N-Qubit W States are Determined by their Bipartite Marginals

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We prove that the most general $W$ class of $N$-qubit states are uniquely determined among arbitrary states (pure or mixed) by just their bipartite reduced density matrices. Moreover, if we consider only pure states, then $(N-1)$ of them are shown to be sufficient.

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Understanding the structure of multi party quantum correlations is an important issue in quantum information. Different types of correlations that a multi-partite state exhibits lead to classification and characterization of quantum states. Essentially the study reveals peculiarity of quantum correlation as compared to its classical analogue. For example, contrary to the quantum case, two different generic trivariate classical probability distributions can have the same bivariate marginals.

One of the basic questions concerning the study of quantum correlations is whether higher order correlations follow from lower order ones. This was first addressed by Linden, Popescu and Wootters\textsuperscript{1} where they proved that a generic 3-qubit pure state is uniquely determined by its two-party reduced states. Extending this proof to more parties having any finite dimension, Linden and Wootters\textsuperscript{2} have given some bounds on the number of reduced parties. An alternative technique to prove the result of\textsuperscript{1} was proposed by Diosi\textsuperscript{3} by making use of the Schmidt decomposition. It was also shown in\textsuperscript{1} that the only exceptional class of 3-qubit pure states not determined uniquely by its bipartite marginals is the Greenberger-Horne-Zeilinger (GHZ) class (a(000) + b(111)). This implies that only these states carry information at the three qubit level, since their correlations are not reducible. Generalizing this result, Walck and Lyons\textsuperscript{4} have shown that GHZ is the only class of $N$-qubit states which are not determined by their $(N-1)$-partite marginals. But generically the “Parts” can determine the “Whole”. Recently, a quantitative measure of the degree of irreducible $K$-particle correlations in an $N$-particle state, based on the maximal entropy construction has been defined by Zhou\textsuperscript{5}, in particular for stabilizer and generalized GHZ states.

It is known\textsuperscript{6} that under Stochastic Local Operation and Classical Communication (SLOCC), there exists two inequivalent classes of 3-qubit genuinely entangled pure states - the GHZ class and the $W$ class (a(001) + b(010) + c(100)). These later states have an interesting property that their entanglement exhibits maximum robustness against the loss of one qubit. This means that the bipartite entanglement left in the system can still be used as a resource to perform information-theoretic tasks, even in the absence of cooperation from the third party. Moreover, the third party cannot destroy the residual entanglement, thereby making $W$ state especially useful for secure communication\textsuperscript{7}. Also the reduced bipartite entangled state can be brought arbitrarily close to a Bell state by means of a filtering measurement\textsuperscript{8}. Motivated by these special features, we investigate the most general $W$ class of states in terms of their irreducible correlations.

It would be interesting to find classes of states which could be determined by fewer than $(N-1)$-partite marginals. However, this task becomes quite challenging since the known techniques cannot be applied to such situations. The present Communication is a first attempt in this direction. We prove that the $N$-qubit pure $W$ class of states ($|W\rangle_N = a_1|0...1\rangle + ... + a_N|1...0\rangle$, all $a_i$ complex) are uniquely determined by their two-party reduced density matrices. There does not exist any other pure or mixed $N$-qubit state sharing the same bipartite marginals.

Before proceeding to the proof, we will adopt some notations, for easier understanding.

Since a Hermitian matrix $A$ is usually identified by the elements $a_{ij}, \forall i \leq j$, a density matrix (written in some basis) is necessarily identified by its upper-half elements $(a_{ij}, \forall i < j)$ together with the diagonal elements $a_{ii}$. The lower-half entries $(a_{ij}, \forall i > j)$ are redundant as they are just complex conjugates of the upper ones. Therefore, we can write a general (possibly mixed) $N$-qubit density matrix in standard Computational Basis (CB) as\textsuperscript{9}

$$
\rho_{M}^{12...N} = \sum_{i=0}^{2^N-1} \sum_{j=i}^{2^N-1} r_{ij} |B_N(i)\rangle \langle B_N(j)| \quad (1)
$$

where $B_N(i)$ is the binary equivalent of the decimal number $i$ in an $N$-bit string.

Another key observation is that to compute the reduced density matrix (RDM) (of some parties) from an $N$-qubit pure state (in CB)

$$
|\psi\rangle_N = \sum_{i=0}^{2^N-1} a_i|B_N(i)\rangle, \quad (2)
$$

we need to find the expressions for only the diagonal entries of that RDM in terms of the state coefficients.

