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THE NECESSARY AND SUFFICIENT CONDITION FOR THE UNIQUENESS OF SCHMIDT DECOMPOSITION AND THE NECESSARY CONDITION FOR THE MAXIMAL VON NEUMANN ENTANGLEMENT ENTROPY

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Schmidt decomposition (SD) has been proven to be an important tool in quantum information and computation. Acín et al. proposed the SD for three qubits, but in the meanwhile, they indicated that it is possible to have two different SDs for the same state. The more challenging quest of finding the sufficient and necessary condition for the uniqueness of SD has never been undertaken. In this paper, we propose a necessary and sufficient condition for the uniqueness of SD for three qubits. By examining the condition, one can tell what state has one SD and what state has two SDs without actually performing the Schmidt decomposition. We investigate the relation between the uniqueness of SD and the von Neumann entanglement entropy (vNEE). To this end, we prove that any state having the maximal vNEE $S(\rho_x) = \ln 2$, $x = A, B$, or C must have a unique SD. This means if a state has two SDs, then the state does not have the maximal vNEE. Therefore, we should not choose a state having two SDs for its maximal vNEE for quantum information theory. In this paper, we also give all the SD states that have the maximal vNEE and a unique SD, as well as all the SD states that have a unique SD.

Keywords: GHZ SLOCC class, LU equivalence, qubits, Schmidt decomposition, von Neumann entanglement entropy (vNEE)

1 Introduction

SD for pure states has proven to be an important tool in quantum information and computation [1, 2, 3]. It is known that for a bipartite system, a pure state of a bipartite system can be written in the following canonical form.

$$|\psi\rangle_{AB} = \sum \lambda_i |i_A\rangle |i_B\rangle, \tag{1}$$

where $|i_A\rangle$ are orthonormal states for system A and $|i_B\rangle$ are orthonormal states for system B, $\lambda_i \geq 0$ and $\sum \lambda_i^2 = 1$. λ_i are referred to Schmidt coefficients. It is known that all the information about the non-local properties that the state possesses is contained in the positive Schmidt coefficients [4].

Quantum entanglement is a unique physical resource in quantum information and computation, such as quantum communication, quantum cryptography, and quantum teleportation [4]. Recently, the entanglement preparation on the quantum cloud was studied [6, 7]. Lots of efforts have been devoted to studying the characterization, the measurement, and the classification of the entanglement via SD [8, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 25]. A method to transform pure states of three qubits into SD under local unitary (LU) operators was proposed [8, 9]. Under Stochastic local operations and classical communication (SLOCC), pure states of three qubits were partitioned into six SLOCC equivalence classes: GHZ, W, A-BC, B-AC, C-AB, and A-B-C [5]. Via the SD of three qubits, it is convenient to study the classification of three qubits under SLOCC and LU [8, 9, 21, 30, 29]. For example, SDs for three qubits were partitioned into five types [8, 9], while SDs for the GHZ SLOCC class were partitioned into ten families under LU [29]. Via SD, Enriquez et al. studied the minimal decomposition entropy [22, 8], Tajima investigated LOCC transformation [23], and Liu et al. studied linear monogamy of entanglement [24]. There is a close relationship between Schmidt decomposition and purification.

Furthermore, Carteret et al. explored the SD for the multipartite system [14]. Kraus transformed a pure state of the multipartite system into a standard form and proved that two states are LU equivalent if and only if their standard forms coincide [26, 27]. Vicente et al. proposed a different decomposition of three qubits by means of five parameters under LU [10]. Li and Qiao proposed the canonical forms for pure and mixed states of multipartite systems with arbitrary dimensions [20].

Acín et al. first proposed SD and investigated the uniqueness of SD for three qubits [8, 9]. A pure state of three qubits has eight complex coefficients while its SD has five non-negative coefficients and a real phase parameter because SD has five local bases product states (LBPS). It is known that a pure state and its SD are equivalent under LU. It is convenient to study entanglement property and entanglement classification via SD. A different SD procedure was proposed in [35].

In [8, 9], the authors indicated that the equation $\det L_0^A = 0$ has generically two different solutions, so two different SDs are possible for the same state. In [8, 9], for the uniqueness of SD, the phase factor is limited to $0 \leq \chi \leq \pi$. It means that the SD with phase of $\chi \in (\pi, 2\pi)$ is discarded. Thus, the SD with the phase of $\chi \in (0, \pi)$ remains. When the phase χ is 0 or π, one of two possible SDs is taken by the smallest λ_1 else the smallest λ_0 [9].

We explain why it is important to discuss the uniqueness of SD below. (1). For the state $|\psi\rangle$ having a unique SD, subjected to local random unitary noise, the SD of $|\psi\rangle$ does not change. That is, $U_1 \otimes U_2 \otimes U_3|\psi\rangle$, where U_i are unitary, and $|\psi\rangle$ have the same SD. It means that though $|\psi\rangle$ becomes a different state, but its SD remains the same. In the case for which a different SD is obtained, it means that the state is interacting with a non-local unitary system. (2). When SD is used for entanglement classification, we need to know how many SDs a state has. Of course, it is easy to partition states with a unique SD via SD. For example, consider the state $-p_1|001\rangle - p_2|010\rangle - p_3|100\rangle + q_0|111\rangle$, where $p_i, i = 1, 2, 3$ and

q_0 are non-zero real numbers, which corresponds to a black hole according to [31], ref. Ex. 8 in Section 4. From Ex. 8, the state has a unique SD. Using the unique SD, we partition the states and the corresponding black holes under LU in [29, 36]. One can also see that when a state has a unique SD, then if another state has a different SD, then the two states are LU inequivalent. But, when a state has two SDs, the situation becomes a bit complicated. (3). It is well known that vNEE is an important entanglement measure for quantum information theory. We will show that a state having the maximal vNEE must have a unique SD. By contrapositive, if a state has two SDs, then it does not have the maximal vNEE.

In this paper, we propose a necessary and sufficient condition for the uniqueness of SD for three qubits. By the condition, one can know a three-qubit pure state has one or two SDs without transforming the state into SD. We investigate the relation between the uniqueness of SD and the maximal vNEE.

2 Steps for Schmidt decomposition

Acín et al. [8] proposed SD for three qubits by transforming any pure three-qubit state into the canonical form (Eq. (14)) under LU. Let $|\psi\rangle$ and $|\psi'\rangle$ be any pure states of three qubits. Then, from [5, 26], $|\psi'\rangle$ is LU equivalent to $|\psi\rangle$ if and only if there are local unitary operators U^A, U^B, and U^C such that $|\psi'\rangle = U^A \otimes U^B \otimes U^C|\psi\rangle$.

The following shows how to find the three unitary matrices U^A, U^B, and U^C to get an SD.

Let $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$ and $|\psi'\rangle = \sum_{i,j,k} c'_{ijk}|ijk\rangle$, with $i, j, k \in \{0, 1\}$, and

$$\begin{aligned} C_0 &= \begin{pmatrix} c_0 & c_1 \\ c_2 & c_3 \end{pmatrix}, C_1 = \begin{pmatrix} c_4 & c_5 \\ c_6 & c_7 \end{pmatrix}, \\ C'_0 &= \begin{pmatrix} c'_0 & c'_1 \\ c'_2 & c'_3 \end{pmatrix}, C'_1 = \begin{pmatrix} c'_4 & c'_5 \\ c'_6 & c'_7 \end{pmatrix}. \end{aligned} \tag{2}$$

Then, from [32, 33, 30], obtain

$$\begin{pmatrix} C'_0 \\ C'_1 \end{pmatrix} = (U^A \otimes U^B) \begin{pmatrix} C_0 \\ C_1 \end{pmatrix} (U^C)^T. \tag{3}$$

Let the unitary matrix $U^A = \left(u^A_{ij}\right), i, j = 0, 1$. Then, from Eq. (3), we have

$$\begin{aligned} \begin{pmatrix} C'_0 \\ C'_1 \end{pmatrix} &= \begin{pmatrix} u^A_{00}U^B & u^A_{01}U^B \\ u^A_{10}U^B & u^A_{11}U^B \end{pmatrix} \begin{pmatrix} C_0 \\ C_1 \end{pmatrix} (U^C)^T \\ &= \begin{pmatrix} U^B L^A_0 (U^C)^T \\ U^B L^A_1 (U^C)^T \end{pmatrix}, \end{aligned} \tag{4}$$

where

$$L^A_0 = u^A_{00}C_0 + u^A_{01}C_1, \tag{5}$$

$$L^A_1 = u^A_{10}C_0 + u^A_{11}C_1. \tag{6}$$

To get SD, choose U^A such that $\det L^A_0 = 0$ as Acín et al. did in [8]. We derive the equation $\det L_0^A = 0$ as follows [30]. Let

$$\alpha = c_0c_3 - c_1c_2, \quad (7)$$
$$\beta = c_0c_7 - c_1c_6 - c_2c_5 + c_3c_4, \quad (8)$$
$$\gamma = c_4c_7 - c_5c_6, \quad (9)$$
$$\tau = \beta^2 - 4\alpha\gamma. \quad (10)$$

Note that for GHZ SLOCC class, $\tau \neq 0$.

