Higher-order singular value decomposition and the reduced density matrices of three qubits

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Abstract
In this paper, we demonstrate that higher-order singular value decomposition (HOSVD) can be used to identify special states in three qubits by local unitary (LU) operations. Since the matrix unfoldings of three qubits are related to their reduced density matrices, HOSVD simultaneously diagonalizes the one-body reduced density matrices of three qubits. From the all-orthogonality conditions of HOSVD, we computed the special states of three qubits. Furthermore, we showed that it is possible to construct a polytope that encapsulates all the special states of three qubits by LU operations with HOSVD.

Keywords Quantum entanglement · Higher-order singular value decomposition · Local unitary equivalence · Three qubits

Mathematics Subject Classification 15A69

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1 Introduction

Being the central characteristic of composite quantum systems, entanglement has been studied extensively in the past from various perspectives, such as the classification of multipartite states [1,2,7,18,19,21], the geometry of quantum state space [5,15,25] and more recently, the resource-theoretic [4,9,11,13] and categorical approach [10,12]. Apart from the fact that entanglement connects deeply to the foundations of quantum theory, it can be utilized as a resource in quantum information processing. From this perspective, it is important to be able to quantify entanglement and classify entangled states based on the computational tasks they can perform.

The Hilbert space of a composite quantum system is described by the tensor product of its subsystems’ Hilbert spaces. This tensor product structure naturally endows tensorial properties to the elements of multipartite states, thus allowing us to employ multilinear algebraic methods on them. As an example, we can apply singular value decomposition (SVD) on the elements of bipartite states and restate it as Schmidt decomposition [22], which is a widely used approach in the local unitary (LU) classification of bipartite states. It is also known that the Schmidt coefficients are LU invariants of the entanglement classes for bipartite states [7,25].

Given the successful precedence in bipartite states, it is natural to consider Schmidt decomposition in the LU classification of multipartite states. This idea turned out to be unsuccessful [23] since multipartite states cannot be generally represented by only the Schmidt coefficients. If one were to follow a similar concept, Schmidt decomposition or equivalently SVD has to be generalized.

As a matter of fact, such a generalization has been considered in the mathematical literature back in 2000 [17]. Particularly, the requirement of matrix diagonalization in SVD is relaxed. This generalized version of SVD is called higher-order singular value decomposition (HOSVD). It is applicable to higher order tensors, which is the tensorial representation of multipartite states. The idea of utilizing HOSVD in the LU classification of multipartite pure states was first suggested in [21]. Subsequently, a general scheme was proposed in [18] to identify the LU equivalence between two multipartite pure states. Later, Li et al. [19] presented a necessary and sufficient criterion to check if two multipartite mixed states are local unitary equivalent or not.

In this paper, we choose a different approach of utilizing HOSVD in finding the special states of three qubits. Instead of focusing on the local symmetries [18,19,21] of multipartite states, we make use of the properties of matrix unfolding and HOSVD to identify the special states of three-qubit pure states by LU operations. We begin by defining the idea of multilinear algebra in Sect. 2. Then, we discuss the matrix unfolding of tensors in Sect. 3. Here, we note that the matrix unfoldings of three-qubit tensor are related to their reduced density matrices. The definition of HOSVD is presented in Sect. 4, whereby HOSVD defines and guarantees the existence of simultaneous diagonalization of one-body reduced density matrices for three qubits. Based on the all-orthogonality conditions of HOSVD, we calculated the special states of three qubits and constructed a polytope of three qubits by LU operations in Sect. 5. The special states of three qubits are in correspondence to an earlier work by [7].
2 Tensors

Tensors are indexed mathematical objects coming from the tensor product of vector spaces and can be regarded as multi-dimensional arrays \[14\]. Let \( X = [\chi_{i_1i_2...i_N}] \in V^{I_1} \otimes V^{I_2} \otimes \cdots \otimes V^{I_n} \otimes \cdots \otimes V^{I_N} \) be a tensor, where \( V^{I_n} \) is the \( n \)th vector space of dimension \( I_n \). The total number of indices \( N \) of a tensor \( X \) is called the order of a tensor. Thus, tensors of order 1 are vectors while tensors of order 2 are matrices. For tensors of order 3 and above, we call them higher-order tensors. The Hilbert space of three qubits, for instance, is the tensor product of three complex vector spaces, \( H = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \). Therefore, any three-qubit states, or tripartite states in general, are tensors of order 3.

Now, let \( V_n = [\nu_{i_n}] \in V^{I_n} \) be vectors (or tensors of order 1) in the \( n \)th vector space \( V^{I_n} \) of dimension \( I_n \). An \( N \)th order tensor \( X = [\chi_{i_1i_2...i_N}] \in V^{I_1} \otimes V^{I_2} \otimes \cdots \otimes V^{I_n} \otimes \cdots \otimes V^{I_N} \) is of rank 1 if it can be written as

\[ X = V_1 \otimes V_2 \otimes \cdots \otimes V_n \otimes \cdots \otimes V_N, \quad (1) \]

or equivalently if its element \( \chi_{i_1i_2...i_N} \) can be written as

\[ \chi_{i_1i_2...i_N} = \nu_{i_1} \nu_{i_2} \cdots \nu_{i_n} \cdots \nu_{i_N}. \quad (2) \]

Rank 1 tensors are also called simple tensors \[24\]. Now, let \( X_r \) be a \( N \)th order tensor of rank 1. Then, the rank of a generic \( N \)th order tensor \( X \) is the minimum number \( R \) of rank 1 tensors \( X_r \) combined linearly to form \( X \) \[20\],

\[ \text{Rank}(X) := \text{Min} \left\{ R : X = \sum_{r=1}^{R} X_r \right\}. \quad (3) \]

As an example, the GHZ state

\[ |\text{GHZ}\rangle = \psi_{111} |111\rangle + \psi_{222} |222\rangle \]

is a third-order tensor of rank 2, while the W state

\[ |\text{W}\rangle = \psi_{112} |112\rangle + \psi_{121} |121\rangle + \psi_{211} |211\rangle \]

is a third-order tensor of rank 3 \[24\]. Even though the idea of tensor rank is not the main focus of this paper, we would like to highlight that tensor rank is related to the transformation of tripartite entangled states through stochastic local operation and classical communication (SLOCC) \[8\] and can be an algebraic measure of entanglement \[6\].

\[ \quad \square \]
3 Matrix unfolding and local transformation of tensors

While it is possible to write down a higher-order tensor by listing its tensor elements, it will be more convenient to devise a standardized way of representing a higher-order tensor as matrices. Such a method is called matrix unfolding [17].

