The power of reduced quantum states

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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.

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-particle 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 \( \rho_{AB} \). We ask how much more information there is in \( \rho_A \) and \( \rho_B \) but no more \( \rho_{AB} \). A simple calculation using Lagrange multipliers shows that \( \hat{\rho}_{AB} \) has the form

\[
\hat{\rho}_{AB} = \exp(\Lambda_A \otimes 1_B + 1_A \otimes \Lambda_B).
\]

In the case that \( \rho_A \) and \( \rho_B \) 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 \( \rho_A \) and \( \rho_B \). Then Eq. (1) defines \( \hat{\rho}_{AB} \) only on the subspace in which it is nonzero, but Eq. (2) remains valid.

The difference \( S(\hat{\rho}_{AB}) - S(\rho_{AB}) \), where \( S \) is the von Neumann entropy, can be interpreted as the amount of information in \( \rho_{AB} \) that is not contained in \( \rho_A \) and \( \rho_B \). In fact \( S(\hat{\rho}_{AB}) - S(\rho_{AB}) \) is equal to the quantum mutual information \( I(\rho_A, \rho_B) \), which measures the degree of correlation in \( \rho_{AB} \). (Alternatively, we could use any measure of the distance between \( \hat{\rho}_{AB} \) and \( \rho_{AB} \) to express the degree of correlation.) We use the word “correlation” rather than entanglement since for mixed states, \( \hat{\rho}_{AB} \) will have greater entropy than \( \rho_{AB} \) if \( \rho_{AB} \) is separable but not of product form. For pure states however \( S(\hat{\rho}_{AB}) = S(\rho_{AB}) \) if and only if \( \rho_{AB} \) is of product form, and in this case the difference \( S(\hat{\rho}_{AB}) - S(\rho_{AB}) \) is, except for a factor of two, the standard measure of bipartite entanglement. We also note that for a pure state with reduced states \( \rho_A \) and \( \rho_B \), 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 will 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 \( \rho_{ABC} \). We ask how much more information there is in \( \rho_{ABC} \) than is already contained in the three reduced states \( \rho_{AB}, \rho_{BC}, \rho_{AC} \).

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 \( \rho_{AB}, \rho_{BC}, \rho_{AC} \) which are supposed to be the reduced states of some (possibly mixed) state of three parties. These three must certainly satisfy some consistency con-
ditions: the reduced state $\rho_A$ can arise from both $\rho_{AB}$ and $\rho_{AC}$, 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. For consider the following set of reduced states which are supposed to be the reduced states of some state of three qubits: $\rho_{AB}$, $\rho_{BC}$, $\rho_{AC}$ are all singlets held between the given pairs, e.g.

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

(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 $\rho_{ABC}$. 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 that has no more information in it than in the reduced states. As in the two-party case we may use Lagrange multipliers to find the state $\tilde{\rho}_{ABC}$ which contains only the information in the reduced states. If $\rho_{ABC}$ has maximal rank, then $\tilde{\rho}_{ABC}$ is of the form

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

(4)

Here $\Lambda_{AB}$, $\Lambda_{BC}$ and $\Lambda_{AC}$ come from the Lagrange multipliers and are to be determined by the condition that the reduced states of $\tilde{\rho}_{ABC}$ be those of $\rho_{ABC}$. 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. For 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

$$\rho_{ABC} = \frac{1}{8} \left( 1 \otimes 1 \otimes 1 + \alpha_i \sigma_i \otimes 1 \otimes 1 + \beta_i \otimes 1 \otimes 1 + \gamma_i \otimes 1 \otimes 1 \right.$$

$$\left. + R_{ij} \sigma_i \otimes \sigma_j \otimes 1 + S_{ijk} \sigma_i \otimes 1 \otimes \sigma_j \right)$$

$$+ T_{ij} \sigma_i \otimes 1 \otimes \sigma_j + Q_{ijk} \sigma_i \otimes \sigma_j \otimes \sigma_k \right),$$

(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 (for consider a density matrix which is of the form $\rho_A \otimes \rho_B \otimes \rho_C$—it has non-zero $Q$). 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 non-maximal 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 non-maximal rank is the set of pure states. As we will 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

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

(6)

The labels within each ket refer to qubits $A$, $B$ and $C$ in that order; in what follows we will continue to identify qubits only by the ordering of the labels. We now show that almost all of these states have no irreducible three-party correlation in the sense developed in this paper. 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 $\omega$ be a three-qubit density matrix whose two-particle reduced states are the same as those of $|\eta\rangle$. We can think of $\omega$ as obtained from a pure state $|\psi\rangle$ of a larger system, consisting of the three qubits and an environment $E$: thus $\omega = \text{Tr}_E |\psi\rangle \langle \psi|$. To get a constraint on the form of $|\psi\rangle$, consider the state $\rho_{AB}$ of qubits $A$ and $B$ as obtained from $|\eta\rangle$:

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

(7)

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

$$|\phi_0\rangle = a|00\rangle + c|01\rangle + d|10\rangle; \quad |\phi_1\rangle = b|00\rangle + e|11\rangle.$$  

(8)

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

$$|\psi\rangle = |\phi_0\rangle |E_0\rangle + |\phi_1\rangle |E_1\rangle$$

(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. (6) and comparing it with Eq. (7), we see that $|E_0\rangle$ and $|E_1\rangle$ must be orthonormal. It will be helpful to expand $|E_0\rangle$ and $|E_1\rangle$ in terms of states of $C$ and states of $E$:

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

(10)

Here the environment states $|e_{ij}\rangle$ are a priori not necessarily either normalized or orthogonal. Combining Eqs. (8), (10) and (9), we can write
that we must have $\omega$. We conclude, again for generic values of the parameters, that any two-party reduced state of the pair $AB$ can be represented as $\rho_{AB} = \sum_{ijkl} \eta_{ijkl} \ket{ijkl} \bra{ijkl}$. By an argument essentially identical to the one leading to Eq. (11), we find that $\ket{\psi} = \sum_{ijkl} a_{ijkl} \ket{ijkl} \bra{ijkl}$. Finally, we note that many of the ideas we have put forward here also shed light on classical probability distributions. For example the idea of characterizing the $n$-party correlations using the information in the $(n-1)$-party marginal distributions. In the 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. For 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 $q_{ijk} = p_{ijk} + \delta(-1)^{(ijk)}$ has the same two-party marginal distributions, where $\delta$ is a constant and $\epsilon(ijk)$ is the parity of the bit string $ijk$.