From Eq. (5), we can calculate $\det L_0^A$. Equation $\det L_0^A = 0$ is equivalent to:

$$\alpha(u_{00}^A)^2 + \beta u_{01}^A u_{00}^A + \gamma(u_{01}^A)^2 = 0. \quad (11)$$

By solving Eq. (11) we can get u_{00}^A and u_{01}^A. U^A is a unitary matrix. Therefore u_{10}^A and u_{11}^A can be obtained via the properties of a unitary matrix. We compute a U^A for each case of α, β, γ, and τ in Table A.1 in Appendix A.

Next, we calculate the Singular Value Decomposition (SVD) of L_0^A to get λ_0. We can get the SVD of L_0^A by considering the degenerate L_0^A: there are unitary matrices U^B and U^C such that

$$U^B L_0^A (U^C)^T = \text{diag}(\lambda_0, 0), \quad (12)$$

where $\lambda_0 \geq 0$, and λ_0 and 0 are called singular values of L_0^A. U^B and U^C can be found following the steps in Appendix B.

Next, with U^B and U^C, we can calculate $U^B L_1^A (U^C)^T$ to get other λ's and the phase. Let

$$U^B L_1^A (U^C)^T = \begin{pmatrix} \lambda_1 e^{i\chi_1} & \lambda_2 e^{i\chi_2} \\ \lambda_3 e^{i\chi_3} & \lambda_4 e^{i\chi_4} \end{pmatrix}. \quad (13)$$

Let $\chi = (\chi_1 - \chi_2 - \chi_3 + \chi_4) \bmod (2\pi)$. From [8, 30], we obtain the SD of $|\psi\rangle$ as follows,

$$\lambda_0|000\rangle + \lambda_1 e^{i\chi}|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle, \quad (14)$$

where $\lambda_i \geq 0$ are called Schmidt coefficients, and $\sum_{i=0}^{4} \lambda_i^2 = 1$; $0 \leq \chi < 2\pi$ is called the phase of the SD. For simplicity, the state in Eq. (14) is written as $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$.

2.1 The number of solutions of Eq. (11) and the number of SDs

In [8], the authors indicated that Eq. (11) has generically two different solutions. Specially when the phase is 0 or π, two canonical forms exist in general [9].

2.1.1 The number of solutions of Eq. (11)

There are three cases for the number of solutions of Eq. (11) (Ref. Table A.1).

Case 1. $\alpha = \beta = \gamma = 0$. For the case, clearly, any unitary matrix satisfies Eq. (11). It means Eq. (11) has infinite solutions.

Case 2. Subcase 2.1. $\alpha = \beta = 0$ but $\gamma \neq 0$, Subcase 2.2. $\alpha \neq 0$ but $\beta = \gamma = 0$, Subcase 2.3. $\alpha\beta\gamma \neq 0$ but $\tau = 0$. For Case 2, one can see that Eq. (11) has one solution.

Case 3. Subcase 3.1. $\alpha = \gamma = 0$ but $\beta \neq 0$, Subcase 3.2. $\alpha = 0$ but $\beta\gamma \neq 0$, Subcase 3.3. $\alpha\beta \neq 0$ but $\gamma = 0$, Subcase 3.4. $\alpha\gamma \neq 0$ but $\beta = 0$, Subcase 3.5. $\alpha\beta\gamma\tau \neq 0$. For case 3, one can see that Eq. (11) has two solutions.

2.1.2 A correspondence between the number of solutions of Eq. (11) and the number of SDs

We have the following cases ((i)-(iv)) for the solutions of Eq. (11) and the corresponding number of SDs.

Case (i). If Eq. (11) has only one solution, then the state has only one SD.

Case (ii). Eq. (11) has two solutions, and the state also has two SDs. For this case, we have the following examples (a), (b), (c), and (d).

(a). For Ex. 2 in Sec. 4, it belongs to Subcase 3.1. The state has two SDs which have the phase of 0.

(b). For Ex.3 in Sec. 4, the state belongs to Subcase 3.2. The state has two SDs. One of them has phase π while the other one's phase cannot be determined.

(c). For Ex. 4 in Sec. 4, it belongs to Subcase 3.2. It has two SDs. One SD has the phase of $-\pi/4$ while the other one has the phase of $\pi - \arctan 2$.

(d). For the state $\lambda_0|000\rangle + \lambda_4|111\rangle$, where $\lambda_0 > 0$, $\lambda_4 > 0$, and $\lambda_0^2 + \lambda_4^2 = 1$, itself is of the form SD. It belongs to Subcase 3.1. Clearly, $\lambda_4|000\rangle + \lambda_0|111\rangle$ is also an SD of that state. This is because $\lambda_4|000\rangle + \lambda_0|111\rangle = \sigma_x \otimes \sigma_x \otimes \sigma_x(\lambda_0|000\rangle + \lambda_4|111\rangle)$. Thus, when $\lambda_0 \neq \lambda_4$, $\lambda_0|000\rangle + \lambda_4|111\rangle$ have two SDs: itself and $\lambda_4|000\rangle + \lambda_0|111\rangle$. But their phases cannot be determined.

Case (iii). Eq. (11) has two solutions, but the state has only one SD. For this case, we have the following examples (a) and (b).

(a). When $\lambda_0 = \lambda_4$, $\lambda_0|000\rangle + \lambda_4|111\rangle$ is just GHZ state $\frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$. For the GHZ state, one can check it has only one SD. i.e. itself though Eq. (11) has two solutions. Generally, if a GHZ state is an SD of a state, then the GHZ state is a unique SD of the state.

(b). For Ex. 8 in Sec. 4, it belongs to case 3.4. For the state, Eq. (11) has two solutions. However, we show it has only one SD in Sec. 4.

Case (iv). Eq. (11) has two solutions, and the state has two SDs ignoring the phases of SDs. We have the following example.

For Ex. 5 in Sec. 4, it belongs to case 3.3. It has two SDs (ignoring phases). However, we know $(1/\sqrt{6}, \sqrt{3}/6e^{i\varphi_2}, 0, 0, \sqrt{3}/2)$ is LU equivalent to $(1/\sqrt{6}, \sqrt{3}/6, 0, 0, \sqrt{3}/2)$ for any phase φ_2 [29]. Thus, we can also say the state has infinite SDs.

For any pure state of three qubits, if it has a unique canonical form in Eq. (14), we say the Schmidt decomposition of the state is unique. In this paper, we give a necessary and sufficient condition to determine a state has one or two SDs without transforming a state into the canonical form in Eq. (14). The condition is expressed via the coefficients c_i. Therefore, it is easy to calculate it.

It is well known that pure states of three qubits were partitioned into six SLOCC classes: GHZ, W, A-BC, B-AC, C-AB, and A-B-C [5]. We can find all the solutions for U^A by solving Eq. (11) for each SLOCC class.

From [28] we obtain Table A.1 in Appendix A, in which num_sol is the number of the solutions of Eq. (11). For $\alpha = \beta = \gamma = \tau = 0$, i.e., for B-AC, C-AB, and A-B-C SLOCC classes in Table A.1, any unitary matrix satisfies Eq. (11), thus there are infinite solutions for Eq. (11).