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Note that we require the expressions (i.e., the complex numbers appearing in the sum) and not the final calculated values (which are always real) of the diagonals. All other non-diagonal entries will be determined from these expressions. To see it explicitly, let us consider the m-partite marginal $\rho^{1i2...-m}$ of $\rho = |\psi\rangle\langle\psi|$, where $\rho^{1i2...-m} = T_{i,m+1}T_{m+2...-1}(\rho)$. This RDM can be written as

$$\rho^{1i2...-m} = \sum_{i=0}^{2^m-1} \sum_{j=0}^{2^{m-1}-1} r_{ij} |B_m(i)\rangle\langle B_m(j)|. \quad (3)$$

Clearly it has $2^m$ diagonal entries ($r_{ii}, \forall i = 0(1)2^m - 1$). To find the expression of $r_{ii}$, we should first write the decimal number $i$ by putting $t_1$, $t_2$,...,$t_m$ (each $t_j$ can take value 0/1) in an $m$-bit binary string. Then taking an N-bit string we put the $t_j$'s at $i$th places respectively (see Fig.1 and then fill the remaining $(N - m)$ places of the string arbitrarily by 0 and 1. These $(N - m)$ places can be filled in $2^{N-m}$ different ways. Hence each $r_{ii}$ will be the sum of $2^{N-m}$ number of terms (each term is of the form $|a_k|^2$, where the decimal number $k$ in the suffix is obtained by converting the binary arrangement to the decimal number). If we write these terms in increasing order of the suffixes, the first term in the expression of $r_{ii}$ will be $|a_{\sum_{j=1}^{t} 2^{N-i_j}}|^2$. (This least suffix is obtained by converting the binary number formed by putting $t_j$'s at $i$th places and filling all other places of the N-bit string by 0). Once we know the expression for $r_{ii}$, the expression for $r_{ij}$ follows trivially. To be explicit, say $r_{ii} = \sum_{k=0}^{2^{N-m}-1} |p_k|^2$ and $r_{ij} = \sum_{k=0}^{2^{N-m}-1} |q_k|^2$ ($p_k$, $q_k$ are some $a_i$'s with the suffix $l$ in increasing order), then $r_{ij} = \sum_{k=0}^{2^{N-m}-1} p_k q_k$. Note that $r_{ii}$, $r_{ij}$ and $r_{jj}$ are the co-efficient of $|B_m(i)\rangle\langle B_m(i)|$, $|B_m(j)\rangle\langle B_m(j)|$ and $|B_m(i)\rangle\langle B_m(j)|$ respectively in the RHS of (3). (See Appendix).

Now we will prove our claim: **N-Qubit Pure W States are Determined by their Bipartite Marginals.**

To prove this we will show that there exists no N-qubit state (rather Density Matrix) having the same bipartite marginals as those of an N-qubit W-state

$$|W\rangle_N = \sum_{i=0}^{N-1} w_{2i} |B_N(2^i)\rangle \quad (4)$$

with $\sum_{i=0}^{N-1} |w_{2i}|^2 = 1$ other than

$$|W\rangle_N < |W| = \sum_{i=0}^{N-1} \sum_{j=i}^{N-1} w_{2i} w_{2j} |B_N(2^i)\rangle\langle B_N(2^j)|. \quad (5)$$

**Proof**

1. Let us first find the bipartite marginals $\rho_{W}^{JK}$ of $|W\rangle_N$. As discussed above, we need to calculate the expressions for only the 4 diagonal elements $r_{ii}, i = 0(1)3$. Since the CB states in (4) contain just one 1, $r_{33} = 0$ in all $\rho_{W}^{JK}$. To find $r_{11}$ (which is the co-efficient of $|01\rangle\langle 01|$), we should put one 1 at $K$th place of N-bit string and there is exactly one such CB in (4) having co-efficient $w_{2N-K}$. Hence $r_{11} = |w_{2N-K}|^2$. Similarly, $r_{22} = |w_{2N-J}|^2$, $r_{00}$ can be obtained from the normalization condition. Thus

$$\rho_{W}^{JK} = (1 - |w_{2N-J}|^2 - |w_{2N-K}|^2) |00\rangle\langle 00| + |w_{2N-K}|^2 |01\rangle\langle 01| + |w_{2N-J}|^2 |10\rangle\langle 10| + w_{2N-K} w_{2N-J} |11\rangle\langle 11| \quad (6)$$

Written in matrix form,

$$\rho_{W}^{JK} = \begin{pmatrix} r_{00} & 0 & 0 & 0 \\ 0 & |w_{2N-K}|^2 & w_{2N-K} w_{2N-J} & 0 \\ 0 & w_{2N-K} w_{2N-J} & |w_{2N-J}|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (7)$$

where $r_{00} = 1 - |w_{2N-J}|^2 - |w_{2N-K}|^2$.

