Classification of arbitrary multipartite entangled states under local unitary equivalence

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Abstract

We propose a practical method for finding the canonical forms of arbitrary dimensional multipartite entangled states, either pure or mixed. By extending the technique developed in one of our recent works, the canonical forms for the mixed $N$-partite entangled states are constructed where they have inherited local unitary symmetries from their corresponding $N + 1$ pure state counterparts. A systematic scheme to express the local symmetries of the canonical form is also presented, which provides a feasible way of verifying the local unitary equivalence for two multipartite entangled states.

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1. Introduction

Entanglement is one of the most important ingredients in quantum information science; it gives impetus to the most extraordinary nonclassical applications, such as teleportation and quantum computation, etc [1]. It is now generally regarded that entanglement is a key physical resource in realizing many quantum information tasks, thus the quantitative and qualitative studies of entanglement become more and more important. Though superficially entangled states show different features—usually not all entangled states are functionally independent—they may be intrinsically the same as far as the entanglement property is concerned. Two entangled states are said to be equivalent in implementing the same quantum information task if they can be obtained with certainty from each other via local operation and classical communication (LOCC). Theoretically, this LOCC equivalent class is such defined that within the class any two quantum states are inter-convertible by local unitary (LU) operators [2].
The characterization of bipartite entangled states under LU equivalence can be well understood by using the singular value (Schmidt) decomposition. However, things turn out to be much more complicated when the multipartite states are concerned. On one hand, the characterization of multipartite entanglement can be done by computing the LU invariants of the quantum states [3]. Two entangled states are LU equivalent if they have the same LU invariants; the relation between LU equivalence for \( n \)-partite pure states and the \((n - 1)\)-partite mixed states has also been observed and is used in constructing the LU invariants [4, 5]. The parameters in local invariants grow dramatically as the number of partite states increases, and the problem of identifying and interpreting independent invariants becomes very complicated [6]. Recently, an operationally meaningful measure has been introduced for three-qubit entanglement [7]. On the other hand, one can choose certain bases and put the quantum states in some canonical (standard) forms. Along this line, a canonical method was proposed in [8], though it was only given in a set of constraints on the coefficients of the quantum state. Later, this method was reformulated into a compact form [9]. By introducing the standard form for multipartite states Kraus proposed a general way to determine the LU transformation between two LU equivalent \( n \)-qubit states [10, 11], however as the dimensions increase, degeneracy emerges between the identical eigenvalues of the one-partite reduced density matrix and the verification of LU equivalence becomes unpractical.

Recently, in [12] we have proposed a practical method for finding the canonical form of a pure multipartite state by using high order singular value decompositions (HOSVDs) and the local symmetry properties of the tensor form quantum states. In this work, we generalize this method to the mixed states where the canonical forms for arbitrary mixed multipartite states are constructed. Also, we develop a systematic scheme to present the local symmetries among the canonical forms, which provides a feasible way to verify the LU equivalence of two quantum states regardless of the degeneracy conditions.

The structure of the paper is as follows. In section 2, we give a brief introduction to the basic technique of HOSVD which is used in our entanglement classification. In section 3, we reformulate the entanglement classification for multipartite pure states under LU in a neater form, and a practical classification method for arbitrary multipartite mixed states is developed where the canonical forms for mixed states are explicitly constructed. After this complete classification of multipartite entangled states with their canonical forms, in section 4 we develop a systematic scheme for verifying the LU symmetry between two entangled states. In section 5, practical examples of three- and four-qubit states are given. Finally, some concluding remarks are presented in section 6.

2. LU equivalence of the multipartite quantum state

A general \( N \)-partite entangled quantum state in the dimensions \( I_1 \times I_2 \times \cdots \times I_N \) can be formulated in the following form:

\[
|\Psi\rangle = \sum_{i_1, i_2, \ldots, i_N} \psi_{i_1 i_2 \ldots i_N} |i_1\rangle |i_2\rangle \ldots |i_N\rangle ,
\]

(1)

where \( \psi_{i_1, i_2, \ldots, i_N} \in \mathbb{C} \) are coefficients of the quantum state in representative bases. Two quantum states are said to be LU equivalent if they are inter-convertible by LU operators, which can be schematically expressed as
Here, the coefficients \( \psi_{i_1 i_2 \cdots i_N} \) can also be treated as the entries of a tensor \( \Psi \) and hence the quantum states can be represented by high order complex tensors. In the tensor form of \( \Psi \), the unitary operator \( U^{(n)} \) acting on the \( n \)th partite is defined as

\[
(U^{(n)} \Psi)_{i_1 i_2 \cdots i_n a_{n+1} a_{n+2} \cdots a_k} = \sum_{i_1, i_2, \ldots, i_N} \psi_{i_1 i_2 \cdots i_N} U^{(n)}_{i_1 i_2 \cdots i_N} \Psi_{i_1 i_2 \cdots i_N a_{n+1} a_{n+2} \cdots a_k}.
\]

For the bipartite pure state, the tensor \( \Psi \) is a matrix \( \Psi = [\psi_{i \in J} \in \mathbb{C}^{I \times I} \) (matrices with complex numbers of \( I \) rows and \( I \) columns) where the dimensions of the Hilbert space for each partite are \( I_1 \) and \( I_2 \) separately. The singular value decomposition (SVD) of the bipartite state \( \Psi \) of dimensions \( I_1 \times I_2 \) reads

\[
\Lambda = U^{(1)} \cdot \Psi \cdot U^{(2)} = \text{diag} \{ \lambda_1, \ldots, \lambda_I \},
\]

where \( \lambda_i \geq 0, \forall i < j, I = \min(I_1, I_2) \). \( \Lambda \) has the following two properties:

1. The singular values \( \lambda_i, i \in \{1, \ldots, I\} \) of matrix \( \Psi \) are uniquely defined.
2. \( \Lambda \) is a diagonal matrix and uniquely defined (with a prescribed order of the singular values).

In this case, the singular values of the quantum state \( \Psi \) readily characterize its entanglement properties under LU equivalence. Two bipartite quantum states are LU equivalent if, and only if, they have the same SVDs.