3 A necessary and sufficient condition for the uniqueness of SD for the phases between 0 and 2π

There is no necessary relation between the number of SDs and the number of solutions to Eq. (11).

3.1 The uniqueness of SD for two qubits

For two qubits, let $|\psi\rangle = \sum_{i=0}^{3} c_i|i\rangle$ be a pure state of two qubits. If $|\psi\rangle$ has a canonical form $\alpha|00\rangle + \beta|11\rangle$ ($\alpha \neq \beta$), then $\beta|00\rangle + \alpha|11\rangle$ is also a canonical form of $|\psi\rangle$ because $\beta|00\rangle + \alpha|11\rangle = \sigma_x \otimes \sigma_x(\alpha|00\rangle + \beta|11\rangle)$. Clearly, $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ is a unique canonical form. One can see the following result holds.

Result 1. A two-qubit state has the maximal vNEE if and only if the state has a unique canonical form.

Under $\alpha \leq \beta$, $\frac{1}{2}|00\rangle + \frac{\sqrt{3}}{2}|11\rangle$ is a unique SD while $\frac{\sqrt{3}}{2}|00\rangle + \frac{1}{2}|11\rangle$ is not an SD. Under $\alpha \leq \beta$, each state has a unique SD. Of course, when each state has a unique SD, Result 1 becomes meaningless.

3.2 The uniqueness of SD for three qubits

For three qubits, from Sec. 2.1, one can see that a three-qubit state may have one or more than one SD. It is known that SD is unique for SLOCC classes A-BC, B-AC, C-AB, and A-B-C when SDs of the SLOCC classes are considered as the ones of two-qubit states, although Eq. (11) has infinite solutions for SLOCC classes B-AC, C-AB, and A-B-C.

To make the Schmidt decomposition unique for all states, the authors of [8, 9] applied the following two restrictions:

Restriction 1. Limiting the phase factor to $[0, \pi]$

Under the restriction, the SD with the phase $\theta \in (\pi, 2\pi)$ is discarded while the SD with the phase $\theta \in (0, \pi)$ remains. For example, for Ex. 4 in Section 4, by the procedure in [5], a calculation yields two SDs $|\Xi_1\rangle = (\frac{\sqrt{2}}{2}, \frac{\sqrt{5}}{4}e^{i(\pi - \arctan 2)}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ and $|\Xi_2\rangle = (\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}e^{-i\frac{\pi}{4}}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. By Restriction 1, $|\Xi_2\rangle$ is discarded. Then, the state has a unique SD $|\Xi_1\rangle$.

Restriction 2. When the phase is 0 or π, arbitrarily taking one of the two SDs

When the phase is 0 or π, there may be two SDs. Then, the one with the smallest λ_1 is taken; when the two SDs have the same λ_1, the one with the smallest λ_0 is taken [9].

For example, for Ex. 2 in Section 4, there are two SDs, which are $|\nu_1\rangle = \{\frac{1}{\sqrt{5}}, (\frac{7}{5})^2\frac{1}{\sqrt{5}}, \frac{7}{25}\frac{1}{\sqrt{5}}, \frac{7}{25}\frac{1}{\sqrt{5}}, \frac{1}{25}\frac{1}{\sqrt{5}}\}$ and $|\nu_2\rangle = \{\frac{2}{\sqrt{5}}, \frac{1}{2}(\frac{7}{5})^2\frac{1}{\sqrt{5}}, \frac{7}{50}\frac{1}{\sqrt{5}}, \frac{7}{50}\frac{1}{\sqrt{5}}, \frac{1}{50}\frac{1}{\sqrt{5}}\}$. For $|\nu_1\rangle$ and $|\nu_2\rangle$, their phases are 0. By Restriction 2, $|\nu_1\rangle$ is discarded. Similarly, take $\alpha|000\rangle + \beta|111\rangle$, where $\alpha < \beta$, as SD for the uniqueness while discard $\beta|000\rangle + \alpha|111\rangle$.

Unfortunately, the two restrictions cannot guarantee the uniqueness of SD for all states. It needs two additional restrictions:

Restriction 3. Ignoring the phases of SDs belonging to W SLOCC class

Let $|W_1\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\varphi}|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle$, where $\lambda_i \neq 0$, $i = 0, 1, 2, 3$. One can see that $|W_1\rangle$ belongs to W SLOCC class. Let $U^A = diag(1, e^{i\theta})$, $U^B = U^C = diag(1, e^{-i\theta})$, and $|W_2\rangle = U^A \otimes U^B \otimes U^C|W_1\rangle$, where θ is any real number. Then, a calculation yields $|W_2\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\varphi'}|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle$, where $\varphi' = \varphi + \theta$. We can make φ' belong to $(0, \pi)$ because θ is any real number. Thus, there are infinite $|W_2\rangle$ which are LU equivalent to $|W_1\rangle$. To make SD unique for $|W_1\rangle$, it needs to ignore the phases. Thus, two

SDs belonging to W SLOCC class are LU equivalent if and only if their Schmidt coefficients are equal, respectively [30]. Thus, the SD of the W SLOCC class is unique under Restriction 3.

Restriction 4. Ignoring the phases of SDs with $\lambda_2\lambda_3 = 0$ and $\lambda_0\lambda_1\lambda_4 \neq 0$

Clearly, the SDs belong to the GHZ SLOCC class. For example, let $|G\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\omega}|100\rangle + \lambda_2|101\rangle + \lambda_4|111\rangle$, where $\lambda_i \neq 0$, $i = 0, 1, 2, 4$. Let $U^A = diag(e^{i\phi}, e^{i2\phi})$, $U^B = diag(e^{-i\phi}, e^{-i\phi})$, and $U^C = diag(1, e^{-i\phi})$, and $|G_1\rangle = U^A \otimes U^B \otimes U^C|G\rangle$, where ϕ is any real number. A calculation yields $|G_1\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\omega'}|100\rangle + \lambda_2|101\rangle + \lambda_4|111\rangle$, where $\omega' = \omega + \phi$. We can make ω' belong to $(0, \pi)$ because ϕ is any real number. Thus, $|G\rangle$ has infinite SDs, which possess the same Schmidt coefficients but different phases. Similarly, there are infinite SDs for $|H\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\varphi}|100\rangle + \lambda_3|101\rangle + \lambda_4|111\rangle$, where $\lambda_i \neq 0$, $i = 0, 1, 3, 4$, and $|Q\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\varphi}|100\rangle + \lambda_4|111\rangle$, where $\lambda_i \neq 0$, $i = 0, 1, 4$. To make SD unique for $|G\rangle$, $|H\rangle$ and $|Q\rangle$, it needs to ignore their phase. Thus, the states $|G\rangle$, $|H\rangle$ and $|Q\rangle$ have a unique SD if and only if $\varrho = 1$ after ignoring their phases [29].

Under the four restrictions, each state of three qubits has a unique SD.

3.3 We don't make SD unique for all states in this paper

From the above discussion, by ignoring the phases of SD, SD of W SLOCC class is unique. While the situation becomes complicated for GHZ SLOCC class. Via Table A.1, one can see that there are always two solutions for Eq. (11) for U^A for GHZ SLOCC class while a state may have one or two SDs. For example, Eq. (11) has two solutions for GHZ state, but GHZ state has a unique SD, i.e., itself.

Clearly, when we make SD unique for all states, it becomes meaningless to say if a state has a property then the state has a unique SD. For example, Result 1 becomes meaningless when each state has a unique SD. We don't make the SD unique for all states in this paper. To consider all the SDs produced by the SD procedure [5,6], Restrictions 1 and 2 in [5,6] are canceled in this paper. We use natural phase to $[0, 2\pi)$ instead of the phases to $[0,\pi]$, thus Ex. 4 in Section 4 has two SDs $|\Xi_1\rangle$ and $|\Xi_2\rangle$. After canceling Restriction 2, then Ex.2 in Section 4 of this paper has two SDS $|\nu_1\rangle$ and $|\nu_2\rangle$.

Some states have a unique SD, and some have two SDs. How do we know that the states in Ex. 6 and Ex. 8 in Section 4 have a unique SD while the states in Ex. 2 and Ex. 4 have two SDs before going through the Schmidt Decomposition procedure? In this paper, we try to answer this question. So far, there is no criteria by which one can determine a three-qubit state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$ has one or two SDs. In this section, we give a necessary and sufficient condition for the uniqueness of SD for the GHZ SLOCC class without performing the procedure for SD.

