

Compatible conditions, entanglement and invariants

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ABSTRACT

To find whether a set of reduced density matrixes come from a common multi-party state is a hard and important problem. In this paper, (1) we introduce a method to find out some polytopes in one-party eigenvalue-space which are sufficient conditions of this problem. (2) We point out that there are some relations between the compatible conditions and the entanglement of pure states. And we show this idea more clearly in the three-qubit case. (3) We investigate the relations between the compatibility problem and the invariants of a matrix-set under some groups. Furthermore, we show that it is one of the reasons why the compatibility problems which involve the multi-party density matrixes are much more difficult than the one-party case.

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1 Introduction

Any N -party quantum state, pure or mixed, can be represented as a positive Hermitian operator $\rho_{12\dots N}$. From this positive operator, we can easily get a set of positive operators $\{\rho_1, \rho_2, \dots, \rho_{12}, \dots, \rho_{12\dots j}\}$ by tracing out some particles. But the inverse problem is far more difficult. To judge whether a given set of positive operators $\{\rho_1, \rho_2, \dots, \rho_{12}, \dots, \rho_{12\dots j}\}$ come from a common positive operator $\rho_{12\dots n}$ is what we concern about in this paper. This problem is called compatibility problem.¹ Since the general problem is too difficult to solve, we simplify this problem to some special situations. We focus on the following problems which have theoretical and practical importance.

1. The compatibility problem between a set of one-party reduced density matrixes $\{\rho_1, \rho_2, \dots, \rho_N\}$ and a N -party pure state $|\Psi_N\rangle$. That is, whether there exists a pure state $|\Psi_N\rangle$ such that its reduced density matrixes are the given ones. The pure-state constraint is a strong one on the positive N -party matrix $\rho_{12\dots N}$, this constraint makes this problem meaningful and much easy to solve. If there is no constraint on the N -party density matrix, this problem is trivial. Obviously, there are some other methods to make this problem nontrivial, such as giving the eigenvalue-spectrum of the N -party matrix $\rho_{12\dots N}$, but this constraint is more difficult than the former.²

2. The compatibility problem between a set of two-party reduced density matrixes and a pure state $|\Psi_N\rangle$. In this problem the pure-state constraint is no longer a condition to make the problem nontrivial, but to make the problem more simple. In any case, the two-party compatibility problem is not trivial.

The problem 1 is much more simple than problem 2 and 3. There are some evidences² that problem 1 only involves the eigenvalues of the reduced density matrixes. And some necessary and sufficient conditions on $C_2^{\otimes N}$ ^{3,4} and $C_3 \otimes C_3 \otimes C_3$ ⁵ systems have been found. But for problem 2 and problem 3, there is no such conditions yet, and these problems do not only involve the eigenvalues of the reduced density matrixes.

Why the compatibility problem is important? First, the compatibility problems have close relations to many-body entanglement which is the central problem of quantum information theory.⁶⁻⁹ It is clear that if there is no entanglement between particles, all of the compatibility problems are trivial. Since the entanglement makes the compatibility problem meaningful and difficult, it is not surprise to obtain some useful entanglement information from the compatible conditions. We can show this more clearly in Sec. III. In addition, the compatible conditions can also help us to understand the structure of pure states,^{10,11} this can also be found in Sec. III.

Second, the compatibility problem is also important in condensed matter physics and chemical physics.^{1,12} Since almost all the interactions in condensed matter physics are local (nearest neighbor interaction), and many physical variants (for example the correlation function) only concerned with a few of particles. We only need only several particles reduced density matrixes and not the whole state of the system. The number of the particles is determined by the form of the interaction (for nearest neighbor interaction, we only need the 2-particle reduced density matrixes). If we get all of the compatible conditions, we can design powerful variational methods to substantially simplify the computation of many physical variants.

2 Sufficient conditions for one-party reduced density matrixes

We begin with choosing a set of states which have the similar properties as set (1). We construct the set by a recursive way. Firstly, we construct the set B_d^2 in the space $C_d \otimes C_d$ as

$$|00\rangle, |11\rangle, \dots, |dd\rangle.$$

If the desired set B_d^k in the space $C_d^{\otimes k}$ are

$$|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_m\rangle.$$

then we construct the set B_d^{k+1} in the space $C_d^{\otimes k+1}$ as

$$\begin{aligned} &|0\rangle \otimes I_k(|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_m\rangle), \\ &|1\rangle \otimes E_k(|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_m\rangle), \\ &|2\rangle \otimes E_k^2(|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_m\rangle), \\ &\vdots \\ &|d-1\rangle \otimes E_k^{d-1}(|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_m\rangle). \end{aligned} \tag{1}$$

where $\{I_k, E_k, \dots, E_k^{d-1}\}$ is a cyclic group on the particle k whose order is d , I_k is the identity of this group, and $E_k|i\rangle_k = |i-1\rangle_k$ ($i = 1, 2, \dots, d-1$), $E_k|0\rangle_k = |d-1\rangle_k$, $E_k|i\rangle_l = |i\rangle_l$ ($k \neq l$). From this

construction, we know that the number of the states in the set $C_d^{\otimes N}$ is d^{N-1} . We can get the following theorem about the set in the space $C_d^{\otimes N}$

Theorem 1: There are no two different states which have more than $N - 2$ identical particles in the same state.