Here we introduce the technique which can be seen as the generalization of SVD to high dimensional multipartite systems—the HOSVD [13]. Let us define the matrix unfolding of the tensor \( \Psi \in \mathbb{C}^{I_1 \times I_2 \cdots I_N} \) with \( n \)th index as

\[
\Psi_{(n)} \in \mathbb{C}^{I_1 \times (I_2 + I_3 + \cdots + I_k - I_{n+1} - I_{n+2} - \cdots - I_N)}.
\]

Here \( \Psi_{(n)} \) is a \( I_1 \times (I_2 + I_3 + \cdots + I_k - I_{n+1} - I_{n+2} - \cdots - I_N) \) matrix. For example, the \( 2 \times 3 \times 4 \) complex tensor \( \Psi \), unfolding with the second and third indexes has the following forms:

\[
\Psi_{(2)} = \begin{pmatrix}
\psi_{111} & \psi_{112} & \psi_{113} & \psi_{121} & \psi_{122} & \psi_{123} & \psi_{131} & \psi_{132} & \psi_{133} & \psi_{211} & \psi_{212} & \psi_{213} & \psi_{221} & \psi_{222} & \psi_{223} & \psi_{231} & \psi_{232} & \psi_{233} & \psi_{311} & \psi_{312} & \psi_{313} & \psi_{321} & \psi_{322} & \psi_{323} & \psi_{331} & \psi_{332} & \psi_{333}
\end{pmatrix},
\]

\[
\Psi_{(3)} = \begin{pmatrix}
\psi_{111} & \psi_{112} & \psi_{113} & \psi_{114} & \psi_{121} & \psi_{122} & \psi_{123} & \psi_{124} & \psi_{131} & \psi_{132} & \psi_{133} & \psi_{134} & \psi_{211} & \psi_{212} & \psi_{213} & \psi_{214} & \psi_{221} & \psi_{222} & \psi_{223} & \psi_{224} & \psi_{231} & \psi_{232} & \psi_{233} & \psi_{234} & \psi_{311} & \psi_{312} & \psi_{313} & \psi_{314} & \psi_{321} & \psi_{322} & \psi_{323} & \psi_{324} & \psi_{331} & \psi_{332} & \psi_{333} & \psi_{334} & \psi_{341} & \psi_{342} & \psi_{343} & \psi_{344} & \psi_{411} & \psi_{412} & \psi_{413} & \psi_{414} & \psi_{421} & \psi_{422} & \psi_{423} & \psi_{424} & \psi_{431} & \psi_{432} & \psi_{433} & \psi_{434} & \psi_{441} & \psi_{442} & \psi_{443} & \psi_{444}
\end{pmatrix}.
\]

For arbitrary \( N \)-partite systems there exists a core tensor \( \Omega \) for each tensor \( \Psi \),

\[
\Omega = U^{(1)} \otimes U^{(2)} \otimes \cdots \otimes U^{(N)} \Psi.
\]

Here \( \Omega \) is of the same order as \( \Psi \) in the Hilbert space of \( I_1 \times I_2 \times \cdots \times I_N \). Any \( N-1 \) order tensor \( \Omega_{i_{n+1} i_{n+2}} \) obtained by fixing the \( n \)th index to \( i \), has the following property:

\[
(\Omega_{i_{n+1} i_{n+2}}, \Omega_{i_{n+1} i_{n+2}}) = \delta_{ij} \left( \sigma_i^{(n)} \right)^2.
\]
where \( \sigma_i^{(n)} \) is called the \( n \)-mode singular value of \( \Psi \) and \( \sigma_i^{(n)} \geq \sigma_j^{(n)} \geq 0, \forall i < j \). The singular value \( \sigma_i^{(n)} \) symbolizes the Frobenius-norm \( \sigma_i^{(n)} = ||\Psi_{i\cdots i}|| = \sqrt{\langle \Omega_{i\cdots i}, \Omega_{i\cdots i} \rangle}, \) where the inner product \( \langle A, B \rangle \equiv \sum_{i_1} \sum_{i_2} \cdots \sum_{i_k} b_{i_1\cdots i_k} a^*_{i_1\cdots i_k} \) (see [13] for details).

In the following we show how to get the core tensor by the LU transformation \( U^{(i)}, i \in \{1, \ldots, N\} \) in equation (7). A quantum state \( \Omega \) with the same dimension as \( \Psi \) is LU equivalent to \( \Psi \) if

\[
\Omega = U^{(1)} \otimes U^{(2)} \otimes \cdots \otimes U^{(N)} \Psi,
\]

where \( U^{(i)}, i \in \{1, \ldots, N\} \) are unitary matrices. In the matrix unfolding form, equation (9) can be rewritten as

\[
\Omega_{(n)} = U^{(n)} \cdot \Psi_{(n)} \cdot (U^{(n+1, \ldots, n-1)})^T.
\]

Here \( U^{(n+1, \ldots, n-1)} \equiv U^{(n+1)} \otimes U^{(n+2)} \otimes \cdots \otimes U^{(N)} \otimes U^{(1)} \otimes \cdots \otimes U^{(n-1)}; \Omega_{(n)} \) and \( \Psi_{(n)} \) have the same dimensions: \( L_i \) rows and \( (I_{n+1} \times I_{n+2} \cdots \times I_N \times I_1 \times \cdots \times I_{n-1}) \) columns. Now consider the particular case where \( U^{(n)} \) is obtained from the SVD of matrix \( \Psi_{(n)} \), i.e.

\[
U^{(n)} \cdot \Psi_{(n)} \cdot V^{(n)} = \text{diag}\{\sigma_1^{(n)}, \sigma_2^{(n)}, \ldots, \sigma_k^{(n)}\},
\]

where \( U^{(n)} \) and \( V^{(n)} \) are unitary matrices, and \( \sigma_1^{(n)} \geq \sigma_2^{(n)} \geq 0, \forall i < j \). Equation (10) now can be written as

\[
\Omega_{(n)} = \text{diag}\{\sigma_1^{(n)}, \sigma_2^{(n)}, \ldots, \sigma_k^{(n)}\} \cdot V^{(n)\dagger} \cdot (U^{(n+1, \ldots, n-1)})^T.
\]

It is clear that \( \Omega_{(n)} \) has orthogonal rows

\[
\langle \Omega_{i\cdots i}, \Omega_{j\cdots j} \rangle = \delta_{jk} \left( \sigma_j^{(n)} \right)^2.
\]

Equation (13) always holds if \( U^{(n+1, \ldots, n-1)} \) is a unitary matrix. In a similar way we can obtain all the other LU matrices \( U^{(i)}, i \in \{1, 2, \ldots, N\} \), and eventually the core tensors \( \Omega \) of \( \Psi \) can then be constructed via equation (9).