One can see that it has a meaning to explore what states have one or two SDs as it has a meaning to study real or complex roots of quadratic equations.

3.4 Uniqueness of SD for the states $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ *of GHZ SLOCC class*

Let $|\Psi\rangle$ be the state $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$. Then, for $|\Psi\rangle$, the following were defined [30, 29].

$$\varrho = \sqrt{(\lambda_0\lambda_4)^2 + |\gamma|^2}/\sqrt{(\lambda_2^2+\lambda_4^2)(\lambda_3^2+\lambda_4^2)}, \tag{15}$$

$$\iota = (\lambda_2\lambda_3 + \gamma^*/\varrho^2)/\lambda_4, \tag{16}$$

$$|\Psi_{\varrho,\iota}\rangle = ((1/\varrho)\lambda_0, \varrho\iota, \varrho\lambda_2, \varrho\lambda_3, \varrho\lambda_4). \tag{17}$$

where $\gamma = \lambda_1\lambda_4 e^{i\chi} - \lambda_2\lambda_3$, γ^* is the complex conjugate of γ.

From [30, 29], it is known that when $\gamma \neq 0$ but $\lambda_2\lambda_3 = 0$, the two states $(\lambda_0, \lambda_1 e^{i\varphi}, \lambda_2, \lambda_3, \lambda_4)$ and $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ for any phases φ and χ are LU equivalent. In this paper, when $\gamma \neq 0$ but $\lambda_2\lambda_3 = 0$, all the states with the same $(\lambda_0, \lambda_1, \lambda_2, \lambda_3, \lambda_4)$ but different phases are considered to be the same for the uniqueness.

Let $|\Upsilon\rangle = (\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ be a complex state with the phase $\chi \neq 0$ or π and $\Pi_{i=0}^4 \lambda_i \neq 0$. It is known that $|\Upsilon\rangle$ with $\varrho = 1$ has one SD, which is its complex conjugate $|\Upsilon^*\rangle = (\lambda_0, \lambda_1 e^{-i\chi}, \lambda_2, \lambda_3, \lambda_4)$, where $|\Upsilon\rangle$ and $|\Upsilon^*\rangle$ are the same ignoring the phases [29]. For the uniqueness, $|\Upsilon\rangle$ with $\varrho = 1$ and its conjugate $|\Upsilon^*\rangle$ are considered to be the same in this paper. Note that when $\varrho \neq 1$, $|\Upsilon\rangle$ and $|\Upsilon^*\rangle$ are LU inequivalent.

For example, $|\Xi_i\rangle$ and their conjugate $|\Xi_i^*\rangle$, $i = 1, 2$, are LU inequivalent. For two qubits, it is known that a state $|\psi\rangle = \sum_{i=0}^3 c_i|i\rangle$ and its conjugate $|\psi^*\rangle = \sum_{i=0}^3 c_i^*|i\rangle$, where c_i^* is the complex conjugate of c_i, are LU equivalent. But, it cannot be guaranteed that a state of three qubits and its conjugate are LU equivalent. This is a difference between two qubits and three qubits. For three qubits, a state with the phases $\varphi \neq 0$ or π and $\Pi_{i=0}^4 \lambda_i \neq 0$ and its conjugate are LU equivalent if and only if $\varrho = 1$ [29].

For GHZ SLOCC class, ignoring the phases of the states with $\gamma \neq 0$ and $\lambda_2\lambda_3 = 0$, one can see that if a state $(\lambda_0', \lambda_1' e^{i\chi'}, \lambda_2', \lambda_3', \lambda_4')$ is LU equivalent to a state $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$, then from [30, 29], the state can be written as

$$(\lambda_0', \lambda_1' e^{i\chi'}, \lambda_2', \lambda_3', \lambda_4') = ((1/\varrho)\lambda_0, \varrho\iota, \varrho\lambda_2, \varrho\lambda_3, \varrho\lambda_4).$$

For the uniqueness of SD for the states $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$, we have the following theorem from [29].

Theorem 1 ([29]) For the states $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$, where $\chi \in [0, 2\pi)$, (1) ignoring the phases of the states with $\gamma \neq 0$ and $\lambda_2\lambda_3 = 0$, and (2) for the states with the phases $\chi \neq 0$ or π and $\Pi_{i=0}^4 \lambda_i \neq 0$, considering a state and its conjugate to be the same whenever they are LU equivalent, then the SD of the states is unique if and only if $\varrho = 1$.

Theorem 1 is equivalent to the following verbose version: Consider the states of GHZ SLOCC class of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$, where $\chi \in [0, 2\pi)$, the condition for the uniqueness of SD is stated as follows:

a). For real positive states of the form $(\lambda_0, \lambda_1, \lambda_2, \lambda_3, \lambda_4)$ with $\gamma = 0$, SD is unique if and only if $\varrho = 1$.

b). For real states of the form $(\lambda_0, \delta\lambda_1, \lambda_2, \lambda_3, \lambda_4)$ with $\delta = \pm 1$ and $\gamma\lambda_2\lambda_3 \neq 0$, SD is unique if and only if $\varrho = 1$.

c). For complex states of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ with $\gamma \neq 0$ and $\lambda_2\lambda_3 = 0$, when ignoring the phase, SD is unique if and only if $\varrho = 1$.

d). For complex states of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ with the phases $\chi \neq 0$ or π and $\Pi_{i=0}^4 \lambda_i \neq 0$, by considering a state and its conjugate state to be the same whenever they are LU equivalent, SD is unique if and only if $\varrho = 1$.

3.5 Uniqueness of SD for any pure state of GHZ SLOCC class

In this subsection, we study the uniqueness of SD for any pure state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$ of GHZ SLOCC class. Note that Eq. (11) has two solutions for GHZ SLOCC class. By solving Eq. (11), we obtain two solutions U^A and $U^{A'}$, and then, from U^A and $U^{A'}$, we obtain L_0^A and $L_0^{A'}$, respectively. Next, we do a SVD of L_0^A and $L_0^{A'}$ to get their SDs: $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ and $(\lambda_0', \lambda_1' e^{i\chi'}, \lambda_2', \lambda_3', \lambda_4')$. However, it is possible for the two SDs to be the same. Theorem 2 states the condition under which the two SDs are the same, i.e., SD of the state $|\psi\rangle$ is unique.

Theorem 2 Let $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$ (with $i, j, k \in \{0, 1\}$) be any state of GHZ SLOCC class. Then SD of the state $|\psi\rangle$ is unique if and only if L_0^A and $L_0^{A'}$ have the same non-zero singular value.

Proof. Let λ_0 and λ_0' be the non-zero singular values of L_0^A and $L_0^{A'}$, respectively. Via steps for SD, from U^A and $U^{A'}$ obtain SD and SD' for $|\psi\rangle$.

$$SD = (\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4), \tag{18}$$

$$SD' = (\lambda_0', \lambda_1' e^{i\chi'}, \lambda_2', \lambda_3', \lambda_4'). \tag{19}$$

Then, if SD is unique for $|\psi\rangle$, it is clear that $\lambda_0 = \lambda_0'$. That is, L_0^A and $L_0^{A'}$ have the same non-zero singular value. Conversely, assume that L_0^A and $L_0^{A'}$ have the same non-zero singular value. That is, $\lambda_0 = \lambda_0'$. We can write SD' as $((1/\varrho)\lambda_0, \varrho\iota, \varrho\lambda_2, \varrho\lambda_3, \varrho\lambda_4)$ because SD' is LU equivalent to SD [29]. Thus, $\lambda_0' = (1/\varrho)\lambda_0$, and then obtain $\varrho = 1$. In light of Theorem 1, SD is unique. Therefore, Theorem 2 holds. □

Let us find the non-zero singular value λ_0 of L_0^A. It is known that the singular values of L_0^A are just the square roots of the eigenvalues of $L_0^A(L_0^A)^H$, where $(L_0^A)^H$ is the Hermitian transpose of L_0^A. Let $S_1 = \sum_{i=0}^3 c_i c_i^*$, $S_2 = \sum_{i=4}^7 c_i c_i^*$, and $S_3 = \sum_{i=0}^3 c_{4+i}^* c_i$, where c_i^* is the complex conjugate of c_i. Then, a calculation yields the non-zero singular value λ_0 of L_0^A:

$$\lambda_0^2 = S_1 u_{00}^A u_{00}^{A\,*} + S_2 u_{01}^A u_{01}^{A\,*} + S_3 u_{00}^A u_{01}^{A\,*} + S_3^* u_{01}^A u_{00}^{A\,*}. \tag{20}$$

Similarly, we can calculate the singular value λ_0' of $L_0^{A'}$:

$$\lambda_0'^2 = S_1 u_{00}'^A u_{00}'^{A*} + S_2 u_{01}'^A u_{01}'^{A*} + S_3 u_{00}'^A u_{01}'^{A*} + S_3^* u_{01}'^A u_{00}'^{A*}, \tag{21}$$

where $u_{ij}'^A$ are entries of $L_0^{A'}$.