**Definition 1** *(Matrix unfolding)* Let $X \in V^{I_1} \otimes V^{I_2} \otimes \cdots \otimes V^{I_n} \otimes \cdots \otimes V^{I_N}$ be an $N$th order tensor, where $V^{I_n}$ is the $n$th vector space of dimension $I_n$. The $n$th matrix unfolding, $X_{(n)}$, is a matrix of size $I_n \times (I_n + 1)$, whereby the tensor element $\chi_{i_1i_2\ldots i_n}$ will be located at the position with row index $i_n$ and column index

\[
(i_n + 1 - 1)I_n + (i_n + 2 - 1)I_n + 1 + \cdots + (i_N - 1)I_1I_2 \cdots I_{n-1} + (i_1 - 1)I_2I_3 \cdots I_n + (i_2 - 1)I_3I_4 \cdots I_{n-1} + \cdots + i_{n-1}.
\] (4)

When the elements of multipartite states are represented as tensors, the matrix unfolding of higher-order tensors allows us to define local transformation of multipartite states [18] in a convenient way, as follow.

**Definition 2** *(Local transformation of tensors)* Let $X \in V^{I_1} \otimes V^{I_2} \otimes \cdots \otimes V^{I_n} \otimes \cdots \otimes V^{I_N}$ be an $N$th order tensor, where $V^{I_n}$ is the $n$th vector space of dimension $I_n$. Let $M^{(n)} \in \text{GL}(V^{I_n})$ be the linear transformation matrix on the vector space $V^{I_n}$. Then, the local transformation of an $N$th order tensor $X$ is given as

\[
X' = M^{(1)} \otimes M^{(2)} \otimes \cdots \otimes M^{(n)} \otimes \cdots \otimes M^{(N)} X,
\] (5)

where $M^{(1)} \otimes M^{(2)} \otimes \cdots \otimes M^{(N)} \in \text{GL}(V^{I_1}) \times \text{GL}(V^{I_2}) \times \cdots \times \text{GL}(V^{I_N})$. The $n$th matrix unfolding of Eq. (5) can be written as

\[
X'_{(n)} = M^{(n)} X_{(n)} \left[ M^{(n+1)} \otimes \cdots \otimes M^{(N)} \otimes M^{(1)} \otimes \cdots \otimes M^{(n-1)} \right]^T,
\] (6)

where the superscript $T$ denotes matrix transpose.

Let $\Psi \in \mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ be the three-qubit tensor. From “Appendix A”, it is shown that the matrix unfoldings, $\Psi_{(i)}$ where $i = 1, 2, 3$, are $\Psi_{A|BC}$, $\Psi_{B|CA}$, and $\Psi_{C|AB}$, respectively. By direct comparison with the reduced density matrices of three qubits, we find that

\[
\rho^{AB} = \Psi_{(3)}^T \Psi_{(3)},
\] (7)

\[
\rho^{CA} = \Psi_{(2)}^T \Psi_{(2)},
\] (8)

\[
\rho^{BC} = \Psi_{(1)}^T \Psi_{(1)},
\] (9)

\[
\rho^{A} = \Psi_{(1)} \Psi_{(1)}^T.
\] (10)
\[
\rho^B = \Psi(2)\Psi^\dagger(2),
\]
\[
\rho^C = \Psi(3)\Psi^\dagger(3),
\]
where overhead bar denotes complex conjugate while superscript \(\dagger\) denotes conjugate transpose.

4 Higher-order singular value decomposition

Having defined tensors and matrix unfolding, our next goal is to introduce a type of tensor decomposition called higher-order singular value decomposition (HOSVD) [17,18], which is the generalized version of singular value decomposition (SVD).

**Theorem 1** (Higher-order singular value decomposition) Let \(X \in \mathbb{C}^{I_1} \otimes \mathbb{C}^{I_2} \otimes \cdots \otimes \mathbb{C}^{I_N}\) be an \(N\)th order complex tensor, where \(\mathbb{C}^{I_n}\) is the \(n\)th complex vector space of dimension \(I_n\). There exists a core tensor \(T\) of \(X\) and a set of unitary matrices \(U^{(1)}, U^{(2)}, \ldots, U^{(n)}, \ldots, U^{(N)}\) such that

\[
X = U^{(1)} \otimes U^{(2)} \otimes \cdots \otimes U^{(n)} \otimes \cdots \otimes U^{(N)} T. \tag{13}
\]

The core tensor \(T\) is also an \(N\)th order complex tensor for which its subtensors \(T_{i_n=\alpha}\), obtained by fixing the \(n\)th index to \(\alpha\), have the properties of

1. All-orthogonality: Two subtensors \(T_{i_n=\alpha}\) and \(T_{i_n=\beta}\) are orthogonal for all possible values of \(n\), \(\alpha\) and \(\beta\), subject to \(\alpha \neq \beta\):

\[
\langle T_{i_n=\alpha}, T_{i_n=\beta} \rangle = \sum_{i_1 \ldots i_{n-1} i_{n+1} \ldots i_N} \bar{t}_{i_1 \ldots i_{n-1} \alpha i_{n+1} \ldots i_N} t_{i_1 \ldots i_{n-1} \beta i_{n+1} \ldots i_N} = 0 \text{ when } \alpha \neq \beta; \tag{14}
\]

2. Ordering:

\[
|T_{i_n=1}| \geq |T_{i_n=2}| \geq \cdots \geq |T_{i_n=I_n}| \geq 0 \tag{15}
\]

for all possible values of \(n\),

where \(t_{i_1 \ldots i_N}\) is the element of the tensor \(T\) and \(|T_{i_n=i}| = \sqrt{\langle T_{i_n=i}, T_{i_n=i} \rangle}\) is called the \(n\)-mode singular value of \(X\), \(\sigma_i^{(n)}\).

Due to Definition 2, Eq. (13) can be rewritten as

\[
X^{(n)} = U^{(n)} T^{(n)} \left[ U^{(n+1)} \otimes U^{(n+2)} \otimes \cdots \otimes U^{(N)} \right. \\
\left. \otimes U^{(1)} \otimes U^{(2)} \otimes \cdots \otimes U^{(n-1)} \right] T, \tag{16}
\]

where \(X^{(n)}\) and \(T^{(n)}\) are \(I_n \times (I_{n+1} I_{n+2} \ldots I_N I_1 I_2 \ldots I_{n-1})\)-complex matrices, and \(U^{(n)}\) are unitary matrices of size \(I_n \times I_n\).
As stated in [17], SVD reduces any real or complex matrix into a diagonal matrix \( \Lambda \) of real entries, whereas HOSVD relaxes this property into a set of all-orthogonality conditions (14). To put this into perspective, instead of requiring the matrix \( \Lambda \) to be diagonal, HOSVD only requires that the row and column vectors of \( \Lambda \) to be orthogonal to each other. In this sense, HOSVD generalizes SVD.