From the construction of the core tensor, two important properties of HOSVD (when compared to its bipartite counterpart) can be concluded:

1. The \( n \)-mode singular values \( \sigma_i^{(n)} \), \( i \in \{1, \ldots, L_i\}, n \in \{1, \ldots, N\} \), of \( \Psi \) are uniquely defined.
2. If \( \forall n \in \{1, \ldots, N\} \) the \( n \)-mode singular values \( \sigma_i^{(n)} \) are all distinct, then \( \Omega_{(n)} = \Theta_{(n)} \Omega_{(n)} \) is also a HOSVD of \( \Psi \) where \( \Theta_{(n)} = \text{diag}\{e^{\mu_1^{(n)}}, \ldots, e^{\mu_{k_n}^{(n)}}\} \). Otherwise, let \( \sigma_1^{(n)} > \sigma_2^{(n)} > \cdots > \sigma_{k_n}^{(n)} \geq 0 \) denote the distinct \( n \)-mode singular values of \( \Omega_{(n)} \) with respective positive multiplicities \( \mu_1^{(n)} \), \( \mu_2^{(n)} \), \ldots, \( \mu_{k_n}^{(n)} \) where \( \sum_{j=1}^{k_n} \mu_j^{(n)} = L_n \). In this case,

\[
\Omega_{(n)} = \bigoplus_{i=1}^{k_n} \mu_i^{(n)} \Omega_{i\cdots i}(n), \quad \Omega_{(n)} \equiv S^{(n)} \Omega_{(n)}
\]

is also a HOSVD of \( \Psi \). Here \( u_i^{(n)} \in \mathbb{C}^{\mu_i^{(n)} \times \mu_i^{(n)}} \) are arbitrary \( \mu_i^{(n)} \times \mu_i^{(n)} \) unitary matrices and constitute the diagonal blocks of \( S^{(n)} \) which are conformal to those \( n \)-mode singular values of \( \Omega_{n} \) with multiplicity.

From the second property it is clear that, unlike the bipartite case, the core tensor \( \Omega \) (HOSVD) of \( \Psi \) is not uniquely defined.
3. Classification under local unitary equivalence

In this section we propose an entanglement classification scheme by decomposing the LU equivalence of the quantum states into two correlated problems: the HOSVD and LU symmetries. First, we give a brief introduction to the entanglement classification of arbitrary dimensional multipartite pure states which was first proposed in [12], then we extend the method to the mixed states, by which the canonical forms for entanglement classes of mixed states under LU equivalence can be constructed neatly.

3.1. LU equivalence for multipartite pure states

Due to the nonuniqueness of the core tensors, \( \Omega \) cannot be identified as the entanglement classes of the quantum states. The philosophy of our scheme in [12] is that if we impose this nonuniqueness as a local symmetry within the core tensors themselves, then we can get the unique canonical forms. That is, if we regard the core tensors \( \Omega \) as a local symmetry within the core tensors themselves, then we can get the canonical forms for entanglement classes of mixed states under LU equivalence.

The core tensors \( \Omega \) of two different core tensors related by local operators as the same entanglement class then the HOSVD can be seen as the entanglement classification of the multipartite state \( \Psi \).

Suppose that the core tensor \( \Omega \) has \( k_n \) distinct \( n \)-mode singular values \( \sigma_i^{(n)} \), \( i \in \{1, 2, \ldots, k_n\} \), each with a multiplicity of \( \mu_i^{(n)} \) where \( \sum_i \mu_i^{(n)} = l_n \). Here we regard these multiplicities as the degeneracies of the singular values which corresponds to the case of the nongeneric states of [10]. From equation (14) we can infer that the LU symmetry which relates two core tensors takes the following form

\[
S = \bigotimes_{n=1}^{N} \bigoplus_{i=1}^{k_n} u_i^{(n)}
\]

The core tensors \( \Omega' \) and \( \Omega \) related by this symmetry now can be written as

\[
\Omega' = S \Omega.
\]

Two different core tensors related by \( S \) belong to the same entanglement class. We can call such a core tensor \( \Omega \) of \( \Psi \) associated with the corresponding local symmetry \( S \) the canonical form of \( \Psi \).

In order to see how this symmetry acts on the core tensors we introduce the technique of vectorization of the matrix. With each matrix \( A = [a_{ij}] \in \mathbb{C}^{I \times J} \), we can associate it with a vector \( \vec{A} \) defined by

\[
\vec{A} \equiv [a_{11}, \ldots, a_{I_1}, a_{12}, \ldots, a_{I_1I_2}, \ldots, a_{I_1I_2\cdots I_J}]^T.
\]

Two tensors \( \Psi \) and \( \Psi' \) of \( I_1 \times I_2 \times \cdots \times I_N \) which are related by local operators \( U^{(n)} \), \( n \in \{1, 2, \ldots, N\} \), can be expressed in the matrix unfolding form with the \( n \)-th index

\[
\Psi'_{(n)} = U^{(n)} \cdot \Psi_{(n)} \cdot (U^{(n+1)} \otimes U^{(n+2)} \otimes \cdots \otimes U^{(N)} \otimes U^{(1)} \otimes \cdots \otimes U^{(m-1)})^T.
\]

With the convention of equation (17), the matrix equation equation (18), can be written as (see [14])

\[
U^{(n+1)} \otimes U^{(n+2)} \otimes \cdots \otimes U^{(N)} \otimes U^{(1)} \otimes \cdots \otimes U^{(m-1)} \otimes U^{(n)} \hat{\Psi}_{(n)} = \hat{\Psi}'_{(n)}.
\]