Then, we derive the condition that L_0^A and $L_0^{A'}$ have the same non-zero singular value by letting $\lambda_0^2 = \lambda_0'^2$ as follows.

$$\begin{aligned} S_1(u_{00}^A u_{00}^{A\,*} - u_{00}'^A u_{00}'^{A*}) &+ S_2(u_{01}^A u_{01}^{A\,*} - u_{01}'^A u_{01}'^{A*}) \\ &+ S_3(u_{00}^A u_{01}^{A\,*} - u_{00}'^A u_{01}'^{A*}) \\ &+ S_3^*(u_{01}^A u_{00}^{A\,*} - u_{01}'^A u_{00}'^{A*}) = \quad 0. \end{aligned} \tag{22}$$

It is clear to see that the above condition is a function of the coefficients c_i. However, the expression is too general to be convenient. In sec. 4, the expression is reduced for different cases.

Theorem 2 can be reduced to five cases of GHZ SLOCC class, which will be discussed in Section 4. Table A.1 in Appendix A includes the five cases as well as the non-GHZ SLOCC class cases.

4 Cases for GHZ SLOCC class

4.1 When $\alpha = 0$, $\gamma = 0$, and $\beta \neq 0$ (Table A.1, Case 2)

When $\alpha = \gamma = 0$ but $\beta \neq 0$, Eq. (11) reduces to the equation $\beta u_{01}^A u_{00}^A = 0$, from which there are the following two solutions for U^A.

Solution 1 is $u_{01}^A = 0$ and $u_{00}^A = e^{i\phi}$, one can get $U^A = diag(e^{i\phi}, e^{i\omega})$.

Solution 2 is $u_{00}^A = 0$ and $u_{01}^A = e^{i\phi}$, one can get the following unitary matrix.

$$U^{A'} = \begin{pmatrix} 0 & e^{i\phi} \\ e^{i\omega} & 0 \end{pmatrix}. \tag{23}$$

For Solution 1, via U^A, clearly $L_0^A = e^{i\phi} C_0$. We do not need to do SVD of L_0^A to get the SD of a state since the singular values of L_0^A are just the square roots of the eigenvalues of $L_0^A (L_0^A)^H$, where $(L_0^A)^H$ is the Hermitian transpose of L_0^A. Let λ_0 and 0 be the singular values of L_0^A. Thus, λ_0^2 and 0 are the eigenvalues of $L_0^A (L_0^A)^H$. A calculation yields

$$\lambda_0^2 = \sum_{i=0}^{3} |c_i|^2 \tag{24}$$

For solution 2, via $U^{A'}$ in Eq. (23), clearly $L_0^{A'} = e^{i\phi} C_1$. Similarly, let λ_0' be the non-zero singular value of $L_0^{A'}$. Then, $(\lambda_0')^2$ is the eigenvalue of $L_0^{A'} (L_0^{A'})^H$. A calculation yields

$$(\lambda_0')^2 = \sum_{i=4}^{7} |c_i|^2. \tag{25}$$

From Theorem 2, we obtain the following.

Corollary 1 When $\alpha = \gamma = 0$ and $\beta \neq 0$, SD is unique if and only if

$$\sum_{i=0}^{3} |c_i|^2 = \frac{1}{2}. \tag{26}$$

Ex. 1. GHZ state $\frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$, which is the maximal entangled state, satisfies $\sum_{i=0}^{3} |c_i|^2 = \frac{1}{2}$. Thus, the GHZ state has a unique SD, i.e., itself. Generally, if a GHZ state is an SD of a state, then the GHZ state is its unique SD.

Ex. 2. For state $\frac{1}{5\sqrt{5}}(|000\rangle + 2|001\rangle + 2|010\rangle + 4|011\rangle + |100\rangle + 3|101\rangle + 3|110\rangle + 9|111\rangle)$, from Eq. (24) we compute $\lambda_0^2 = 1/5$; from Eq. (25), we compute $(\lambda_0')^2 = 4/5$. Therefore, the state has two SDs [30]: $\left(\frac{1}{\sqrt{5}}, (\frac{7}{5})^2 \frac{1}{\sqrt{5}}, \frac{7}{25}\frac{1}{\sqrt{5}}, \frac{7}{25}\frac{1}{\sqrt{5}}, \frac{1}{25}\frac{1}{\sqrt{5}}\right)$ and $\left(\frac{2}{\sqrt{5}}, (\frac{7}{5})^2 \frac{1}{2\sqrt{5}}, \frac{7}{50}\frac{1}{\sqrt{5}}, \frac{7}{50}\frac{1}{\sqrt{5}}, \frac{1}{50}\frac{1}{\sqrt{5}}\right)$.

4.2 When $\alpha = 0$, $\gamma \neq 0$, *and* $\beta \neq 0$ *(Case 4, Table A.1)*

For the case, Eq. (11) reduces to $u_{01}^A(\beta u_{00}^A + \gamma u_{01}^A) = 0$, from which there are two solutions for U^A.

Solution 1. $u_{01}^A = 0$ and $u_{00}^A = e^{i\phi}$. Thus, the unitary matrix $U^A = diag(e^{i\phi}, e^{i\omega})$.

Solution 2. $u_{00}^A = -\frac{\gamma}{\beta}u_{01}^A$, where $u_{01}^A \neq 0$. Via the properties of the unitary matrix, a complicated calculation yields

$$U^{A'} = \frac{|\beta|}{\sqrt{|\beta|^2 + |\gamma|^2}} \begin{pmatrix} -\frac{\gamma}{\beta}e^{i\phi} & e^{i\phi} \\ e^{i\omega} & \frac{\gamma^*}{\beta^*}e^{i\omega} \end{pmatrix} \tag{27}$$

For Solution 1, clearly $L_0^A = e^{i\phi}C_0$. Let λ_0 be the non-zero singular value of L_0^A. Similarly, a calculation yields

$$\lambda_0^2 = \sum_{i=0}^{3} |c_i|^2. \tag{28}$$

Solution 2. Via $U^{A'}$ in Eq. (27), clearly $L_0^{A'} = -\frac{\gamma}{\beta}\frac{|\beta|e^{i\phi}}{\sqrt{|\beta|^2+|\gamma|^2}}C_0 + \frac{|\beta|e^{i\phi}}{\sqrt{|\beta|^2+|\gamma|^2}}C_1$. Let λ_0' be the non-zero singular value of $L_0^{A'}$. A calculation yields

$$(\lambda_0')^2 = \frac{|\beta|^2}{|\beta|^2 + |\gamma|^2}\left(1 + \left(|\frac{\gamma}{\beta}|^2 - 1\right)\sum_{i=0}^{3}|c_i|^2 + 2[\text{real}(-\frac{\gamma}{\beta}\sum_{i=0}^{3}c_i c_{i+4}^*)]\right), \tag{29}$$

where c_i^* is the complex conjugate of c_i.

From Theorem 2, we obtain the following.