2. Now let us suppose that there exists an N-qubit density matrix $\rho_{M}^{12...N}$ given by (1), which has the same bipartite marginals as $|W\rangle_N$. In matrix form, all bipartite marginals $\rho_{M}^{JK}$ of $\rho_{M}^{12...N}$ will have four diagonal elements $d_{i}^{JK}$ at (i,i) positions, $i = 1(1)4$. Let us first calculate the diagonal element $d_{4}^{JK}$ at (4,4) position of $\rho_{M}^{JK}$. Obviously, this will be a sum of $2^{N-2}$ number of diagonal terms ($r_{ii}$) of $\rho_{M}^{12...N}$. To see explicitly which $r_{ii}$'s will appear in the sum, we observe that the suffixes $i$ will vary over the decimal numbers obtained by converting the N-bit binary numbers having 1 fixed at $J$th & $K$th places and arbitrarily 0/1 at the remaining (N-2) places. (As an illustration, Fig.2 shows how to get the least suffix there). Hence the terms $r_{ii}$’s for the suffixes $i = 0$ and $i = 2^{j-1} \forall j = 1(1)N$ will not appear in the expression of $d_{4}^{JK}$ for any $J,K$ as the binary representation of these numbers can have at most one 1 (but we need at least two 1).

3a. Now comparing the (4,4) position of $\rho_{M}^{JK}$ and $\rho_{W}^{JK}$, it follows that $d_{4}^{JK} = 0 \forall J,K$. Since the diagonal elements $r_{ii} \geq 0 \forall i$, it follows that all $r_{ii}$ appearing in
the expression of $d_4^{1K}$ should individually be zero. Hence it implies (from step 2) that the only non-zero diagonal elements of $\rho^{12...N}_M$ are $r_{ii}$ for $i = 0$ & $i = 2^{-j} \forall j = 1(1) N$.

3b. Next considering $d_3^{1K}$ for any fixed $K$ and comparing with the element at (3, 3) position of $\rho^{1K}_M$, we get $r_{2N-1} = |w_{2N-1}|^2$. Similarly comparing (2, 2) position of $\rho^{1K}_M$ and $\rho^{1K}_W$, it follows that $r_{2N-K-K} = |w_{2N-K}|^2 \forall K = 1(1) N$ i.e., $r_{2^j 2^j} = |w_{2^j}|^2 \forall i = 0 \to (N - 2)$.

3c. Finally, from normalization condition $\sum_{i=0}^{2^{N-1}} r_{ii} = 1 = \sum_{i=0}^{N-1} |w_{2i}|^2$, we get $r_{00} = 0$. Thus collecting the results of steps 3a & 3b we get

$$r_{2^j 2^j} = |w_{2^j}|^2, \forall i = 0(1) N - 1 \tag{8}$$

and all other $r_{ii}$ in $\rho^{12...N}_M$ are zero.

4. Now we will use the fact that if a diagonal element of a positive semidefinite (PSD) matrix is zero, then all elements in the row and column containing that element should be zero \[11]. Hence (using the final result of step 3c) it follows that

$$\rho^{12...N}_M = \sum_{i=0}^{N-1} \sum_{j=i}^{N-1} r_{2^j 2^j} |B_N(2^j)\rangle \langle B_N(2^j)| \tag{9}$$

where $r_{2^j 2^j}$ are given by (8). Note that $\rho^{12...N}_M$ in eqn. (9) reduces to the same form as $|W_N\rangle \langle W_N|$ given in (5).

5. The non-diagonal element $r_{2^j 2^j}$ at $(2^j, 2^j)$ place of $\rho^{12...N}_M$ is found to be $w_{2^j} \bar{w}_{2^j}$ by comparing the elements at (2, 3) position of $\rho^{1(N-j)(N-j)}_M$ and $\rho^{12...N}_W$. Thus $r_{2^j 2^j} = w_{2^j} \bar{w}_{2^j}$ and hence it follows that $\rho^{12...N}_M = |W_N\rangle \langle W_N|$. 

In the above analysis considering mixed states, we needed all $N^2C_2$ number of bipartite marginals to determine $|W_N\rangle$. However, if restricted to pure states only, then it can be shown that we require only $(N - 1)$ bipartite marginals $\rho^{1K}_W$, where one of the parties is fixed and the other varies over all the remaining $(N - 1)$ parties. Without loss of generality, we can take the first party as the fixed one and thus $\rho^{1K}_W \forall K = 2(1) N$ are sufficient to determine $|W_N\rangle$.