This can be seen as a unitary transformation of a \( I_1 \times I_2 \times \cdots \times I_N \) vector \( \vec{\Psi}_{(n)} \) to \( \vec{\Psi}'_{(n)} \). On choosing \( n = N \), we have the simple form of equation (19)

\[
U^{(1)} \otimes \cdots \otimes U^{(N)} \hat{\Psi}_{(N)} = \hat{\Psi}'_{(N)}.
\]
Here the symmetry between their core tensors, equation (16), can be similarly represented as
\[
\tilde{\Omega}_N = S \tilde{\Omega}_N = S \left( \bigoplus_{n=1}^{N} \bigoplus_{j=1}^{k_n} u_j^{(n)} \right) = \tilde{\Omega}_N,
\]
(21)
where \( u_j^{(n)} \) is a \( \mu_j^{(n)} \times \mu_j^{(n)} \) unitary matrix and \( \sum_{i=1}^{k_n} \mu_j^{(n)} = I_k \). In the block-diagonalized form, equation (21) is
\[
\begin{pmatrix}
 u_1^{(1)} \otimes \cdots \otimes u_1^{(N)} & 0 & \cdots & 0 \\
 0 & u_1^{(1)} \otimes \cdots \otimes u_2^{(N)} & \cdots & 0 \\
 \vdots & \vdots & \ddots & \vdots \\
 0 & 0 & \cdots & u_{k_1}^{(1)} \otimes \cdots \otimes u_{k_2}^{(N)}
\end{pmatrix} \cdot \tilde{\Omega}_N = \tilde{\Omega}_N',
\]
(22)
We can set \( u_j^{(n)} = e^{i\theta_j} \) if the multiplicity \( \mu_j^{(n)} = 1 \). In all, we have the following theorem which has been stated in [12].

**Theorem 1.** The core tensors \( \Omega \) associated with the local symmetry group \( S \) is the canonical form of the multipartite pure state and is the entanglement class under LU equivalence.

From this theorem, we can form a more general point of view for the equivalent entanglement class. Any subset of the quantum states in the form of the multipartite pure state and is the entanglement class under LU equivalence.

From the quantum state point of view, tensor \( \Omega \) now is decomposed into several invariant subtensors (denoted by \( \omega \)) of the Hilbert space of \( I_1 \times I_2 \times \cdots \times I_N \) under the transformation \( S \). The dimensions of these subtensors conform to the direct-summed subgroups of \( S \) in equation (22). For example equation (22) can be written as
\[
\begin{pmatrix}
 u_1^{(1)} \otimes \cdots \otimes u_1^{(N)} & 0 & \cdots & 0 \\
 0 & u_1^{(1)} \otimes \cdots \otimes u_2^{(N)} & \cdots & 0 \\
 \vdots & \vdots & \ddots & \vdots \\
 0 & 0 & \cdots & u_{k_1}^{(1)} \otimes \cdots \otimes u_{k_2}^{(N)}
\end{pmatrix} \cdot \begin{pmatrix}
 \overline{\alpha}_{r_1} \\
 \overline{\alpha}_{r_2} \\
 \vdots \\
 \overline{\alpha}_{r_n}
\end{pmatrix} = \begin{pmatrix}
 \overline{\alpha}_{r_1} \\
 \overline{\alpha}_{r_2} \\
 \vdots \\
 \overline{\alpha}_{r_n}
\end{pmatrix},
\]
(26)
Figure 1. The wiggled line represents $U\Psi$ and it forms an orbit with an irregular shape; the circular line represents $S\Omega$ and it forms a well-structured orbit. $\Omega = U_0\Psi$ and $\Omega' = U'_0\Psi'$ both are the core tensors on the $S\Omega$ orbit.

where $\vec{\omega}_i$ and $\vec{\omega}'_i$ are the segments of the column vectors $\Omega_{(N)}$ and $\Omega'_{(N)}$ with the dimension conformal to the diagonal blocks $u^{(1)}_{i_1} \otimes \cdots \otimes u^{(N)}_{i_N}$. $\vec{\omega}$s are just the vector forms of the subtensors $\omega$.

3.2. LU equivalence for multipartite mixed states

The classification of the entanglement for mixed states is generally believed to be more complicated than for pure states in many cases. However in the case of LU equivalence, it has been noticed that an $n$-partite pure state is related to its $(n - 1)$-partite mixed state [5]. Here we generalize our entanglement classification method developed for multipartite pure states to the case of arbitrary dimensional $N$-partite mixed states.

Consider a mixed $N$-partite quantum state $\rho$ which is generally expressed as

$$\rho = \sum_i p_i^2 |\psi_i\rangle \langle \psi_i|, \quad (27)$$

where $\sum_i p_i^2 = 1$, $p_i \in \mathbb{R}^+$, $|\psi_i\rangle$ are $N$-partite pure states. We add an additional 0th partite to the original $N$-partite mixed state $\rho$ and formulate an $N + 1$ pure quantum state of the following form

$$\Psi_0 = \sum_i p_i |\tilde{i}\rangle |\psi_i\rangle, \quad (28)$$

where $|\tilde{i}\rangle$ are the bases of the 0th partite. For this quantum state, we have the following fact:

$$\text{Tr}_0[|\Psi_0\rangle \langle \Psi_0|] = \sum_{n,i,j} p_ip_j \langle n|\tilde{i}\rangle \langle \psi_j| \langle j|n\rangle$$

$$= \sum_{n,i,j} p_ip_j \langle j|n\rangle \langle n|\tilde{i}\rangle \langle \psi_i| \langle \psi_j|$$

$$= \sum_i p_i^2 |\psi_i\rangle \langle \psi_i| = \rho. \quad (29)$$
Further, we have, if $\Psi_0 = U(0) \otimes E(1) \otimes \cdots \otimes E(N) \Psi_0 \equiv U(0) \Psi_0$, where $E$ is unit matrix,

\[
\text{Tr}_0[\Psi_0] = \text{Tr}_0[\Psi_0]\langle \Psi_0 | = \sum_{n,i,j} p_ip_j (nU(0)^\dagger j) \langle \psi_i | \langle j | U(0)^\dagger | n \rangle = \sum_{n,i,j} p_ip_j (\langle j | U(0)^\dagger | n \rangle \langle n | U(0)^\dagger | j \rangle) \langle \psi_i | = \rho = \text{Tr}_0[\Psi_i] \langle \Psi_0 |. \quad (30)
\]

From the above two facts we can state that the following relation

\[
\rho = \sum_{i=1}^r p_i^2 \langle \psi_i | \Psi_i \rangle \quad (31)
\]

forms a bijection between $\rho$ and $\Psi_0$. Defining this bijection as a map between $\Psi_0$ and $\rho$, we have the following proposition.