By comparison, the all-orthogonality conditions (40)–(42) in “Appendix B” are the same as the off-diagonal terms of the one-body reduced density matrices \( \rho^A \), \( \rho^B \) and \( \rho^C \), respectively. This means that HOSVD simultaneously diagonalizes the one-body reduced density matrices of three qubits,

\[
\begin{align*}
\rho^A &= U^{(1)} \rho_d^A U^{(1)\dagger}, \\
\rho^B &= U^{(2)} \rho_d^B U^{(2)\dagger}, \\
\rho^C &= U^{(3)} \rho_d^C U^{(3)\dagger},
\end{align*}
\]

where

\[
\begin{align*}
\rho_d^A &= T_{(1)} T_{(1)}^\dagger = \begin{pmatrix}
\sigma_1^{(1)2} & 0 \\
0 & \sigma_2^{(1)2}
\end{pmatrix}, \\
\rho_d^B &= T_{(2)} T_{(2)}^\dagger = \begin{pmatrix}
\sigma_1^{(2)2} & 0 \\
0 & \sigma_2^{(2)2}
\end{pmatrix}, \\
\rho_d^C &= T_{(3)} T_{(3)}^\dagger = \begin{pmatrix}
\sigma_1^{(3)2} & 0 \\
0 & \sigma_2^{(3)2}
\end{pmatrix},
\end{align*}
\]

and \( T_{(1)}, T_{(2)} \) and \( T_{(3)} \) are the 1-, 2- and 3-matrix unfolding of \( \mathcal{T}_\psi \). In this case, we can say that Eqs. (17)–(19) are the spectral theorem of Hermitian matrices [3] in disguise.

By Definition 2, HOSVD is a local unitary (LU) transformation, hence the three-qubit tensor \( \Psi \) and the core tensor \( \mathcal{T}_\psi \) are LU equivalent.

5 Determining special three-qubit states

5.1 All-orthogonality conditions of three qubits

Besides diagonalizing the one-body reduced density matrices of three qubits, we found that it is possible to make use of the all-orthogonality conditions from HOSVD to determine the special states of three qubits. To show this, we must first combine the three equations (40)–(42) together. By rearranging Eqs. (40) and (41), we get

\[
\begin{align*}
t_{111} &= \frac{\bar{t}_{221}(t_{121} t_{212} - t_{122} t_{211}) + t_{112}(|t_{122}|^2 - |t_{121}|^2)}{t_{121} t_{221} - t_{122} t_{211}}, \\
t_{222} &= \frac{\bar{t}_{112}(t_{121} t_{212} - t_{122} t_{211}) + t_{221}(|t_{122}|^2 - |t_{121}|^2)}{t_{212} t_{211} - \bar{t}_{122} t_{121}}.
\end{align*}
\]
Substituting the above equations in (42) and comparing the real and imaginary parts, we get

\[ |t_{112}|^2 (|t_{122}|^2 - |t_{212}|^2) + |t_{121}|^2 (|t_{221}|^2 - |t_{122}|^2) + |t_{211}|^2 (|t_{212}|^2 - |t_{221}|^2) = 0, \]

(25)

\[ \bar{t}_{112}\bar{t}_{221}(t_{122}t_{211} - t_{121}t_{212}) + \bar{t}_{121}\bar{t}_{212}(t_{112}t_{221} - t_{122}t_{211}) + \bar{t}_{122}\bar{t}_{211}(t_{121}t_{212} - t_{112}t_{221}) = 0. \]

(26)

By adding some self-canceling terms, Eq. (25) becomes

\[ |t_{112}|^2 \left[ \sigma_1^{(1)2} - \sigma_1^{(2)2} \right] + |t_{211}|^2 \left[ \sigma_1^{(2)2} - \sigma_1^{(3)2} \right] + |t_{121}|^2 \left[ \sigma_1^{(3)2} - \sigma_1^{(1)2} \right] = 0, \]

(27a)

\[ |t_{221}|^2 \left[ \sigma_1^{(1)2} - \sigma_1^{(2)2} \right] + |t_{122}|^2 \left[ \sigma_1^{(2)2} - \sigma_1^{(3)2} \right] + |t_{212}|^2 \left[ \sigma_1^{(3)2} - \sigma_1^{(1)2} \right] = 0. \]

(27b)

We note that Eqs. (27a) and (27b) are equivalent. Meanwhile, it is possible to rewrite Eq. (26) as

\[ (t_{112}t_{221} - t_{121}t_{212})(\bar{t}_{121}\bar{t}_{212} - \bar{t}_{122}\bar{t}_{211}) - (\bar{t}_{112}\bar{t}_{221} - \bar{t}_{121}\bar{t}_{212})(t_{121}t_{212} - t_{122}t_{211}) = 0, \]

(28a)

\[ (t_{112}t_{221} - t_{122}t_{211})(\bar{t}_{121}\bar{t}_{212} - \bar{t}_{112}\bar{t}_{221}) - (\bar{t}_{112}\bar{t}_{221} - \bar{t}_{122}\bar{t}_{211})(t_{121}t_{212} - t_{112}t_{221}) = 0, \]

(28b)

\[ (t_{122}t_{211} - t_{121}t_{212})(\bar{t}_{122}\bar{t}_{211} - \bar{t}_{121}\bar{t}_{221}) - (\bar{t}_{122}\bar{t}_{211} - \bar{t}_{121}\bar{t}_{212})(t_{112}t_{221} - t_{122}t_{211}) = 0. \]

(28c)

Similarly, Eqs. (28a), (28b) and (28c) are equivalent.

### 5.2 Separability conditions of three qubits

With HOSVD, we found that elements of the core tensor \([t_{ijk}] \in T_\psi\) have to satisfy only one separability condition, i.e. Eq. (64) to show the bi-separability of \(C|AB\). In other words, we can derive Eqs. (59)–(63) with Eqs. (23), (24) and (64). Similarly, the following Eqs. (29) and (30) are the only condition to show the bi-separability of \(A|BC\) and \(B|CA\), respectively:

\[ t_{112}t_{221} = t_{212}t_{121}, \]

(29)

\[ t_{112}t_{221} = t_{211}t_{122}. \]

(30)

Equations (28a), (28b) or (28c) inform us about the separability of three qubits. For bi-separable and completely separable states, these equations are automatically satisfied. Meanwhile, for genuinely entangled three-qubit states, Eqs. (28a), (28b) or (28c) determine the linear dependency of the complex phases between \(\bar{t}_{112}\bar{t}_{221}t_{122}t_{211}\),
Table 1 HOSVD of three qubits and their respective cases