We will now prove this second claim: Among pure states, $N$-Qubit W States are Determined by their $N$-1 Bipartite Marginals $\rho^{1K}_W$, $K = 2(1) N$.

To prove this claim it suffices to show that there exists no $N$-qubit pure state $|\psi\rangle_N$ given by eqn. (2) having the same bipartite marginals.

**Proof**

1. First compare the entries at (4, 4) position of $\rho^{1K}_W$ and $\rho^{1K}_W \forall K = 2(1) N$. This will make the last (arranged in increasing order of the suffix) $2^{N-1} - 1$ number of coefficients vanish, i.e., $a_i = 0 \forall i = 2^{N-1} + 1 \to 2^N - 1$ [The decimal numbers generated by placing 1 at 1st & Kth places and filling all other places arbitrarily by 0/1 \forall K = 2(1) N].

2. Now look at the entries at (3, 3) position of $\rho^{1K}_W$. For all values of $K$ there is only one term $|a_{2N-1}|^2$ in common and this is the term with least suffix. (The common bit 1 at Most Significant Place has decimal value $2^{N-1}$). All remaining $2^{N-2} - 1$ terms of each $\rho^{1K}_W$ are nothing but the terms considered in step 1 (as the suffixes generated will be $> 2^{N-1}$). So the only non-zero term at (3, 3) position of each $\rho^{1K}_W$ is the common term $|a_{2N-1}|^2$ which when compared with $\rho^{1K}_W$ gives

$$|a_{2N-1}| = |w_{2N-1}| \tag{10}$$

3. The element at (2, 3) place of $\rho^{1K}_W$ is the sum of products of corresponding $a_i$’s appearing at (2, 2) position and complex conjugate of $a_i$’s appearing at (3, 3) position. The term with least suffix at (2, 2) position is $|a_{2N-K}|^2$. Hence (by step 2, $|a_{2N-1}|^2$ is the only non-zero term at (3, 3) position and this is the least suffix term there) comparing with $\rho^{1K}_W$,

$$a_{2N-K} \bar{a}_{2N-1} = w_{2N-K} \bar{w}_{2N-1}$$

$$\Rightarrow a_{2N-K} \bar{w}_{2N-1} = \bar{a}_{2N-1} = e^{i\phi}$$

$$\Rightarrow a_{2N-K} = e^{i\phi} w_{2N-K}, \forall K = 1(1) N \tag{11}$$

where $\phi = arg(a_{2N-1}) - arg(w_{2N-1})$ is a fixed number.

4. Next consider the entries at (2, 2) position of $\rho^{1K}_W$. For all $K$, the sum there starts with the least suffix term $|a_{2N-K}|^2 = |w_{2N-K}|^2$ (by (11)). So comparison with $\rho^{1K}_W$ will make the remaining $2^{N-2} - 1$ terms vanish.

5. Finally, the normalization condition gives $a_0 = 0$. Therefore,

$$|\psi\rangle_N = \sum_{i=0}^{2^{N-1}} a_i |B_N(i)\rangle = e^{i\phi} \sum_{i=1}^{N} w_{2^i} |B_N(2^i)\rangle = |W_N\rangle$$

In conclusion, we have shown that the $N$-qubit W class of states are uniquely determined by just their bipartite marginals. This reveals that we do not require information regarding the reduced states beyond the bipartite level. In other words, the $N$-party correlations in $W$ states are reducible to 2-party correlations. Therefore, any higher party $W$ state can be constructed from bipartite reduced density matrices. Recently, a lot of effort has been devoted to experimental generation of multi-qubit $W$ states by different methods \[12]. We hope that our result may be useful to make the process easier as it is sufficient to consider only bipartite marginals. In a slightly different context, such investigations are being carried out in molecular physics, viz., construction of density matrices of an $N$-electron system from its bipartite marginals (see \[3\] for references).
Another notable point is that for $|W\rangle_N$, the loss of any $N-2$ parties still leaves it in a bipartite entangled state

$$\rho_{JK}^{\mu} = (|\psi^+\rangle J_{JK} (|\psi^+\rangle + (1 - w_{2N-J}) - w_{2N-K}|00\rangle\langle 00|)$$

where $|\psi^+\rangle J_{JK} = w_{2N-J}|01\rangle + w_{2N-J}|10\rangle$, which can be distilled. It has been suggested in the literature that the entanglement of $W$ state is readily bipartite. Our result confirms this. As $|W\rangle_N$ can be determined uniquely from bipartite marginals, any property of the whole state should be characterized by these marginals. Thus the total entanglement in $W$ state should essentially be characterized by the bipartite entanglement present in it. Also it is very likely that there exists a close relation between the determination of $|W\rangle_N$ from bipartite marginals and the saturation of the general monogamy inequality for bipartite entanglement. However, further investigation is required in order to establish this.