**Proposition 2.** An arbitrary dimensional mixed $N$-partite state $\rho'$ is LU equivalent to $\rho$, i.e.

\[
\rho' = U(1) \otimes U(2) \otimes \cdots \otimes U(N) \rho U(1)^\dagger \otimes U(2)^\dagger \otimes \cdots \otimes U(N)^\dagger \quad (32)
\]

if, and only if, its pure state counterpart $\Psi_0'$ is LU equivalent to $\Psi_0$, i.e.

\[
\Psi_0' = U(0) \otimes U(1) \otimes \cdots \otimes U(N) \Psi_0. \quad (33)
\]

**Proof.** First, if

\[
\rho' = \sum_{i=1}^r p_i^2 \langle \psi_i | \rho U(1)^\dagger \otimes U(2)^\dagger \otimes \cdots \otimes U(N)^\dagger \sum_{i=1}^r p_i^2 | \psi_i \rangle \langle \psi_i |
\]

where $| \psi_i \rangle = U(1) \otimes U(2) \otimes \cdots \otimes U(N) | \psi_i \rangle$, then $\Psi_0'$ corresponding to $\rho'$ is

\[
\Psi_0' = \sum_{j=1}^r p_j | j \rangle \langle j | = \sum_{j=1}^r p_j | j \rangle U(1)^\dagger \otimes U(2)^\dagger \otimes \cdots \otimes U(N)^\dagger | \psi_j \rangle
\]

\[
\rho' = \sum_{j=1}^r p_j | j \rangle \langle j | \otimes \cdots \otimes U(N)^\dagger \sum_{j=1}^r p_j | j \rangle | \psi_j \rangle
\]

That is, $\Psi_0'$ is LU equivalent to $\rho_0$.

Second if $\Psi_0' = U(0) \otimes \cdots \otimes U(N) \Psi_0$, then

\[
\rho' = \sum_{i=1}^r p_i^2 \langle \psi_i | \Psi_i \rangle \langle \Psi_i | \Psi_0 \rangle
\]

\[
= \text{Tr}_0[\Psi_0] \sum_{i=1}^r p_i^2 \langle \psi_i | \langle \Psi_i | \Psi_0 \rangle = \text{Tr}_0[\Psi_0] \sum_{i=1}^r p_i^2 \langle \psi_i | \langle \Psi_0 | \Psi_0 \rangle
\]

\[
= U(1) \otimes \cdots \otimes U(N) \sum_{i=1}^r p_i^2 | \psi_i \rangle \langle \psi_i | U(1)^\dagger \otimes \cdots \otimes U(N)^\dagger
\]

\[
= U(1) \otimes \cdots \otimes U(N) \rho U(1)^\dagger \otimes \cdots \otimes U(N)^\dagger. \quad (36)
\]

Here we have used the fact of equation (30), that is, $\rho'$ is LU equivalent to $\rho$. \hfill \lozenge
We can now conclude that: if $\rho'$ is LU equivalent to $\rho$ then their corresponding pure states $\Psi'_0$ and $\Psi_0$ can be related by LU operators; if $\Psi'$ is LU equivalent to $\Psi_0$ then their reduced matrices $\rho'$ and $\rho$ are LU equivalent. We may construct the core tensor $\Omega_0$ from $\Psi_0$, then we trace out the 0th partite from the core tensor $\Omega_0$ and obtain the canonical form for $\rho$, that is

$$\Upsilon = \text{Tr}_0[(\Omega_0)\langle \Omega_0 \rangle].$$

(37)

**Theorem 3.** The canonical form $\Upsilon$ is of the entanglement class of the mixed state $\rho$ up to a local symmetry inherited from $\Omega_0$.

This method provides a simple way to construct the canonical form for the mixed $N$-partite state $\rho$: first construct the $N+1$-partite pure state $\Psi'_0$ from $\rho$; then compute the core tensor $\Omega_0$ of $\Psi_0$; finally we arrive at the canonical form by tracing out the 0th partite $\Upsilon = \text{Tr}_0[\Omega_0\langle \Omega_0 \rangle]$.

**4. The local symmetries of the canonical form**

We have constructed the canonical forms for both pure and mixed multipartite states. In all, the construction of the canonical forms will result in a general form of equation (22) whether the state is pure or not. With this direct summed forms of the symmetries, in this section we develop a practical scheme to verify the LU equivalence of two quantum states which have the same singular values and same degeneracies for each partite.

**4.1. A general form of the local unitary symmetry**

We start from a general case, that is we have $k_n$ distinct $n$-mode singular values $\sigma_{i_n}^{(n)}$, $i_n \in \{1, 2, \ldots, k_n\}$, each with multiplicities of $\mu_{i_n}^{(n)}$ where \(\sum_{i_n=1}^{k_n} \mu_{i_n}^{(n)} = I_n\). We define the $n$-mode singular value vector $\vec{\sigma}^{(n)}$ for the matrix unfolding form of $\Omega^{(n)}$

$$\vec{\sigma}^{(n)} \equiv \left\{ \begin{array}{c} \sigma_{1_1}^{(n)}, \sigma_{1_2}^{(n)}, \ldots, \sigma_{1_{\mu_{1_1}^{(n)}}}^{(n)} \\ \vdots \\ \sigma_{k_n}^{(n)}, \sigma_{k_n}^{(n)}, \ldots, \sigma_{k_n \mu_{k_n}^{(n)}}^{(n)} \end{array} \right\}^T,$$

(38)

where $\sigma_{i}^{(n)} > \sigma_{j}^{(n)} \geq 0, \forall \ i < j$. The local symmetry corresponding to this partite is

$$S^{(n)} \equiv \left( \begin{array}{c} u_1^{(n)} \\ \vdots \\ u_{k_n}^{(n)} \end{array} \right),$$

(39)

where $u_i^{(n)}$, $i \in \{1, \ldots, k_n\}$ are unitary with the dimension $\mu_i^{(n)} \times \mu_i^{(n)}$.