Corollary 2 When $\alpha = 0$, $\gamma \neq 0$, and $\beta \neq 0$, SD is unique if and only if

$$\sum_{i=0}^{3}|c_i|^2 = \frac{|\beta|^2}{|\beta|^2 + |\gamma|^2}\left(1 + \left(|\frac{\gamma}{\beta}|^2 - 1\right)\sum_{i=0}^{3}|c_i|^2 + 2[\text{real}(-\frac{\gamma}{\beta}\sum_{i=0}^{3}c_i c_{i+4}^*)]\right). \tag{30}$$

Ex. 3. For state $\frac{1}{2\sqrt{2}}(|000\rangle + |001\rangle + 010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle - |111\rangle))$, $\lambda_0^2 = 1/2, (\lambda_0')^2 = 1/4$. Therefore there are two SDs: $\left(\frac{1}{2}, 0, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$, and $\left(\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}\right)$

Ex. 4. For state $\frac{1}{2\sqrt{2}}(|000\rangle + |001\rangle + 010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle - i|111\rangle))$, $\lambda_0^2 = 1/2$, $(\lambda_0')^2 = 1/8$, there are two SDs: $\left(\frac{\sqrt{2}}{2}, \frac{\sqrt{5}}{4}e^{i(\pi - \arctan 2)}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$ and $\left(\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}e^{-i\frac{\pi}{4}}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$.

4.3 When $\alpha \neq 0$, $\gamma = 0$, *and* $\beta \neq 0$ *(Case 6, Table A.1)*

Eq. (11) reduces to $u_{00}^A(au_{00}^A + \beta u_{01}^A) = 0$, which has two solutions for U^A.

Solution 1. $u_{00}^A = 0$ and then $u_{01}^A = e^{i\phi}$. Then, obtain the following unitary matrix,

$$U^A = \begin{pmatrix} 0 & e^{i\phi} \\ e^{i\omega} & 0 \end{pmatrix}. \tag{31}$$

Solution 2. $u_{01}^A = -\frac{\alpha}{\beta}u_{00}^A$, where $u_{00}^A \neq 0$. Via the properties of the unitary matrix, a complicated calculation yields

$$U^{A'} = \frac{|\beta|}{\sqrt{|\beta|^2 + |\alpha|^2}} \begin{pmatrix} e^{i\phi} & -\frac{\alpha}{\beta}e^{i\phi} \\ \frac{\alpha^*}{\beta^*}e^{i\omega} & e^{i\omega} \end{pmatrix}. \tag{32}$$

For solution 1, via U^A in Eq. (31), clearly $L_0^A = e^{i\phi} C_1$. Let λ_0 be the non-zero singular value of L_0^A. A calculation yields

$$\lambda_0^2 = \sum_{i=4}^{7} |c_i|^2. \tag{33}$$

For solution 2, via $U^{A'}$ in Eq. (32), clearly $L_0^{A'} = \frac{|\beta| e^{i\phi}}{\sqrt{|\beta|^2+|\alpha|^2}} C_0 - \frac{\alpha}{\beta} \frac{|\beta| e^{i\phi}}{\sqrt{|\beta|^2+|\alpha|^2}} C_1$. Let λ_0' be the non-zero singular value of $L_0^{A'}$. A calculation yields

$$(\lambda_0')^2 = \frac{|\beta|^2}{|\beta|^2+|\gamma|^2} \left(\left(1 - |\frac{\alpha}{\beta}|^2\right) \sum_{i=0}^{3} |c_i|^2 + |\frac{\alpha}{\beta}|^2 + 2[\text{real}(-\frac{\alpha}{\beta} \sum_{i=0}^{3} c_i^* c_{i+4})] \right). \tag{34}$$

From Theorem 2, we obtain the following.

Corollary 3 When $\alpha \neq 0$, $\gamma = 0$, and $\beta \neq 0$, SD is unique if and only if

$$\sum_{i=4}^{7} |c_i|^2 = \frac{|\beta|^2}{|\beta|^2+|\gamma|^2} \left(\left(1 - |\frac{\alpha}{\beta}|^2\right) \sum_{i=0}^{3} |c_i|^2 + |\frac{\alpha}{\beta}|^2 + 2[\text{real}(-\frac{\alpha}{\beta} \sum_{i=0}^{3} c_i^* c_{i+4})] \right). \tag{35}$$

Ex. 5. For state $\frac{1}{2\sqrt{3}}(3|000\rangle + |011\rangle + \sqrt{2}|111\rangle)$ (from [14]), $\lambda_0^2 = 1/6$, $(\lambda_0')^2 = 1/2$. Therefore, there are two SDs. The two SDs are given by [30] as follows: $(1/\sqrt{6}, \sqrt{3}/6, 0, 0, \sqrt{3}/2)$ and $(\sqrt{2}/2, 1/2, 0, 0, 1/2)$. Here, we disregard the phases.

4.4 When $\alpha\gamma \neq 0$ (Cases 7.1 and 7.3, Table A.1)

For the case when $u_{01}^A = 0$, then $u_{00}^A \neq 0$ and $\det L_0^A = \alpha (u_{00}^A)^2 \neq 0$. Similarly, when $u_{00}^A = 0$, then $u_{01}^A \neq 0$ and $\det L_0^A = \gamma (u_{01}^A)^2 \neq 0$. So, for this case, clearly $u_{01}^A u_{00}^A \neq 0$ to make $\det L_0^A = 0$. Let $t = \frac{u_{00}^A}{u_{01}^A}$, therefore $t \neq 0$. Eq. (11) becomes

$$\alpha t^2 + \beta t + \gamma = 0. \tag{36}$$

From $u_{00}^A = u_{01}^A t$ and via the properties of a unitary matrix, a straightforward and complicated calculation yields

$$U^A = \begin{pmatrix} \frac{t}{\sqrt{|t|^2+1}} e^{i\phi} & \frac{1}{\sqrt{|t|^2+1}} e^{i\phi} \\ \frac{1}{\sqrt{|t|^2+1}} e^{i\omega} & -\frac{t^*}{\sqrt{|t|^2+1}} e^{i\omega} \end{pmatrix}. \tag{37}$$

For GHZ SLOCC class, $\tau \neq 0$. Thus, Eq. (36) has two solutions: $t = \frac{-\beta \pm \sqrt{\tau}}{2\alpha}$.

Solution 1. Let $p = \frac{-\beta + \sqrt{\tau}}{2\alpha}$. Via U^A in Eq. (37), clearly $L_0^A = \frac{p e^{i\phi}}{\sqrt{|p|^2+1}} C_0 + \frac{e^{i\phi}}{\sqrt{|p|^2+1}} C_1$. Let λ_0 be the non-zero singular value of L_0^A. A calculation yields

$$\lambda_0^2 = \frac{1}{|p|^2+1} \left(1 + \left(|p|^2 - 1\right) \sum_{i=0}^{3} |c_i|^2 + 2[\text{real}(p \sum_{i=0}^{3} c_i c_{i+4}^*)] \right). \tag{38}$$

Solution 2. Let $q = \frac{-\beta - \sqrt{\tau}}{2\alpha}$. Via U^A in Eq. (37), clearly $L_0^{A'} = \frac{q e^{i\phi}}{\sqrt{|q|^2+1}} C_0 + \frac{e^{i\phi}}{\sqrt{|q|^2+1}} C_1$. Let λ_0' be the non-zero singular value of $L_0^{A'}$. A calculation yields

$$(\lambda_0')^2 = \frac{1}{|q|^2+1}\left(1+(|q|^2-1)\sum_{i=0}^{3}|c_i|^2+2[\mathrm{real}(q\sum_{i=0}^{3}c_ic_{i+4}^*)]\right). \tag{39}$$

4.4.1 When $\alpha\beta\gamma\tau \neq 0$ (Case 7.3, Table A.1)

From Theorem 2 and Eqs. (38, 39) we obtain the following Corollary.

Corollary 4 When $\alpha\beta\gamma\tau \neq 0$, we can conclude that SD is unique if and only if

$$\begin{aligned} & \frac{1}{|p|^2+1}\left(1+\left(|p|^2-1\right)\sum_{i=0}^{3}|c_i|^2+2[\mathrm{real}(p\sum_{i=0}^{3}c_ic_{i+4}^*)]\right) \\ = & \frac{1}{|q|^2+1}\left(1+(|q|^2-1)\sum_{i=0}^{3}|c_i|^2+2[\mathrm{real}(q\sum_{i=0}^{3}c_ic_{i+4}^*)]\right). \end{aligned} \tag{40}$$

Ex. 6. For state $\frac{2}{\sqrt{10}}(|000\rangle+\frac{1}{2}(|011\rangle+|100\rangle)+|111\rangle)$, $\lambda_0^2=(\lambda_0')^2=9/50$. When ignoring the phase, it has a unique SD: $\frac{3\sqrt{2}}{10}|000\rangle-\frac{2}{5}\sqrt{2}|100\rangle+\frac{1}{\sqrt{2}}|111\rangle$.