It is natural to ask whether $|W\rangle_N$ can uniquely be determined by arbitrary $(N-1)$-partite marginals. We have verified that the answer is in the affirmative only for $N = 3, 4$. This is due to the fact that up to $N = 4$, any set of $(N-1)$ number of bipartite marginals covering the parties would automatically correlate all the parties. However, for $N \geq 5$, there always exist some set which would not correlate all the parties. For example, for $N = 5$, the set $\{\rho_1^{12}, \rho_1^{13}, \rho_1^{23}, \rho_1^{34}\}$ cannot determine $|W\rangle_5$ uniquely.

Another interesting issue would be to find if $(N-1)$ is the optimal number or $|W\rangle_N$ can be determined by less number of bipartite marginals. It is tempting to think that it is sufficient to take $[\frac{N+1}{2}]$ bipartite marginals (since this is the minimum number required to cover all parties). However, this is not the case. For even $N$, one particular coverage can be achieved by taking the marginals $\rho_{J(j+1)}^{12}$, $J = 1(2)(N-1)$. But such a coverage does not determine $|W\rangle_N$ uniquely. For example

$|W\rangle_4 = a|0001\rangle + b|0010\rangle + c|0100\rangle + d|1000\rangle$ and $|W\rangle_4 = e ^ {i \theta} (a|0001\rangle + b|0010\rangle + c|0100\rangle + d|1000\rangle)$ share the same $\rho_{12}^4$ and $\rho_{34}^4$. The reason for this indeterminacy is that $\rho_{12}^4$ and $\rho_{34}^4$ can be viewed as local marginals and they do not capture the entire correlation. So it is necessary to take into account one more marginal to correlate them. Similar argument holds for the general case.

We have presented the first example of a class of $N$-party quantum states determinable from fewer than $(N-1)$-partite marginals. It is also worth finding other classes determinable from $K$-partite reduced matrices for $K < (N-1)$. The method developed here can be readily applied to identify states which exhibit $K$-party correlations. It also needs to be checked whether $W$ is the only class whose correlations can be reduced to 2-party level.

We hope this work would provide some insight into the general problem of reducibility of multi-party quantum correlations, and shed light on its close connection with quantum entanglement.

We thank Sandu Popescu for bringing to our attention the paper [1] which has inspired the present work.

**Appendix**

Here we will explicitly show how one can obtain the off diagonals from the expression of the diagonal elements, by considering a simple example.

Let us determine the bipartite RDM $\rho_{ij}^2$ from $|\psi\rangle = \frac{1}{\sqrt{7}}(|001\rangle + i|111\rangle)$.

In matrix form, $\rho = |\psi\rangle \langle \psi| = [r_{ij}]_{1\leq i,j\leq 3}$ and $\rho_{ij}^2 = [R_{kj}]_{1\leq j,k\leq 3}$. Then the diagonal terms are given by

$$R_{00} = r_{00} + r_{11} = |0|^2 + |\frac{1}{\sqrt{7}}|^2 = \frac{2}{7}$$

$$R_{11} = r_{22} + r_{33} = |0|^2 + |0|^2 = 0$$

$$R_{22} = r_{44} + r_{55} = |0|^2 + |0|^2 = 0$$

$$R_{33} = r_{66} + r_{77} = |0|^2 + |\frac{1}{\sqrt{7}}|^2 = \frac{2}{7}$$

Now from the explicit expression (and not from their calculated final real values $\frac{2}{7}$ and 0) of these diagonal entries, we can get the off-diagonal terms. For example, $R_{33} = \sum_{\text{corresponding terms}} (\text{complex number appearing in } R_{22}) (\text{conjugate of complex number appearing in } R_{33}) = 0(0) + 0(\frac{1}{\sqrt{7}}) = 0$

Similarly, $R_{03} = 0(0) + \frac{1}{\sqrt{7}}(\frac{1}{\sqrt{2}}) = -\frac{1}{2}$

Following matrix form:

$$\begin{bmatrix}
    r_{00} & r_{01} & \cdots & r_{02N-1} \\
    r_{10} & r_{11} & \cdots & r_{12N-1} \\
    \vdots & \vdots & \ddots & \vdots \\
    r_{2N-1} & \cdots & \cdots & r_{2N-1}
\end{bmatrix}$$

[10] If possible let $d_i < 0$ in a PSD matrix $A$. Then taking $|\psi\rangle = [0, \ldots, 1, \ldots, 0]^T$, $\langle \psi|A|\psi\rangle = d_i < 0$, a contradiction.

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