The total LU symmetry $S = \bigotimes_i S^{(i)}$ of the core tensor $\Omega$ is

$$\left( \begin{array}{c} u_1^{(1)} \\ \vdots \\ u_{k_1}^{(1)} \end{array} \right) \otimes \cdots \otimes \left( \begin{array}{c} u_1^{(N)} \\ \vdots \\ u_{k_N}^{(N)} \end{array} \right) \cdot \vec{\Omega}_N = \vec{\Omega'}_N,$$

(40)

which is just equation (22). We then define the ‘singular value matrix’ $\Sigma$ of the core tensor

$$\Sigma \equiv \{ \vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}, \ldots, \vec{\sigma}^{(N)} \},$$

(41)
where it is uniquely defined according to the properties of HOSVD. Quantum states with different singular value matrices are apparently LU inequivalent. Then the core tensors which have the same singular value matrix belong to the same entanglement class if, and only if, they satisfy equation (26). In equation (26), the verification of the LU equivalence of two core tensors turns to finding the solutions of the following equation groups with varying \( r \)

\[
\mu^{(n)}_i = 1, \quad \mu^{(n)}_i = 1 \in \{1, \ldots, n\}
\]

\[
\omega^{(i_1)}_{i_2} \cdots \omega^{(i_J)}_{i_J} \omega^{(i_{n-J+1})} \cdots \omega^{(i_{n+1})} = \omega^{(i_{n-J+1})} \cdots \omega^{(i_{n+1})}
\]

\[
\exp \left( i \sum \theta^{(n)}_{i_i} \right) \omega^{(i_1)}_{i_2} \cdots \omega^{(i_J)}_{i_J} \omega^{(i_{n-J+1})} \cdots \omega^{(i_{n+1})} = \omega^{(i_{n-J+1})} \cdots \omega^{(i_{n+1})}
\]

\[
\exp \left[ i \left( \theta^{(1)}_{i_1} + \theta^{(2)}_{i_2} + \cdots + \theta^{(N)}_{i_N} \right) \right] \omega^{(i_1)}_{i_2} \cdots \omega^{(i_J)}_{i_J} \omega^{(i_{n-J+1})} \cdots \omega^{(i_{n+1})} = \omega^{(i_{n-J+1})} \cdots \omega^{(i_{n+1})}
\]

Thus we can pick the subtensor \( \omega \) out of the tensor \( \Omega \) and apply the HOSVD to it recursively.

As the fine-grained process goes, the recursion will result in two cases: 1, that the singular values are all distinct for all the partite; 2, that the singular values are all the same for all the partite.

For the first case, if \( \forall i \in \{1, \ldots, k_n\} \) and \( \forall n \in \{1, \ldots, N\} \), the singular value multiplicity \( \mu_i^{(n)} = 1 \), then \( k_n = I_n \) and

\[
U^{(n)} = \begin{pmatrix}
\exp(i\theta^{(1)}_{i_1}) & 0 & \cdots & 0 \\
0 & \exp(i\theta^{(2)}_{i_2}) & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \exp(i\theta^{(N)}_{i_N})
\end{pmatrix},
\]

\[
equation (26) turns to
\exp \left[ i \left( \theta^{(1)}_{i_1} + \theta^{(2)}_{i_2} + \cdots + \theta^{(N)}_{i_N} \right) \right] \omega^{(i_1)}_{i_2} \cdots \omega^{(i_J)}_{i_J} \omega^{(i_{n-J+1})} \cdots \omega^{(i_{n+1})} = \omega^{(i_{n-J+1})} \cdots \omega^{(i_{n+1})}
\]

These are \( I_1 \times I_2 \times \cdots \times I_N \) linear equations for \( I_1 + I_2 + \cdots + I_N \) phase variables and it can be verified immediately whether they have consistent solutions. The quantum states are LU equivalent if, and only if, there is at least one solution to this linear equation group.

4.2. A completely degenerate state for all the partite

In the completely degenerate state, the reduced density matrix for each partite is proportional to the unit matrix. Consider an arbitrary \( N \)-partite pure state with the dimension \( I_1 \times I_2 \times \cdots \times I_N \).

The complete degenerate state is that \( \forall n \in \{1, 2, \ldots, N\} \)

\[
\rho_n = \text{Tr}_{\{\omega\}}[\Omega] = \frac{1}{I_n} E.
\]

The core tensor has the following form

\[
\Omega = \sum_{i_n} |i_n\rangle \sum_{\omega^{(i_n)}_{i_n}} \omega^{(i_n)}_{i_n} |i_1i_2 \cdots i_n-1i_n+1 \cdots i_N\rangle
\]

\[
= \sum_{i_n} |i_n\rangle \langle \omega^{(i_n)}_{i_n} |, \quad n \in \{1, \ldots, N\},
\]

where \( \langle \omega^{(i_n)}_{i_n} | \omega^{(i_n)}_{i_n} \rangle = \frac{1}{I_n} \delta_{i_n}^{i_n} \). The local symmetry \( S \) takes the following form

\[
\Omega^{(N)} = S \cdot \Omega^{(N)} = \bigotimes_n U^{(n)} \cdot \Omega^{(N)}.
\]