We can point out that the set constructed by our method is the maximal one which satisfies the theorem 1. And adding any state into this basis set will make the theorem not be hold. As the above special case, there are some other sets satisfy the same conditions. All of the maximal sets can also be found by operating an element $E_1^k \otimes E_2^l \cdots \otimes E_N^m$ of the group $G_c(d, d \cdots, d)$ on the original set (5). Here $\{I_k, E_k, \cdots, E_k^{d-1}\}$ is a cycle group operating on the k th particle as before. It is obvious that not every element of this group operate on the initial basis will generate a new set, there are many degenerate cases.

Since the number of parameters in the states space which spanned by B_d^N is far more than the number of the eigenvalues in the one-party density matrix eigenvalues space, it is difficult to get the explicit form of the eigenvalue space. But we can also use these states to get a polytope in the eigenvalues space of the one-party density matrixes. Any state in the space spanned by the set B_d^N can be written as $|\varphi\rangle = \sum_{i=1}^{d^{N-1}} \alpha_i |\varphi_i\rangle$. For the property of this set, any eigenvalues of one-party density matrix can be expressed as the sum of some coefficients' square $|\alpha_i|^2$. That is, the eigenvalues of one-party density matrixes of $|\varphi\rangle$ are linear combination of $|\alpha_i|^2$. For convenience, we define a vector V which is a point in the eigenvalues space. This vector V can be divided into N segments, the i th segments is constructed by d eigenvalues of the i th one-party reduced density matrix. We also define another vector $V' = (|\alpha_1|^2, |\alpha_2|^2, \cdots, |\alpha_{d^{N-1}}|^2)$ which is a point in the d^{N-1} -dimension space. Now we denote the set in the eigenvalues space, which can be gotten by the space spanned by B_d^N , as Q and the set which is formed by V' as P . We note that the coefficients $|\alpha_i|^2$ must satisfy the conditions $\sum_{i=1}^{d^{N-1}} |\alpha_i|^2 = 1$. So all of the vectors V' construct the standard simplex in $(d^{N-1} - 1)$ -dimension space. Since the eigenvalues of one-party density matrixes are linear combination of $|\alpha_i|^2$, Q can be found by operating a linear transformation on the set P . Using the simple property of the projection of the polytopes, we know that the set Q is also a polytope whose dimension is $rank(M)$ where matrix M is the linear transformation between P and Q . Here the rank of the matrix M is just the number of independent eigenvalues of one-party density matrixes, that is $N(d - 1)$. From this conclusion, we can find that the polytope which we have found before is not trivial, at least, it is not a zero measure set in eigenvalue-space. Even more, we have the following proposition from the projection theory¹³

Proposition : Let $\pi : P \rightarrow Q$ be a projection of polytopes. Then for every face of Q , F , the preimage $\pi^{-1}(F) = \{y \in P : \pi(y) \in F\}$ is a face of P . Furthermore, if F, G are faces of Q , then $F \subseteq G$ holds if and only if $\pi^{-1}(F) \subseteq \pi^{-1}(G)$.

Now from this proposition, we can find that all of the vertexes of the projection polytope Q are projection of some faces of the initial polytope P . If the vertex A of Q is the projection of a face B of P . Since we know the linear transformation M , it is easy to find the coordinates of A (A is a vertex of Q) through the coordinates of the vertexes of B (B is a face of P). So we can find all of the vertexes of Q by the vertexes of P . Since P is the standard simplex in $(d^{N-1} - 1)$ -dimension space, we know all of it's vertexes. They are $(100 \cdots 00), (010 \cdots 00), \cdots (00 \cdots 01)$ and there are one to one correspondence between them and the basis in (5). There are no degenerate on these vertexes under the linear transformation A . So we can construct a direct one to one correspondence between the vertexes of the projection polytope Q and the basis set (5). That is, we project every basis $|\Psi\rangle = |i_1 i_2 \cdots i_N\rangle$ to the vertex whose coordinates are $\{\{i_1\}, \{i_2\}, \cdots, \{i_N\}\}$ where $\{i_j\}$ means that only the (i_j) th eigenvalue is 1 and the others are zeroes. So we can get a polytope Q with d^{N-1} vertexes. For every set, we can

find a polytope Q_i . Of course, some polytopes are the same, some are overlapped. Then we can get the largest set which guarantees the existence of a pure state by union all of the polytopes, that is, $Q = \cup_{j=1}^{d^N} Q_j$.