Ex. 7. For state $\frac{1}{2\sqrt{2}}((\sqrt{2}+1)|000\rangle+|011\rangle-(\sqrt{2}-1)|100\rangle+|111\rangle)$. $\lambda_0^2=1/2$, $(\lambda_0')^2=1/6$. Therefore, it has two SDs (We ignore their phases) [30]: $(1/\sqrt{6},\sqrt{3}/6,0,0,\sqrt{3}/2)$, and $(\sqrt{2}/2,1/2,0,0,1/2)$.

Note that the state in Ex. 7 is LU equivalent to the state in Ex. 5.

4.4.2 when $\beta=0$ and $\alpha\gamma\neq 0$ (Case 7.1, Table A.1)

In this case, $t=\pm\sqrt{-\frac{\gamma}{\alpha}}$. Let $p=\sqrt{-\frac{\gamma}{\alpha}}$ and $q=-\sqrt{-\frac{\gamma}{\alpha}}$.

From Theorem 2 and Eqs. (38, 39) we obtain the following Corollary.

Corollary 5 When $\beta=0$ and $\alpha\gamma\neq 0$, SD is unique if and only if

$$\mathrm{real}\left(\sqrt{-\frac{\gamma}{\alpha}}\sum_{i=0}^{3}c_ic_{i+4}^*\right)=0. \tag{41}$$

Specially, when $\sum_{i=0}^{3}c_ic_{i+4}^*=0$, SD is unique. When all c_i are real, SD is unique if and only if $\sum_{i=0}^{3}c_ic_{i+4}=0$ or $\frac{\gamma}{\alpha}>0$.

Ex. 8. For the state $-p_1|001\rangle-p_2|010\rangle-p_3|100\rangle+q_0|111\rangle$, where $p_i, i=1,2,3$ and q_0 are non-zero real numbers, which corresponds to a black hole according to [31], one can see that $\sum_{i=0}^{3}c_ic_{i+4}=0$. Therefore, it has a unique SD.

5 A necessary condition for LU equivalence for GHZ SLOCC class

It is known that two states of the GHZ SLOCC class are considered LU equivalent if their SDs are the same, which requires computing the SD of each state. Now we can have a new necessary condition for LU equivalence for GHZ SLOCC class without actually computing the SD of the state.

Let $|\psi_1\rangle$ and $|\psi_2\rangle$ be two pure states of GHZ SLOCC class, $SD_1=(\lambda_0,\lambda_1e^{i\chi},\lambda_2,\lambda_3,\lambda_4)$ and $SD_1'=(\lambda_0',\lambda_1'e^{i\chi'},\lambda_2',\lambda_3',\lambda_4')$ be two SDs of $|\psi_1\rangle$. Note that SD_1 and SD_1' may be the same. Let $SD_2=(\eta_0,\eta_1e^{i\varphi},\eta_2,\eta_3,\eta_4)$ and $SD_2'=(\eta_0',\eta_1'e^{i\varphi'},\eta_2',\eta_3',\eta_4')$ be two SDs of $|\psi_2\rangle$.

Table 1. Values of $\alpha_A, \alpha_B,$ and α_C.

α_A	$J_2 + J_3 + J_4$
α_B	$J_1 + J_3 + J_4$
α_C	$J_1 + J_2 + J_4$

Note that SD_2 and SD_2' may be the same. We can compute λ_0, λ_0', η_0, and η_0' without transforming the states into SDs.

From Theorem 2, we get the following.

Theorem 3 If two states $|\psi_1\rangle$ and $|\psi_2\rangle$ of GHZ SLOCC class are LU equivalent, then the multisets $\{\lambda_0, \lambda_0'\} = \{\eta_0, \eta_0'\}$.

From Theorem 3, if $\{\lambda_0, \lambda_0'\} \neq \{\eta_0, \eta_0'\}$, then $|\psi_1\rangle$ and $|\psi_2\rangle$ are LU inequivalent.

6 Any state having the maximal vNEE must have a unique SD

vNEE is defined as

$$S(\rho) = -\sum \eta_i \ln \eta_i, \tag{42}$$

where $\eta_i \geq 0$ are the eigenvalues of ρ, and $\sum_i \eta_i = 1$. Note that $0 \ln 0 = 0$. In this section, we investigate the relation between the uniqueness of SD and the maximal vNEE. To this end, we explore what states with a unique SD have the maximal vNEE.

We use the notations $J_1 = |\lambda_1\lambda_4 e^{i\chi} - \lambda_2\lambda_3|^2$, $J_i = (\lambda_0\lambda_i)^2$, $i = 2, 3, 4$, where J_i, $i = 1, 2, 3, 4$, are LU invariant and defined in [8]. It is known that $\rho_A = (tr_{BC})(\rho_{ABC})$, where ρ_{ABC} is the density matrix.

We derived vNEE $S(\rho_\mu)$ for the states of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ in Eq.(14), where $\mu \in \{A, B, C\}$ as follows [34].

$$S(\rho_\mu) = -\left(\tfrac{1+\sqrt{1-4\alpha_\mu}}{2} \ln \tfrac{1+\sqrt{1-4\alpha_\mu}}{2} + \tfrac{1-\sqrt{1-4\alpha_\mu}}{2} \ln \tfrac{1-\sqrt{1-4\alpha_\mu}}{2}\right) \tag{43}$$

where $0 \leq \alpha_\mu \leq 1/4$. (see Table 1.) We showed that $S(\rho_\mu)$ increases strictly monotonically as α_μ increases. Thus, $S(\rho_\mu) = \ln 2$ if and only if $\alpha_\mu = 1/4$. It is well known that the maximal vNEE is $\ln 2$.

We calculated the maximal vNEE for real states $(\lambda_0, \pm\lambda_1, \lambda_2, \lambda_3, \lambda_4)$ of GHZ SLOCC class in [36], and will compute the maximal vNEE for complex states $(\lambda_0, \lambda_1 e^{i\phi}, \lambda_2, \lambda_3, \lambda_4)$ of GHZ SLOCC class below. We give all the SD states that have the maximal vNEE and a unique SD and also give all the SD states that have a unique SD in Appendix C.

6.1 *The states having the maximal vNEE* $S(\rho_A) = S(\rho_B) = S(\rho_C) = \ln 2$ *have a unique SD which is GHZ state*

It is known that a state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ in Eq.(14) has the maximal vNEE $S(\rho_A) = S(\rho_B) = S(\rho_C) = \ln 2$ if and only if the state is GHZ state [34]. Generally, for any state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$, it has the maximal vNEE $S(\rho_A) = S(\rho_B) = S(\rho_C) = \ln 2$ if and only if it has a unique SD GHZ state.

6.2 The states having the maximal vNEE $S(\rho_A) = \ln 2$ while $S(\rho_B) < \ln 2$ and $S(\rho_C) < \ln 2$ have a unique SD

First consider the states of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ in Eq.(14). Since $S(\rho_A) = \ln 2$, $\alpha_A = 1/4$. Thus, we have the following equation.

$$\alpha_A = J_2 + J_3 + J_4 = 1/4. \tag{44}$$

From Eq. (44), obtain

$$\lambda_0^2(\lambda_2^2 + \lambda_3^2 + \lambda_4^2) = \lambda_0^2(1 - \lambda_0^2 - \lambda_1^2) = 1/4, \tag{45}$$

and then

$$\lambda_0^4 - \lambda_0^2(1 - \lambda_1^2) + 1/4 = 0. \tag{46}$$

The above equation has solutions for λ_0^2 if and only if the discriminant $(1-\lambda_1^2)^2 - 1 \geq 0$, i.e., $(1-\lambda_1^2)^2 \geq 1$. Clearly, $(1-\lambda_1^2)^2 \geq 1$ if and only if $\lambda_1 = 0$. Then, obtain

$$\lambda_1 = 0, \lambda_0 = 1/\sqrt{2} \tag{47}$$

and the state:

$$|\kappa\rangle = \frac{1}{\sqrt{2}}|000\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle, \tag{48}$$

where $\lambda_2\lambda_3 \neq 0$.