| Case | States |
|------|--------|
| 1. \(\sigma_1^{(1)^2} = \sigma_1^{(2)^2} = \sigma_1^{(3)^2}\) | (a) General states,  
\(|t_{121}|^2 + |t_{122}|^2 = |t_{211}|^2 + |t_{212}|^2\),  
\(|t_{112}|^2 + |t_{122}|^2 = |t_{211}|^2 + |t_{222}|^2\)  
(b) Generalized GHZ states,  
\(|\text{GHZ}| = t_{111} \langle 111 | + t_{222} \langle 222 |\)  
(c) Completely separable states,  
\(|\text{Sep}| = t_{111} \langle 111 |\) |
| 2. \(\sigma_1^{(1)^2} = \sigma_1^{(2)^2}, \sigma_1^{(2)^2} = \sigma_1^{(3)^2}\), or \(\sigma_1^{(2)^2} = \sigma_1^{(3)^2}\) | (a) (1) \(\sigma_1^{(1)^2} = \sigma_1^{(2)^2}, (\sigma_1^{(1)^2}, \sigma_1^{(2)^2}, \sigma_1^{(3)^2}) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\),  
\(|t_{121}|^2 = |t_{211}|^2, |t_{122}|^2 = |t_{212}|^2\)  
(2) \(\sigma_1^{(1)^2} = \sigma_1^{(3)^2}, (\sigma_1^{(1)^2}, \sigma_1^{(2)^2}, \sigma_1^{(3)^2}) = (\frac{1}{2}, \sigma_1^{(2)^2}, \frac{1}{2})\),  
\(|t_{121}|^2 = |t_{211}|^2, |t_{122}|^2 = |t_{222}|^2\)  
(3) \(\sigma_1^{(2)^2} = \sigma_1^{(3)^2}, (\sigma_1^{(1)^2}, \sigma_1^{(2)^2}, \sigma_1^{(3)^2}) = (\sigma_1^{(1)^2}, \frac{1}{2}, \frac{1}{2})\),  
\(|t_{112}|^2 = |t_{212}|^2, |t_{122}|^2 = |t_{221}|^2\)  
(b) (1) \(\sigma_1^{(3)^2} > \sigma_1^{(1)^2} = \sigma_1^{(2)^2}\),  
\(|S_1| = t_{111} \langle 111 | + t_{112} \langle 112 | + t_{221} \langle 221 | + t_{222} \langle 222 |\),  
\(\tilde{t}_{111}/t_{112} + \tilde{t}_{221}/t_{222} = 0\)  
(2) \(\sigma_1^{(2)^2} > \sigma_1^{(1)^2} = \sigma_1^{(3)^2}\),  
\(|S_2| = t_{111} \langle 111 | + t_{121} \langle 121 | + t_{212} \langle 212 | + t_{222} \langle 222 |\),  
\(\tilde{t}_{111}/t_{121} + \tilde{t}_{212}/t_{222} = 0\)  
(3) \(\sigma_1^{(1)^2} > \sigma_1^{(2)^2} = \sigma_1^{(3)^2}\),  
\(|S_3| = t_{111} \langle 111 | + t_{122} \langle 122 | + t_{211} \langle 211 | + t_{222} \langle 222 |\),  
(\tilde{t}_{111}/t_{211} + \tilde{t}_{122}/t_{222} = 0\)  
(c) (1) Bi-separable state \(C|AB\),  
\(|\text{Bi-Sep}_{C|AB}| = t_{111} \langle 111 | + t_{221} \langle 221 |\)  
(2) Bi-separable state \(B|CA\),  
\(|\text{Bi-Sep}_{B|CA}| = t_{111} \langle 111 | + t_{212} \langle 212 |\)  
(3) Bi-separable state \(A|BC\),  
\(|\text{Bi-Sep}_{A|BC}| = t_{111} \langle 111 | + t_{122} \langle 122 |\) |
Table 1 continued

| Case | States |
|------|--------|
| 3. $\sigma_1^{(1)2} \neq \sigma_1^{(2)2} \neq \sigma_1^{(3)2}$ | (a) General states, $\sigma_1^{(1)2} + \sigma_1^{(2)2} - \sigma_1^{(3)2} \leq 1$; $\sigma_1^{(1)2} + \sigma_1^{(3)2} - \sigma_1^{(2)2} \leq 1$; $\sigma_1^{(2)2} + \sigma_1^{(3)2} - \sigma_1^{(1)2} \leq 1$ |

However, since the complex phases will be canceled out in Eqs. (27a) or (27b), their linear dependency is not important to us for the rest of the discussion.

### 5.3 Special states of three qubits and its polytope

Once we simultaneously diagonalized the one-body reduced density matrices of three qubits, there are three ways Eqs. (27a) or (27b) can be satisfied. By exploring all three possibilities in “Appendix D”, we determine the special states in each case. Table 1 summarizes our findings according to the behavior of the largest eigenvalue ($\sigma_1^{(n)2}$ where $n = 1, 2, 3$) of one-body reduced density matrices of three qubits.

In [26], the authors showed the construction of the entanglement polytope of three qubits by stochastic local operation and classical communication (SLOCC). Here, we show that it is also possible to construct a polytope of three qubits via the $n$-mode singular values classified by the local unitary (LU) operations through HOSVD. Due to the ordering property of higher-order singular value decomposition (HOSVD), we only need to consider the range $0.5 \leq \sigma_1^{(n)2} \leq 1$ when plotting the polytope. Combining with other constraints discussed in “Appendix D”, we plot the polytope of three qubits by LU operations in Fig. 1. We find that the polytope perfectly includes all the special states that we discovered by HOSVD.

### 5.4 The exceptional states of three qubits

In this subsection, we would like to make a comparison between our results and that in [7]. We summarize their classification in Table 2. Since it was shown that exceptional states have enlarged stabilizers, we choose to include the stabilizers in the table.

In Table 3, we check each of the exceptional states in [7] to see if they are in the higher order singular value decomposition (HOSVD) form, and their respective one-
body reduced density matrices. Of all the exceptional states, only Slice states are not in the HOSVD form. Therefore, we compute the eigenvalues of its one-body reduced density matrices in Table 3. In addition, we note that the generic states in [7] are not exceptional states, since their stabilizers are discrete.

By comparison, it is not difficult to see that the set of special states ($|S_1\rangle$, $|S_2\rangle$, $|S_3\rangle$) correspond to the Slice states in [7], while ($|B_1\rangle$, $|B_2\rangle$) corresponds to the Beechnut states. Because of this correspondence, we choose to label those special states as they are.
Table 2  Local unitary classification of three qubits [7] and the stabilizers of respective exceptional states

| Local unitary classes | Exceptional states and their stabilizers |
|-----------------------|-----------------------------------------|
| 1. Generic states     | Generic three-qubit states              |
|                       | $\text{Stab} = \{(e^{i\varphi}, U, V, W) = (1, 1, 1, 1)\}$ |
| 2. Bystander’s states | (a) $T_2$ is singular, i.e. $|\psi\rangle = \psi_{211} |211\rangle$ |
|                       | $\text{Stab} = \{(e^{i\varphi}, U, V, W) = \left[ e^{i\varphi}, \left( \begin{array}{cc} e^{i\varphi} & 0 \\ 0 & e^{-i\varphi} \end{array} \right) \right]\}$ |
|                       | (b) $T_2$ is not singular, i.e. $|\psi\rangle = \psi_{211} |211\rangle + \psi_{222} |222\rangle$ |
|                       | (i) If $|\psi_{211}| \neq |\psi_{222}|$ |
|                       | $\text{Stab} = \{(e^{i\varphi}, U, V, W) = \left[ e^{i\varphi}, \left( \begin{array}{cc} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{array} \right) \right]\}$ |
|                       | (ii) If $|\psi_{211}| = |\psi_{222}|$ |
|                       | $\text{Stab} = \{(e^{i\varphi}, U, V, W) = \left[ e^{i\varphi}, \left( \begin{array}{cc} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{array} \right) \right]\}$ |
| 3. Slice states       | States of the form $|\psi\rangle = p |111\rangle + bc |221\rangle + bd |222\rangle$ and its qubit-relabeling permutations |
|                       | (a) If $u_{12} = 0$, |
|                       | $\text{Stab} = \{(e^{i\varphi}, U, V, W) = \left[ \epsilon_1, e^{i\theta \sigma_3}, e^{e^{-i\theta \sigma_3}}, \epsilon_1 \epsilon_2 \right]\}$ |
|                       | (b) If $u_{11} = 0$, then $p^2 = |b|^2 (|c|^2 + |d|^2)$ |
|                       | $\text{Stab} = \{(e^{i\varphi}, U, V, W) = \left[ \epsilon_1, e^{i\theta \sigma_3}, \epsilon_2 e^{-i\theta \sigma_3}, \epsilon_1 \epsilon_2 \right]\}$ |