This can be seen as a fine-grained LU classification problem of the subtensor \( \omega \). Thus we can pick the subtensor \( \omega \) out of the tensor \( \Omega \) and apply the HOSVD to it recursively.
An arbitrary unitary matrix is unitarily equivalent to a diagonal matrix, that is
\[
U^{(n)} = X^{(n)} \odot \Phi^{(n)} \odot X^{(n)},
\]
where \(X^{(n)}\) is a unitary matrix and \(\Phi^{(n)} = \text{diag}\{e^{i\phi_1^{(n)}}, \ldots, e^{i\phi_{n}^{(n)}}\}\) is the conjugate class of \(U^{(n)}\). Equation (48) now turns to
\[
\bigotimes_n \Phi^{(n)} \bigotimes_n X^{(n)} = \bigotimes_n X^{(n)} \odot \Omega.'
\]
Equation (50) corresponds to the \(I_1 \times I_2 \times \cdots \times I_N\) homogeneous equations, which in the detailed form of equation (50) look like
\[
\sum_{i_1 \cdots i_N} x_{i_1}^{(1)} x_{j_1}^{(2)} \cdots x_{j_N}^{(N)} \cdot (e^{i\phi_{i_1}^{(1)} + \phi_{j_1}^{(2)} + \cdots + \phi_{j_N}^{(N)}}) a_{i_1i_2 \cdots i_N} - a'_{i_1i_2 \cdots i_N} = 0.
\]
Here we represent \(x_{ij}\) as the elements of matrix \(X\). This is a typical equation group of \(I_1 \times I_2 \times \cdots \times I_N\) equations for \(I_1^2 + I_2^2 + \cdots + I_N^2\) complex parameters \(x_{ij}^{(n)}\) (note we first solve the parameters \(x_{ij}^{(n)}\) then impose the unitary condition on the matrix \(X^{(n)}\)).

For this kind of nonlinear equation there exists a simple tool called ‘linearization’ or ‘relinearization’ [15, 16]. The key algorithms rely on the fact that for \(N > 2\) multipartite quantum states, when the dimensions or number of parties increase, the number of equations grows much more quickly than the number of parameters. Generally equation (51) would turn out to be an over-defined system of equations which means that there are more equations than unknown parameters.

The linearization technique goes as follows. Regard each monomial of the matrix elements as a new variable
\[
v_{i_1i_2 \cdots i_N} = x_{i_1}^{(1)} x_{j_1}^{(2)} \cdots x_{j_N}^{(N)},
\]
then there will be \((I_1 \times I_2 \times \cdots \times I_N)^2\) such variables \(v\). Equation (51) now can be written as
\[
\sum_{i_1 \cdots i_N} v_{i_1i_2 \cdots i_N} \cdot (e^{i\phi_{i_1}^{(1)} + \phi_{j_1}^{(2)} + \cdots + \phi_{j_N}^{(N)}}) a_{i_1i_2 \cdots i_N} - a'_{i_1i_2 \cdots i_N} = 0.
\]
For the sake of simplicity we use the convention that I represents the value of the bit string \((i_1i_2 \cdots i_N)\), i.e. \(I = 1 = (1 \cdots 1)\) and \(I = 2 = (1 \cdots 2)\), etc. Define \(o_{ij} \equiv e^{i\phi_{i_1}^{(1)} + \phi_{j_1}^{(2)} + \cdots + \phi_{j_N}^{(N)}} a_{ij} - a'_i\) where \(j = (j_1j_2 \cdots j_N)\). Equation (53) can be reformulated as
\[
o_{ij} \cdot v_{ij} = 0,
\]
where the dot means the summation over \(i\). Taking a \(2 \times 2 \times 2\) system as an example, we have
\[
o_{11} v_{11} + o_{12} v_{12} + o_{13} v_{13} + o_{14} v_{14} + o_{23} v_{23} + o_{25} v_{25} + o_{35} v_{35} + o_{37} v_{37} + o_{38} v_{38} = 0.
\]
There are eight such equations for \(j\) runs from 1 to 8. The solution can be expressed as
\[
\begin{pmatrix}
  v_{j_1} \\
v_{j_2} \\
v_{j_3} \\
\vdots \\
v_{j_8}
\end{pmatrix} = c_2 \begin{pmatrix}
o_{21} \\
o_{22} \\
o_{23} \\
\vdots \\
o_{28}
\end{pmatrix} + c_3 \begin{pmatrix}
o_{31} \\
o_{32} \\
o_{33} \\
\vdots \\
o_{38}
\end{pmatrix} + \cdots + c_8 \begin{pmatrix}
o_{81} \\
o_{82} \\
o_{83} \\
\vdots \\
o_{88}
\end{pmatrix},
\]
where \(c_n\) are new parameters. Clearly, equation (56) is a under-defined equation group for variables \(v_{ij}\). However, there are additional equations between the products of \(v_{ij}\), i.e.
\[
v_{i_1i_2 \cdots i_N} v_{j_1j_2 \cdots j_N} v_{k_1k_2 \cdots k_N} = v_{i_1j_1k_1} v_{i_2j_2k_2} v_{i_3j_3k_3} \cdots v_{i_Nj_Nk_N}.
\]
This relation is inherited from equation (52) as
\[ x_{i_1}^{(1)} \cdots x_{i_n}^{(n)} = x_{i_1}^{(1)} \cdots x_{i_n}^{(n)} \]
\[ = x_{i_1}^{(1)} \cdots x_{i_n}^{(n)} \]
\[ x_{i_1}^{(1)} \cdots x_{i_n}^{(n)} = x_{i_1}^{(1)} \cdots x_{i_n}^{(n)} \]
\[ \cdots \]
\[ \times x_{i_1}^{(1)} \cdots x_{i_n}^{(n)} = x_{i_1}^{(1)} \cdots x_{i_n}^{(n)} \] (58)

For example in the $2 \times 2 \times 2$ system we have $v_{111,111}v_{112,112} = v_{111,121}v_{111,112}$ or simply $v_{11}v_{12} = v_{13}v_{12}$. This imposes an additional equation between parameters $v_{ij}$, and can also be viewed as an equation in the (smaller number of) parameters $c_{ij}$ expressing them. The new system of equations can be derived from all the possible relations of the type of equation (57).

In solving the equations on $c_{ij}$ we can use the linearization method recursively.

Here we give two simple examples of how we can get the canonical forms of the arbitrary quantum state, and how we can verify whether two quantum states in the canonical forms can be related by LU symmetry $S$. As the entanglement classification of the mixed states can be reduced to a specific pure state case, here we only give examples of pure states.

