0$ and $b \neq 0$, there do exist other three-qubit states — e.g., a mixture of $|000\rangle$ and $|111\rangle$ — having the same two-party reduced states.

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