6 Conclusion

From the all-orthogonality conditions of higher-order singular value decomposition (HOSVD) for three qubits, we derived Eq. (27a) or equivalently Eq. (27b) that the $n$-mode singular values have to satisfy. We studied all possible scenarios that satisfy Eq. (27a) and computed all the special states of three qubits. Algebraically, the special states of three qubits are special zeroes of the polynomial (27a). The correspondence between the special states in our work with the exceptional states found in [7] shows that we recovered the LU classification of three qubits by using HOSVD.
Table 2  continued

| Local unitary classes | Exceptional states and their stabilizers |
|-----------------------|----------------------------------------|
| 4. GHZ states         | States of the form $|\psi\rangle = p|111\rangle + q|222\rangle$ |
|                       | (a) If $u_{12} = 0$,  |
|                       | $\text{Stab} = \left\{ (e^{i\phi}, U, V, W) = \left[ \epsilon_1, e^{i\theta}, e^{i\alpha}, e^{i\beta} \right] \right\}$  |
|                       | where $\theta + \alpha + \beta = 0(\text{mod } \pi)$.  |
|                       | (b) If $|q| = p$,  |
|                       | $\text{Stab} = \left\{ (e^{i\phi}, U, V, W) = \left[ e^{i\phi}, 0, 0, e^{-i\phi} \right] \right\}$  |
|                       | where $\theta + \alpha + \beta = \pi/2(\text{mod } \pi)$.  |
| 5. Beechnut states    | States of the following forms:  |
|                       | $|\psi\rangle = wc|111\rangle + b|212\rangle + c|221\rangle$ |
|                       | $|\psi\rangle = wc|112\rangle + b|211\rangle + c|222\rangle$  |
|                       | $\text{Stab} = \left\{ (e^{i\phi}, U, V, W) = \left[ e^{i\phi}, e^{i\theta}, e^{i\alpha}, e^{-i\beta} \right] \right\}$ |

Table 3  Local unitary classification of three qubits [7] and its one-body reduced density matrices

| Local unitary classes | HOSVD form | One-body reduced density matrices |
|-----------------------|------------|----------------------------------|
| 1. Generic states     | No         | $\rho^A, \rho^B, \rho^C$ are generic one-body reduced density matrices of three qubits |
| 2. Bystander’s states (a) | Yes | $\rho^A = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \rho^B = \rho^C = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ |
| Bystander’s states (b) (i) | Yes | $\rho^A = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \rho^B = \rho^C = \begin{pmatrix} |\psi_{211}\rangle^2 & 0 \\ 0 & |\psi_{222}\rangle^2 \end{pmatrix}$ |
| Bystander’s states (b) (ii) | Yes | $\rho^A = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \rho^B = \rho^C = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$ |
| 3. Slice states       | No         | $\rho^A = \rho^B = \begin{pmatrix} p^2 & 0 \\ 0 & |b\rangle^2 \end{pmatrix}, \rho^C = \begin{pmatrix} |bc\rangle^2 & |b\rangle^2 \bar{c}d \\ |b\rangle^2 \bar{c}d & |bd\rangle^2 \end{pmatrix}$ |
|                       | Eigenvalues of $\rho^C$ are $1\pm\sqrt{1-4p^2|bd|^{-2}}$. |
|                       | Any qubit-relabeling permutation results in the same set of reduced density matrices |
Table 3 continued

| Local unitary classes | HOSVD form | One-body reduced density matrices |
|-----------------------|------------|-----------------------------------|
| 4. GHZ states         | Yes        | $\rho^A = \rho^B = \rho^C = \begin{pmatrix} p^2 & 0 \\ 0 & |q|^2 \end{pmatrix}$ |
| 5. Beechnut states    | Yes        | $\rho^A = \begin{pmatrix} |wc|^2 & 0 \\ 0 & |b|^2 + |c|^2 \end{pmatrix}$, $\rho^B = \begin{pmatrix} |wc|^2 + |b|^2 & 0 \\ 0 & |c|^2 \end{pmatrix}$, $\rho^C = \begin{pmatrix} |wc|^2 + |c|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}$ or $\rho^C = \begin{pmatrix} |b|^2 & 0 \\ 0 & |wc|^2 + |c|^2 \end{pmatrix}$ |

As we have shown in Sect. 4, HOSVD simultaneously diagonalizes three-qubit states through LU actions, therefore our results are with respect to the LU equivalence. In comparison to the entanglement polytope constructed in [26] which is based on the stochastic local operation and classical communication (SLOCC) equivalence, we did not recover the inequality

$$\sigma_1^{(1)} + \sigma_1^{(2)} + \sigma_1^{(3)} \leq 2.$$  

This inequality separates the GHZ- and W-polytope in [26]. It will be an interesting problem to check if HOSVD can be used to classify multipartite states by SLOCC. Technically, HOSVD can be used to characterize LU entanglement classes of multipartite states with more than three subsystems (for example, four qubits) or of higher local dimensions (for example, three qutrits). However, due to the multiplicative nature of tensor product, the complexity of the computation will increase exponentially. Another future problem that can be tackled is to simplify such calculation.

In summary, we studied explicitly the matrix unfolding and HOSVD [17] for three qubits. We showed that the matrix unfoldings of three qubits are related to their reduced density matrices, while HOSVD simultaneously diagonalizes the one-body reduced density matrices of three qubits. Due to the all-orthogonality conditions from HOSVD, we identified the special states of three qubits. Since the special states are in correspondence to the exceptional states [7], we completely classified three-qubit states by LU operations in this sense. In addition, we proved that a three-qubit core tensor needs to satisfy only one bi-separability condition to be bi-separable. We further constructed a polytope of three qubits by LU operations that contains all the special states of three qubits that we found.