3 Relations between the compatibility problems and entanglement

The necessary and sufficient compatible conditions between N one-party reduced qubit density matrixes and a pure state in $C_2^{\otimes N}$ are in the following

$$\sum_{i \neq k, i=1}^N \lambda_1^\dagger(i) \geq \lambda_1^\dagger(k) \quad (k = 1, 2, \dots, N), \quad (2)$$

where $\lambda_1^\dagger(i)$ is the smaller eigenvalue of the one-party density matrix ρ_i . These conditions are first gotten by Higuchi.³ The points that satisfy these conditions form a polytopes, Bravyi⁴ first given all of the vertexes of this polytopes, they are vectors

$$(00 \dots 0), \left(\frac{1}{2} \frac{1}{2} 0 \dots 0\right), \left(\frac{1}{2} \frac{1}{2} \frac{1}{2} 0 \dots 0\right), \dots, \left(\frac{1}{2} \frac{1}{2} \dots \frac{1}{2}\right). \quad (3)$$

and any particle permutation of these vertexes. For convenience in the following, we denote A_k ($k \geq 2$) as the vertexes set gotten by exchanging any of particles in the vertex $(\frac{1}{2} \dots \frac{1}{2} 0 \dots 0)$ (there are $k \frac{1}{2}$ in this vertex), especially, the set A_1 is a one-point set $\{(00 \dots 0)\}$. To make it clear, we first focus on the three-qubit case. In this case, we can draw these conditions in a three-dimension smaller-eigenvalue space (Fig 1). For pure states in the $C_2^{\otimes 3}$, there is a classification which is given by Acin *et al.*²² They divided the pure states into several classes. We can find from figure 1 that some classes of this classification have clear geometric meanings, they are some faces of this polytopes. The following facts can be found in this figure, the detailed proofs of these facts are given in the Appendix.

1. All the separable states (type 1) are on the point A (000), and vice versa.
2. All the biseparable states (type 2a), i.e. one of the particle does not entangled with the other two particles, are on the line AB_1, AB_2 and AB_3 , and vice versa.
3. All the generalized GHZ states (type 2b) are on the line AC. And for every point on the line AC, we can find a generalized GHZ state which have the given eigenvalues.
4. All the tri-Bell states (type 3a) are on the triangles $\Delta B_2B_3A, \Delta B_1B_3A, \Delta B_1B_2A$ and $\Delta B_1B_2B_3$. And for every point in these triangles, we can find a tri-Bell state which have the given eigenvalues.
5. All the extended GHZ states (type 3b) are on the triangles $\Delta CB_3A, \Delta CB_2A$ and ΔCB_1A . And for every point in these triangles, we can find a extended GHZ state which have the given eigenvalues.
6. All the W states²³(type 4a) are in the tetrahedron $AB_1B_2B_3$, and for every point in this tetrahedron, we can find a W state which have the given eigenvalues. This fact does not mean that the W state in the three-qubit pure-state space has none zero measure, since the projection from the state space to the smaller-eigenvalue space is not linear.

From these facts, the relations between the compatible polytopes of the one-party reduced density matrixes and the classification or entanglement of the three-qubit case are clear. Almost all of the types classified by Acin are corresponded with some geometry body. We also can see that there are some overlaps between the different types, this is due to the degenerate of the one-party reduced density matrixes. We believe that the degeneracy will be deleted if we get all of the necessary and sufficient conditions of any k -party reduced density matrixes.

4 Compatible problems and invariants

It is not surprised to find that the compatible conditions between a set of density matrixes and a multi-party state have close relations with the invariants of a set of matrixes under some groups. If we want to solve the compatible problem, we must find out all of the invariants. We can see in the following that this is a very difficult problem. Firstly, we point out that if three two-qubit density matrixes can come from a pure state, then we can find all of the invariants of the three-qubit pure state under $U(2) \otimes U(2) \otimes U(2)$ group from these matrixes. As Sudbery^{27,28} *et al.* point out that there are five independent invariants for three-qubit pure states under $U(2) \otimes U(2) \otimes U(2)$ group. They are $tr(\rho_A^2)$, $tr(\rho_B^2)$, $tr(\rho_C^2)$, $tr(\rho_B \otimes \rho_A \rho_{AB})$ and $\tau_{A,BC} = \tau_{A(BC)} - \tau_{AB} - \tau_{AC}$, where τ_{AB} is the concurrence¹⁵ of two-qubit density matrix ρ_{AB} , $\tau_{A(BC)}$ is equal to $det(A)$ under the pure state situation.²⁴ By the definition of these invariants, they can be completely determined by these reduced density matrixes. Of course, the pure state is determined uniquely under the local unitary. Generally, if all of the invariants of a pure state can be determined by some reduce density matrixes, then the pure state can be determined by the reduced density matrixes uniquely.