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Appendix

Consider an arbitrary pure state $|\eta\rangle = \sum_{ijkl} a_{ijkl} |ijkl\rangle$ of three qubits $A$, $B$ and $C$. We give an alternative derivation that for generic $a_{ijkl}$, $|\eta\rangle$ 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 will 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

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

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

$$\sum_{k} \langle e_{ik} | e_{lk} \rangle = \delta_{il}. \quad (16)$$

Similarly, by considering $AC$ and $BC$ we see that

$$|\psi\rangle = \sum_{ijkl} a_{ijkl} |ijkl\rangle |f_{ij}\rangle = \sum_{ijkl} a_{ijkl} |ijkl\rangle |g_{ij}\rangle. \quad (17)$$

Finally, we note that many of the ideas we have put forward here also shed light on classical probability distributions. For example the idea of characterizing the $n$-party correlations using the information in the $(n-1)$-party marginal distributions. In the 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. For 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 $q_{ijk} = p_{ijk} + \delta(-1)^{(ijk)}$ has the same two-party marginal distributions, where $\delta$ is a constant and $\epsilon(ijk)$ is the parity of the bit string $ijk$.

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with $\sum_i \langle f_i | f_{i'} \rangle = \delta_{ii'}$ and $\sum_i \langle g_i | g_{i'} \rangle = \delta_{ii'}$. Here we regard the coefficients $a_{ijk}$ as fixed—that is, the state $\langle \eta \rangle$ is fixed—and we are looking for environment vectors $|e_{ik}\rangle$, $|f_{i}\rangle$ and $|g_{i}\rangle$ 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 $|e_{10}\rangle$, $|f_{10}\rangle$ and $|f_{11}\rangle$:

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

$$a_{100}|e_{00}\rangle + a_{101}|e_{10}\rangle = a_{100}|f_{00}\rangle + a_{110}|f_{11}\rangle.$$  

(18)

(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 $|e_{ik}\rangle$ to $|g_{i}\rangle$ and $|f_{i}\rangle$ to $|g_{i}\rangle$ can be solved fully, and one finds that the general solution for the vectors $|e_{ik}\rangle$ is

$$|e_{01}\rangle = (a_{011}a_{101} - a_{111}a_{001})|v\rangle$$

$$|e_{10}\rangle = (a_{000}a_{101} - a_{100}a_{010})|v\rangle$$

$$|e_{00}\rangle = (a_{100}a_{011} + a_{101}a_{010})|v\rangle + |w\rangle$$

$$|e_{11}\rangle = (a_{000}a_{111} + a_{010}a_{110})|v\rangle + |w\rangle,$$

(20)

the vectors $|v\rangle$ and $|w\rangle$ being arbitrary. The corresponding expressions for the $f$ and $g$ vectors can be obtained from Eq. (21) 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. (10) which constrains the $e$ vectors. It is helpful to rewrite Eq. (21) in terms of a new arbitrary vector $|z\rangle$ that replaces $|w\rangle$:

$$|e_{01}\rangle = \alpha|v\rangle$$

$$|e_{10}\rangle = |z\rangle$$

$$|e_{00}\rangle = |z\rangle + \gamma|v\rangle,$$

(21)

where $\alpha = a_{011}a_{101} - a_{111}a_{001}$, $\beta = a_{000}a_{110} - a_{100}a_{010}$ and $\gamma = a_{000}a_{111} + a_{010}a_{101} - a_{100}a_{010} - a_{111}a_{000}$. In terms of these parameters, the orthonormality condition of Eq. (10) is expressed by the following three equations

$$\langle z|z\rangle + |\alpha|^2 \langle v|v\rangle = 1$$

$$\langle z|z\rangle + (|\beta|^2 + |\gamma|^2)\langle v|v\rangle + \gamma\langle z|v\rangle + \bar{\gamma}\langle v|z\rangle = 1$$

$$\bar{\alpha}\gamma\langle v|v\rangle + \beta\langle z|v\rangle + \bar{\alpha}\langle v|z\rangle = 0.$$  

(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 $\langle v|v\rangle$, $\text{Re} \langle z|v\rangle$ and $\text{Im} \langle z|v\rangle$. For generic values of $\alpha$, $\beta$ and $\gamma$, these three equations are linearly independent, so that the only solution is $\langle v|v\rangle = 0$. This in turn implies, by Eq. (21), that $|e_{01}| = |e_{10}| = 0$ and $|e_{00}| = |e_{11}|$. 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 $3 \times 3$ 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 $\alpha$ and $\beta$ to zero, thus bringing $|\eta\rangle$ to the form

$$|p_A\rangle|p_B\rangle|0\rangle + |q_A\rangle|q_B\rangle|1\rangle.$$  

(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. (23). 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. mixtures of $|000\rangle$ and $|111\rangle$—having the same two-party reduced states.

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