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Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.
Appendices

A The matrix unfolding and local unitary transformation of three qubits

In this section, we shall demonstrate the procedure of matrix unfolding for the case of three qubits. From Definition 1, given the three-qubit state,

$$|\psi\rangle = \sum_{i_1,i_2,i_3=1}^2 \psi_{i_1i_2i_3} |i_1i_2i_3\rangle,$$  \hspace{1cm} (31)

one can denote its tensorial form as $\Psi = [\psi_{i_1i_2i_3}] \in H = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$. The 1-, 2- and 3-matrix unfoldings of $\Psi$ are given as the following:

- The first matrix unfolding, $\Psi_{(1)}$, is an $I_1 \times (I_2 I_3) = 2 \times 4$ matrix with tensor elements $\psi_{i_1i_2i_3}$ situated at position with row index $i_1$ and column index $(i_2 - 1)I_3 + i_3 = 2(i_2 - 1) + i_3$,

$$\Psi_{(1)} = \begin{pmatrix} \psi_{111} & \psi_{112} & \psi_{121} & \psi_{122} \\ \psi_{211} & \psi_{212} & \psi_{221} & \psi_{222} \end{pmatrix}. \hspace{1cm} (32)$$

- The second matrix unfolding, $\Psi_{(2)}$, is an $I_2 \times (I_3 I_1) = 2 \times 4$ matrix with tensor elements $\psi_{i_1i_2i_3}$ situated at position with row index $i_2$ and column index $(i_3 - 1)I_1 + i_1 = 2(i_3 - 1) + i_1$,

$$\Psi_{(2)} = \begin{pmatrix} \psi_{111} & \psi_{211} & \psi_{112} & \psi_{212} \\ \psi_{121} & \psi_{221} & \psi_{122} & \psi_{222} \end{pmatrix}. \hspace{1cm} (33)$$

- The third matrix unfolding, $\Psi_{(3)}$, is an $I_3 \times (I_1 I_2) = 2 \times 4$ matrix with tensor elements $\psi_{i_1i_2i_3}$ situated at position with row index $i_3$ and column index $(i_1 - 1)I_2 + i_2 = 2(i_1 - 1) + i_2$,

$$\Psi_{(3)} = \begin{pmatrix} \psi_{111} & \psi_{121} & \psi_{211} & \psi_{221} \\ \psi_{112} & \psi_{122} & \psi_{212} & \psi_{222} \end{pmatrix}. \hspace{1cm} (34)$$

These matrix unfoldings are the matrices $\Psi_{A|BC}$, $\Psi_{B|CA}$, and $\Psi_{C|AB}$ used in the literature (see, for example [16]).

For three qubits, its local unitary (LU) transformation can be defined as the action of the LU operators $U^{(1)} \otimes U^{(2)} \otimes U^{(3)} \in \text{SU}(2) \times \text{SU}(2) \times \text{SU}(2)$ acting on the three-qubit state,

$$U^{(1)} \otimes U^{(2)} \otimes U^{(3)} |\psi\rangle = \sum_{j_1,j_2,j_3=1}^2 \sum_{i_1,i_2,i_3=1}^2 u^{(1)}_{j_1i_1} u^{(2)}_{j_2i_2} u^{(3)}_{j_3i_3} \psi_{i_1i_2i_3} |j_1j_2j_3\rangle.$$  \hspace{1cm} (35)
From Definition 2, the tensorial form of Eq. (35) can be rewritten as

\[ \Psi' = U^{(1)} \otimes U^{(2)} \otimes U^{(3)} \Psi. \] (36)

From Eqs. (10) and (36), we can show that

\[ \rho'^A = U^{(1)} \Psi_{(1)} \Psi_{(1)}^\dagger \]
\[ = U^{(1)} \Psi_{(1)} \left[ U^{(2)} \otimes U^{(3)} \right]^T \left\{ U^{(1)} \Psi_{(1)} \left[ U^{(2)} \otimes U^{(3)} \right]^T \right\}^\dagger \]
\[ = U^{(1)} \Psi_{(1)} \left[ U^{(2)} \otimes U^{(3)} \right]^T \left[ U^{(2)} \otimes U^{(3)} \right] \Psi_{(1)}^\dagger U^{(1)} U^{(1)} \]
\[ = U^{(1)} \rho^A U^{(1)} U^{(1)} \]. (37)

Similar procedure can be performed on Eqs. (11) and (12) to get Eqs. (38) and (39), respectively:

\[ \rho'^B = U^{(2)} \rho^B U^{(2)} \]
\[ \rho'^C = U^{(3)} \rho^C U^{(3)} \]. (38) (39)

The simple exercise above shows that Eq. (36) is indeed a LU action and the one-body reduced density matrices \( \rho'^A, \rho'^B, \rho'^C \) will fall under the same LU equivalence classes as \( \rho^A, \rho^B, \rho^C \).

**B Higher-order singular value decomposition on three qubits**

In this section, we apply higher-order singular value decomposition (HOSVD) to three qubits. From Eq. (14), the core tensor elements of three qubits \( T_\Psi = [t_{11213}] \) satisfy the following all-orthogonality conditions,

\[ \tilde{t}_{1111}t_{121} + \tilde{t}_{121}t_{212} + \tilde{t}_{112}t_{121} + \tilde{t}_{122}t_{222} = 0, \] (40)
\[ \tilde{t}_{111}t_{121} + \tilde{t}_{112}t_{121} + \tilde{t}_{112}t_{122} + \tilde{t}_{122}t_{222} = 0, \] (41)
\[ \tilde{t}_{111}t_{112} + \tilde{t}_{112}t_{212} + \tilde{t}_{112}t_{212} + \tilde{t}_{221}t_{222} = 0. \] (42)

The \( n \)-mode singular values are given as

\[ \sigma_1^{(1)} = \sqrt{|t_{111}|^2 + |t_{112}|^2 + |t_{121}|^2 + |t_{122}|^2}, \] (43)
\[ \sigma_2^{(1)} = \sqrt{|t_{211}|^2 + |t_{212}|^2 + |t_{221}|^2 + |t_{222}|^2}, \] (44)
\[ \sigma_1^{(2)} = \sqrt{|t_{111}|^2 + |t_{112}|^2 + |t_{211}|^2 + |t_{212}|^2}. \] (45)
\[ \sigma_2^{(2)} = \sqrt{|t_{121}|^2 + |t_{122}|^2 + |t_{221}|^2 + |t_{222}|^2}, \quad (46) \]
\[ \sigma_1^{(3)} = \sqrt{|t_{111}|^2 + |t_{121}|^2 + |t_{211}|^2 + |t_{221}|^2}, \quad (47) \]
\[ \sigma_2^{(3)} = \sqrt{|t_{112}|^2 + |t_{122}|^2 + |t_{212}|^2 + |t_{222}|^2}. \quad (48) \]

The normalization condition of probability amplitudes tells us that the square of the singular values for a particular matrix unfolding should sum up to be 1, i.e.
\[ \sigma_1^{(1)^2} + \sigma_2^{(1)^2} = 1, \quad (49) \]
\[ \sigma_1^{(2)^2} + \sigma_2^{(2)^2} = 1, \quad (50) \]
\[ \sigma_1^{(3)^2} + \sigma_2^{(3)^2} = 1. \quad (51) \]

Due to the ordering property of HOSVD, \( \sigma_1^{(n)^2} \geq \sigma_2^{(n)^2} \) for \( n = 1, 2, 3 \).