We randomly generate a $2 \times 2 \times 2$ pure state $\Psi$ with the matrix unfolding
\[ \Psi_{(1)} = \begin{pmatrix} 0.0260603 & 1.05491 & -3.69051 & 0.437711 \\ 1.25266 & 1.07259 & 3.2378 & 1.5625 \end{pmatrix}. \] (63)

From the algorithm of equation (12), the singular value matrix $\Sigma$ is
\[ \begin{pmatrix} \sigma_{1}^{(1)} & \sigma_{1}^{(2)} & \sigma_{1}^{(3)} \\ \sigma_{2}^{(1)} & \sigma_{2}^{(2)} & \sigma_{2}^{(3)} \end{pmatrix} = \begin{pmatrix} 5.039966 & 5.31586 & 5.17055 \\ 2.27534 & 1.5202 & 1.95825 \end{pmatrix}. \] (64)

5. Examples of the canonical form for three-and four-qubit states

Here we give two simple examples of how we can get the canonical forms of the arbitrary quantum state, and how we can verify whether two quantum states in the canonical forms can be related by LU symmetry $S$. As the entanglement classification of the mixed states can be reduced to a specific pure state case, here we only give examples of pure states.

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From the algorithm of equation (12), the singular value matrix $\Sigma$ is
\[ \begin{pmatrix} \sigma_{1}^{(1)} & \sigma_{1}^{(2)} & \sigma_{1}^{(3)} \\ \sigma_{2}^{(1)} & \sigma_{2}^{(2)} & \sigma_{2}^{(3)} \end{pmatrix} = \begin{pmatrix} 5.039966 & 5.31586 & 5.17055 \\ 2.27534 & 1.5202 & 1.95825 \end{pmatrix}. \] (64)
The core tensor then is (unfolding with the first index)

\[
\Omega_{(1)} = \begin{pmatrix} -5.01792 & 0.2815 & -0.354882 & -0.0862168 \\ 0.19519 & 1.72088 & -1.17941 & -0.886923 \end{pmatrix}.
\]  

We give another example of a four-qubit state with degenerate singular values. Two \(2 \times 2 \times 2 \times 2\) quantum states

\[
\Psi_{(1)} = \frac{1}{\sqrt{10}} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 2 \end{pmatrix},
\]

\[
\Psi'_{(1)} = \frac{1}{\sqrt{10}} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & -2 \end{pmatrix}.
\]  

are already the core tensors. The singular value matrices for them are the same

\[
\begin{pmatrix} \sigma_{1}^{(1)} & \sigma_{2}^{(1)} & \sigma_{1}^{(3)} & \sigma_{1}^{(4)} \\ \sigma_{2}^{(1)} & \sigma_{2}^{(3)} & \sigma_{2}^{(4)} \end{pmatrix} = \begin{pmatrix} 1 & 4 & 4 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} \sigma_{1}^{(1)} & \sigma_{1}^{(2)} & \sigma_{1}^{(3)} & \sigma_{1}^{(4)} \\ \sigma_{2}^{(1)} & \sigma_{2}^{(2)} & \sigma_{2}^{(3)} & \sigma_{2}^{(4)} \end{pmatrix}.
\]  

In the vector forms of the matrix unfolding of \(\Psi_{(1)}\) and \(\Psi'_{(1)}\), the symmetry \(S\) takes the following form:

\[
S = \begin{pmatrix} e^{\theta_{1}^{(2)} + \theta_{1}^{(3)}} U^{(4)} \otimes U^{(1)} & 0 & 0 \\ 0 & e^{\theta_{2}^{(2)} + \theta_{2}^{(3)}} U^{(4)} \otimes U^{(1)} & 0 \\ 0 & 0 & e^{\theta_{2}^{(2)} + \theta_{2}^{(3)}} U^{(4)} \otimes U^{(1)} \end{pmatrix}.
\]  

The core tensors are then divided into four segments correspondingly

\[
\bar{\omega}_{1} = \frac{1}{\sqrt{10}} [1, 0, 0, 1]^T, \quad \bar{\omega}'_{1} = \frac{1}{\sqrt{10}} [1, 0, 0, 1]^T.
\]  

\[
\bar{\omega}_{2} = \frac{1}{\sqrt{10}} [0, 0, 0, 0]^T, \quad \bar{\omega}'_{2} = \frac{1}{\sqrt{10}} [0, 0, 0, 0]^T.
\]  

\[
\bar{\omega}_{3} = \frac{1}{\sqrt{10}} [0, 0, 0, 0]^T, \quad \bar{\omega}'_{3} = \frac{1}{\sqrt{10}} [0, 0, 0, 0]^T.
\]  

\[
\bar{\omega}_{4} = \frac{1}{\sqrt{10}} [2, 0, 0, 2]^T, \quad \bar{\omega}'_{4} = \frac{1}{\sqrt{10}} [2, 0, 0, -2]^T.
\]  

By transferring all the above equations into equation (26) we have the following effective equations:

\[
e^{\theta_{1}^{(2)} + \theta_{1}^{(3)}} U^{(4)} \otimes U^{(1)} \bar{\omega}_{1} = \bar{\omega}'_{1},
\]

\[
e^{\theta_{2}^{(2)} + \theta_{2}^{(3)}} U^{(4)} \otimes U^{(1)} \bar{\omega}_{4} = \bar{\omega}'_{4}.
\]  

The components of \(\bar{\omega}_{1}\), \(\bar{\omega}'_{1}\) and \(\bar{\omega}_{4}\), \(\bar{\omega}'_{4}\) in equations (68, 71) bring a contradiction to equations (72, 73). Now it is clear that there are no solutions for \(U^{(4)}\) and \(U^{(1)}\), and thus the four-qubit states \(\Psi_{(1)}\) and \(\Psi'_{(1)}\) are LU inequivalent.
6. Conclusions

In summary, by using the tensor decomposition method we have generalized the entanglement classification under LU equivalence to arbitrary dimensional multipartite mixed states. The classification actually reduces to the construction of the canonical forms of the corresponding \( N+1 \)-partite pure states. With the analysis of the local symmetry in the canonical form, the core tensor can be decomposed into a series of subtensors which are transformed independently under the local symmetry. Based on this recognition of the entanglement structure, a practical scheme is also developed for the verification of LU equivalence of two multipartite entangled states. In the verification procedure, only in the worst case of complete degeneracy for all the partite do we need to solve multivariate polynomial equations. The well-developed methods and algorithms on solving such polynomial equations not only provide the formula for finding the solutions but also impose well-formed structures among the solutions [18] which would shed new light on the complete understanding of multipartite entanglement.

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