Secondly, we point out why the compatible problem of the multi-party density problem is much more difficult than the one-party problem. To make this idea more clear, we introduce the following definition.

Definition: A set of reduced matrixes $S = \{\rho_{I_1}, \rho_{I_2}, \dots, \rho_{I_k}\}$ is called locally equivalent to another set of reduced matrixes $S' = \{\rho'_{I_1}, \rho'_{I_2}, \dots, \rho'_{I_k}\}$ (where $I_j (j = 1, 2, \dots, k)$ are subset of $\{1, 2, \dots, n\}$), if there exists local unitary operators U_1, U_2, \dots, U_n such that $\rho_{I_j} = U_{I_j}^\dagger \rho'_{I_j} U_{I_j} (j = 1, 2, \dots, k)$ where U_{I_j} is the tensor product of $U_i (i \in I_j)$.

The relations between the compatible problem and this definition are clear, if the reduced matrixes in the set S are compatible, the matrixes in S' are compatible too. So the compatible conditions can only deal with the invariants of a set of matrixes under the local unitary group. If all of the matrixes in the set $S (S')$ are one-party density matrixes, this problem is trivial. Whether these two sets are locally equivalent is completely determined by the eigenvalues of the corresponding density matrixes and these eigenvalues are the only invariants under the local unitary transformation. But when there are some multi-party density matrixes in the set, the situation is different. There are two main difficulties. The first, the invariants of the multi-party density matrixes under the local unitary group are difficult to find. The second, the things even worse, all of the invariants of the multi-party density matrixes²⁹ under local unitary group are not enough. We need some other conditions. This can be seen in the following simple example. We consider the set $S = \{\rho_{12}, \rho_{23}, \rho_{13}\}$ and $S' = \{\rho'_{12}, \rho'_{23}, \rho'_{13}\}$. If these two sets are locally equivalent, it is easy to find that density matrixes ρ_{12} and ρ'_{12} , ρ_{23} and ρ'_{23} and ρ_{13} and ρ'_{13} must have the same invariants under the group $U_1 \otimes U_2$, $U_2 \otimes U_3$, $U_1 \otimes U_3$, respectively. These invariants have already completely solved by Linden *et al.*²⁹. It means that there exist unitary matrixes to make $\rho'_{12} = u_{11}^\dagger \otimes u_{21}^\dagger \rho_{12} u_{11} \otimes u_{21}$, $\rho'_{23} = u_{22}^\dagger \otimes u_{31}^\dagger \rho_{23} u_{22} \otimes u_{31}$ and $\rho'_{13} = u_{12}^\dagger \otimes u_{32}^\dagger \rho_{13} u_{12} \otimes u_{32}$. But these conditions can not guarantee $u_{11} = u_{12}$, $u_{21} = u_{22}$ and $u_{31} = u_{32}$. The latter requirements even can

not get by invariants under some group.

5 Conclusion

In this paper, we introduce a method to find some polytopes in the eigenvalues space of the one-party density matrixes. This method has been proved to be very strong for the $C_2^{\otimes n}$ space, but whether it is also strong for the other situation is an open question. Since the complexity of the compatibility problem comes from entanglement of the state, it is not surprise that we can find some entanglement information from the compatible conditions. We use the necessary and sufficient conditions of the $C_2^{\otimes n}$ one-party compatibility problem, especially the $C_2^{\otimes 3}$ case, to show that we can get some information indeed. We find there are some correspondences between some classes of the pure states and some polytope sets. But this correspondence is not exact, there are some overlap between them. This degenerate phenomena can be viewed as the limits of the one-party density matrixes. If we can find out all of the compatibility problems, we prefer to believe that we can get almost all of the entanglement information of the pure states. We also point out that to find out the compatibility problem of the multi-party density matrixes are much more difficult than the one-party case. The multi-party compatible problem is not only involved with the invariants of a matrix under local unitary, but also needs some other invariants which can not get by local group. How to find all of the invariants of a set of matrixes is another open question, of course, this problem has close relations with entanglement of states.

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