\textbf{C Separability conditions of three qubits}

The separability of three qubits can be checked by the separability conditions. In order to derive the separability conditions, for example the bi-separability conditions of \( C|AB \), we can first define the following states
\[ |\psi_C\rangle = c_1 |1\rangle + c_2 |2\rangle, \]
\[ |\psi_{AB}\rangle = a_{11} |11\rangle + a_{12} |12\rangle + a_{21} |21\rangle + a_{22} |22\rangle. \]

With the tensor product of \( |\psi_{AB}\rangle \) and \( |\psi_C\rangle \), one can compare the coefficients and conclude that a three-qubit state is bi-separable with respect to \( AB \) and \( C \) if it satisfies the following conditions:
\[ \psi_{111}\psi_{222} = \psi_{112}\psi_{221}, \quad (52) \]
\[ \psi_{111}\psi_{212} = \psi_{211}\psi_{112}, \quad (53) \]
\[ \psi_{121}\psi_{222} = \psi_{221}\psi_{122}, \quad (54) \]
\[ \psi_{111}\psi_{122} = \psi_{112}\psi_{121}, \quad (55) \]
\[ \psi_{211}\psi_{222} = \psi_{212}\psi_{221}, \quad (56) \]
\[ \psi_{211}\psi_{122} = \psi_{212}\psi_{121}. \quad (57) \]

The bi-separability conditions of \( A|BC \) and \( B|CA \) can be derived by the same way. For complete separability, the three-qubit states would satisfy an extra condition besides Eqs. (52)–(57), i.e.
\[ \psi_{211}\psi_{122} = \psi_{212}\psi_{121} = \psi_{112}\psi_{221}. \quad (58) \]

With respect to the core tensor of three qubits, we rewrite Eqs. (52)–(57) as
\[ t_{111}t_{222} = t_{112}t_{221}. \quad (59) \]
\[ t_{111}t_{212} = t_{211}t_{112}, \quad (60) \]
\[ t_{121}t_{222} = t_{221}t_{122}, \quad (61) \]
\[ t_{111}t_{122} = t_{112}t_{211}, \quad (62) \]
\[ t_{211}t_{222} = t_{121}t_{221}, \quad (63) \]
\[ t_{211}t_{122} = t_{212}t_{221}. \quad (64) \]

**D Special states of three qubits**

In this section, we will show explicitly all the possible ways to satisfy Eqs. (27a) or (27b).

**D.1 Case 1:** \( \sigma_1^{(1)2} = \sigma_1^{(2)2} = \sigma_1^{(3)2} \)

Under this condition, Eq. (27a) is satisfied automatically. In addition, the following equations have to be satisfied:

\[ |t_{121}|^2 + |t_{122}|^2 = |t_{211}|^2 + |t_{212}|^2, \quad (65) \]
\[ |t_{112}|^2 + |t_{122}|^2 = |t_{211}|^2 + |t_{221}|^2. \quad (66) \]

If we set \( |t_{112}|^2 = |t_{121}|^2 = |t_{122}|^2 = |t_{211}|^2 = |t_{212}|^2 = |t_{221}|^2 = 0 \), we get the generalized GHZ states,

\[ |\text{GHZ}\rangle = t_{111} |111\rangle + t_{222} |222\rangle, \quad (67) \]

which is a special state under this condition.

With HOSVD, the completely separable states have the following one-body reduced density matrices

\[ \rho_d^A = \rho_d^B = \rho_d^C = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (68) \]

Therefore, completely separable states are also under this condition.

**D.2 Case 2: Either** \( \sigma_1^{(1)2} = \sigma_1^{(2)2}, \sigma_1^{(1)2} = \sigma_1^{(3)2} \) or \( \sigma_1^{(2)2} = \sigma_1^{(3)2} \)

For each of the possibilities, we list down the additional conditions that have to be satisfied and the respective special states.

1. If \( \sigma_1^{(1)2} = \sigma_1^{(2)2} \), then it is necessary that \( |t_{121}|^2 = |t_{211}|^2 \) and \( |t_{122}|^2 = |t_{212}|^2 \).

From Eq. (23), we have

\[ t_{111} = -\frac{\bar{t}_{221}(t_{121}t_{212} - t_{122}t_{211})}{t_{212}\bar{t}_{211} - t_{122}\bar{t}_{121}}. \]
Computing $|t_{111}|^2$, it is not difficult to show that

$$|t_{111}|^2 = \frac{\tilde{t}_{221}(t_{121}t_{212} - t_{122}t_{211})}{t_{121}\tilde{t}_{211} - t_{122}\tilde{t}_{212}} \left[ \frac{t_{121}(\tilde{t}_{121}\tilde{t}_{212} - \tilde{t}_{122}\tilde{t}_{211})}{\tilde{t}_{121}\tilde{t}_{211} - \tilde{t}_{122}\tilde{t}_{212}} \right]$$

$$= |t_{221}|^2.$$ 

Similarly, we can show that $|t_{222}|^2 = |t_{112}|^2$. This implies that the $n$-mode singular values become

$$\sigma_1^{(1)2} = \sigma_1^{(2)2} = \frac{1}{2},$$

$$\sigma_2^{(1)2} = \sigma_2^{(2)2} = \frac{1}{2},$$

$$\sigma_1^{(3)2} = 2(|t_{111}|^2 + |t_{121}|^2),$$

$$\sigma_2^{(3)2} = 2(|t_{112}|^2 + |t_{122}|^2).$$

This corresponds to states where $(\sigma_1^{(1)2}, \sigma_1^{(2)2}, \sigma_1^{(3)2}) = (\frac{1}{2}, \frac{1}{2}, \sigma_1^{(3)2})$.

A special state under this condition is when $|t_{121}|^2 = |t_{211}|^2 = |t_{222}|^2 = 0$, i.e.

$$|S_1⟩ = t_{111} |111⟩ + t_{112} |112⟩ + t_{221} |221⟩ + t_{222} |222⟩,$$  \hspace{1cm} (69)

$$\tilde{t}_{111}t_{112} + \tilde{t}_{221}t_{222} = 0.$$  \hspace{1cm} (70)

Equation (70) enables us to write

$$|t_{221}|^2 = \frac{|t_{111}|^2 |t_{112}|^2}{|t_{222}|^2}.$$ 

Hence,

$$\sigma_1^{(3)2} = |t_{111}|^2 + \frac{|t_{111}|^2 |t_{112}|^2}{|t_{222}|^2}$$

$$= \frac{|t_{111}|^2}{|t_{222}|^2}(|t_{222}|^2 + |t_{112}|^2)$$

$$= \frac{|t_{111}|^2}{|t_{222}|^2} \sigma_2^{(3)2}.$$ 

Since $\sigma_1^{(3)2} + \sigma_2^{(3)2} = 1$, we find that equation above transforms into the followings:

$$\sigma_1^{(3)2} = \frac{|t_{111}|^2}{|t_{111}|^2 + |t_{222}|^2},$$

$$\sigma_2^{(3)2} = \frac{|t_{222}|^2}{|t_{111}|^2 + |t_{222}|^2}.$$
From the ordering property of HOSVD, we have $\sigma_1^{(3)2} \geq \sigma_2^{(3)2}$, which leads us to conclude that $|t_{111}|^2 \geq |t_{222}|^2$. Now,

$$
\sigma_1^{(3)2} - \sigma_1^{(1)2} = |t_{221}|^2 - |t_{112}|^2
= \frac{|t_{111}|^2 |t_{112}|^2}{|t_{222}|^2} - |t_{112}|^2
= \frac{|t_{112}|^2}{|t_{222}|^2} (|t_{111}|^2 - |t_{222}|^2).
$$

Since $\sigma_1^{(3)2} \neq \sigma_1^{(1)2}$, we conclude that $\sigma_1^{(3)2} > \sigma_1^{(1)2}$.

2. If $\sigma_1^{(1)2} = \sigma_1^{(3)2}$, then it is necessary that $|t_{112}|^2 = |t_{211}|^2$ and $|t_{122}|^2 = |t_{221}|^2$. Using a similar proof from above, this corresponds to states where $(\sigma_1^{(1)2}, \sigma_1^{(2)2}, \sigma_1^{(3)2}) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

A special state under this condition is when $|t_{112}|^2 = |t_{211}|^2 = |t_{122}|^2 = |t_{221}|^2 = 0$, i.e.

$$
|S_2\rangle = t_{111} |111\rangle + t_{121} |121\rangle + t_{212} |212\rangle + t_{222} |222\rangle, \quad (71)
$$

$$
\bar{t}_{111} t_{121} + \bar{t}_{212} t_{222} = 0. \quad (72)
$$

Here, $\sigma_1^{(2)2} > \sigma_1^{(1)2}$.

3. If $\sigma_1^{(2)2} = \sigma_1^{(3)2}$, then it is necessary that $|t_{112}|^2 = |t_{121}|^2$ and $|t_{122}|^2 = |t_{221}|^2$. Using a similar proof from above, this corresponds to states where $(\sigma_1^{(1)2}, \sigma_1^{(2)2}, \sigma_1^{(3)2}) = (\sigma_1^{(2)2}, \frac{1}{2}, \frac{1}{2})$.

A special state under this condition is when $|t_{112}|^2 = |t_{121}|^2 = |t_{122}|^2 = |t_{221}|^2 = 0$, i.e.

$$
|S_3\rangle = t_{111} |111\rangle + t_{122} |122\rangle + t_{211} |211\rangle + t_{222} |222\rangle, \quad (73)
$$

$$
\bar{t}_{111} t_{122} + \bar{t}_{121} t_{222} = 0. \quad (74)
$$

Here, $\sigma_1^{(1)2} > \sigma_1^{(2)2}$.

We also note that the bi-separable states fall under this case. For example, the HOSVD of the bi-separable state $C|AB$ has the following one-body reduced density matrices:

$$
\rho_d^A = \rho_d^B = \begin{pmatrix} |t_{111}|^2 & 0 \\ 0 & |t_{221}|^2 \end{pmatrix}, \quad (75)
$$

$$
\rho_d^C = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (76)
$$
D.3 Case 3: $\sigma_1^{(1)2} \neq \sigma_1^{(2)2} \neq \sigma_1^{(3)2}$

Since there is no special requirements on the $n$-mode singular values ($\sigma_1^{(n)2}$ where $n = 1, 2, 3$), this is where a generic genuinely entangled three-qubit state would be located. By rearranging the terms in Eq. (27a), we arrive at the following form:

$$a\sigma_1^{(1)2} + b\sigma_1^{(2)2} + c\sigma_1^{(3)2} = 0,$$

where $a = |t_{112}|^2 - |t_{121}|^2$, $b = |t_{211}|^2 - |t_{112}|^2$ and $c = |t_{121}|^2 - |t_{211}|^2$. This is an equation of a plane that cuts through the origin with normal vector $n = (a, b, c)$ and an extra condition of $a + b + c = 0$. Without loss of generality, we consider the case when $c = -(a + b)$, with $a$ and $b$ being positive. Equation (77) will then become

$$a(\sigma_1^{(1)2} - \sigma_1^{(3)2}) + b(\sigma_1^{(2)2} - \sigma_1^{(3)2}) = 0$$

$$\Rightarrow a(\sigma_1^{(1)2} + \sigma_1^{(2)2} - \sigma_1^{(3)2}) + b(\sigma_1^{(1)2} + \sigma_1^{(2)2} - \sigma_1^{(3)2}) = a\sigma_1^{(1)2} + b\sigma_1^{(2)2}$$

$$\Rightarrow \sigma_1^{(1)2} + \sigma_1^{(2)2} - \sigma_1^{(3)2} = \frac{a}{a + b}\sigma_1^{(2)2} + \frac{b}{a + b}\sigma_1^{(1)2}. \quad (78)$$

Equation (78) shows that the sum $\sigma_1^{(1)2} + \sigma_1^{(2)2} - \sigma_1^{(3)2}$ is a convex combination of $\sigma_1^{(1)2}$ and $\sigma_1^{(2)2}$. Since $0.5 \leq \sigma_1^{(1)2}, \sigma_1^{(2)2} \leq 1$, the upper bound of Eq. (78) is therefore $1$, i.e.

$$\sigma_1^{(1)2} + \sigma_1^{(2)2} - \sigma_1^{(3)2} \leq 1. \quad (79)$$

Similar argument can be carried out for $b = -(a + c)$ and $a = -(b + c)$, leading us to

$$\sigma_1^{(1)2} + \sigma_1^{(3)2} - \sigma_1^{(2)2} \leq 1, \quad (80)$$

$$\sigma_1^{(2)2} + \sigma_1^{(3)2} - \sigma_1^{(1)2} \leq 1. \quad (81)$$

If we let $|t_{112}|^2 = |t_{121}|^2 = |t_{211}|^2 = 0$, then $|t_{222}|^2$ has to be zero as well due to the all-orthogonality conditions (40), (41) and (42). Similarly, we can let $|t_{122}|^2 = |t_{212}|^2 = |t_{221}|^2 = 0$ and $|t_{111}|^2$ is automatically zero. We will then have the following equivalent special states,

$$|B_1\rangle = t_{111}|111\rangle + t_{122}|122\rangle + t_{212}|212\rangle + t_{221}|221\rangle, \quad (82)$$

$$|B_2\rangle = t_{112}|112\rangle + t_{121}|121\rangle + t_{211}|211\rangle + t_{222}|222\rangle. \quad (83)$$

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