Thus, we show that if a state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_A) = \ln 2$ while $S(\rho_B) < \ln 2$ and $S(\rho_C) < \ln 2$, then the state must be $|\kappa\rangle$. One can verify that $|\kappa\rangle$ has a unique SD, i.e., itself, and for the state $|\kappa\rangle$, $\alpha_A = 1/4$ and so $S(\rho_A) = \ln 2$. We calculate $S(\rho_B)$ and $S(\rho_C)$ for $|\kappa\rangle$ as follows. $\alpha_B = J_1 + J_3 + J_4 = \lambda_2^2\lambda_3^2 + \frac{1}{2}\lambda_3^2 + \frac{1}{2}\lambda_4^2 < \frac{1}{2}(\lambda_2^2 + \lambda_3^2 + \lambda_4^2) = \frac{1}{4}$. Similarly, $\alpha_C < \frac{1}{4}$. So, $S(\rho_B) < \ln 2$ and $S(\rho_C) < \ln 2$.

Generally, for any state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$ of three qubits, if it has the maximal vNEE $S(\rho_A)$ $(= \ln 2)$ while $S(\rho_B) < \ln 2$ and $S(\rho_C) < \ln 2$, then its SD has the same vNEE. Clearly, the SD must be $|\kappa\rangle$. Thus, $|\psi\rangle$ has a unique SD (i.e., $|\kappa\rangle$). Conversely, if $|\psi\rangle$ has a SD $|\kappa\rangle$, then $|\psi\rangle$ also has the maximal vNEE $S(\rho_A) = \ln 2$ while $S(\rho_B) < \ln 2$ and $S(\rho_C) < \ln 2$.

We can conclude (i). The state $|\kappa\rangle$ has a unique SD. (ii). The state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ in Eq.(14) has the maximal vNEE $S(\rho_A) = \ln 2$ while $S(\rho_B) < \ln 2$ and $S(\rho_C) < \ln 2$ if and only if the state is $|\kappa\rangle$. (iii). For any state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$, it has the maximal vNEE $S(\rho_A) = \ln 2$ while $S(\rho_B) < \ln 2$ and $S(\rho_C) < \ln 2$ if and only if it has a unique SD $|\kappa\rangle$.

6.3 The states having the maximal vNEE $S(\rho_A) = S(\rho_B) = \ln 2$ while $S(\rho_C) < \ln 2$ have a unique SD

First consider the state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ in Eq.(14). Since $S(\rho_A) = S(\rho_B) = \ln 2$, then we have the following equations

$$\alpha_A = J_2 + J_3 + J_4 = 1/4, \tag{49}$$

$$\alpha_B = J_1 + J_3 + J_4 = 1/4. \tag{50}$$

Then, from the above, obtain

$$J_1 = J_2. \tag{51}$$

Similarly, from Eq. (49) we obtain

$$\lambda_1 = 0, \lambda_0 = 1/\sqrt{2}. \tag{52}$$

From Eqs. (51, 52),

$$\lambda_2\lambda_3 = \lambda_0\lambda_2 = \frac{1}{\sqrt{2}}\lambda_2. \tag{53}$$

From Eq. (53), If $\lambda_2 \neq 0$, then $\lambda_3 = \frac{1}{\sqrt{2}}$. However, it is impossible because $\sum_{i=0}^{4} \lambda_i^2 = 1$. Therefore, $\lambda_2 = 0$ and then, we obtain

$$|\varpi\rangle = \frac{1}{\sqrt{2}}|000\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle, \tag{54}$$

where $\lambda_3 \neq 0$.

Thus, we show that if a state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_A) = S(\rho_B) = \ln 2$ while $S(\rho_C) < \ln 2$, then the state must be $|\varpi\rangle$. One can verify that $|\varpi\rangle$ satisfies Eq. (26). It means $|\varpi\rangle$ has a unique SD, i.e., itself. A calculation yields that $S(\rho_A) = S(\rho_B) = \ln 2$ for $|\varpi\rangle$. Since $\lambda_3 \neq 0$, $S(\rho_C) < \ln 2$.

Similarly, we can conclude:

(i). $|\varpi\rangle$ has a unique SD.

(ii). The state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_A) = S(\rho_B) = \ln 2$ while $S(\rho_C) < \ln 2$ if and only if the state is $|\varpi\rangle$.

(iii). For any state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$, it has the maximal vNEE $S(\rho_A) = S(\rho_B) = \ln 2$ while $S(\rho_C) < \ln 2$ if and only if it has a unique SD $|\varpi\rangle$.

6.4 The states having the maximal vNEE $S(\rho_A) = S(\rho_C) = \ln 2$ and $S(\rho_B) < \ln 2$ have a unique SD

First consider the state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ in Eq.(14). Since $S(\rho_A) = S(\rho_C) = \ln 2$, then we have the following equations:

$$\alpha_A = J_2 + J_3 + J_4 = 1/4, \tag{55}$$

$$\alpha_C = J_1 + J_2 + J_4 = 1/4. \tag{56}$$

Then, from the above two equations, obtain

$$J_1 = J_3. \tag{57}$$

Similarly, from Eq. (55), obtain

$$\lambda_1 = 0, \lambda_0 = 1/\sqrt{2} \tag{58}$$

From Eqs. (57, 58),

$$\lambda_2\lambda_3 = \lambda_0\lambda_3 = \frac{1}{\sqrt{2}}\lambda_3. \tag{59}$$

From the above equation, one can see that if $\lambda_3 \neq 0$ then $\lambda_2 = \frac{1}{\sqrt{2}}$. It is impossible. So, $\lambda_3 = 0$. Then, obtain the following state

$$|\xi\rangle = \frac{1}{\sqrt{2}}|000\rangle + \lambda_2|101\rangle + \lambda_4|111\rangle, \tag{60}$$

where $\lambda_2 \neq 0$.

Thus, we show that if a state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_A) = S(\rho_C) = \ln 2$ while $S(\rho_B) < \ln 2$, then the state must be $|\xi\rangle$. A calculation yields that $S(\rho_A) = S(\rho_C) = \ln 2$ for $|\xi\rangle$. Since $\lambda_2 \neq 0$, $S(\rho_B) < \ln 2$.

Similarly, we can conclude (i). $|\xi\rangle$ has a unique SD. because $|\xi\rangle$ satisfies Eq. (26), (ii). The state in the form of $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_A) = S(\rho_C) = \ln 2$ while $S(\rho_B) < \ln 2$ if and only if the state is $|\xi\rangle$. (iii). For any state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$, it has the maximal vNEE $S(\rho_A) = S(\rho_C) = \ln 2$ while $S(\rho_B) < \ln 2$ if and only if it has a unique SD $|\xi\rangle$.

6.5 The states having the maximal vNEE $S(\rho_B) = S(\rho_C) = \ln 2$ while $S(\rho_A) < \ln 2$ have a unique SD

First consider the state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ in Eq.(14). Clearly, that $S(\rho_B) = S(\rho_C) = \ln 2$ implies

$$\alpha_B = J_1 + J_3 + J_4 = 1/4 \tag{61}$$

$$\alpha_C = J_1 + J_2 + J_4 = 1/4 \tag{62}$$

Then from Eqs. (61, 62), obtain $J_2 = J_3$, and then $\lambda_2 = \lambda_3$. From the definition of α_B, obtain

$$\lambda_1^2\lambda_4^2 - 2\lambda_1\lambda_2^2\lambda_4\cos\phi + \lambda_2^4 + \lambda_0^2\lambda_2^2 + \lambda_0^2\lambda_4^2 - 1/4 = 0 \tag{63}$$

Note that $\sum_{i=0}^4 \lambda_i^2 = 1$. By substituting λ_0 with $(1 - (\lambda_1^2 + 2\lambda_2^2 + \lambda_4^2))$, obtain from Eq. (63)

$$\lambda_1^2\lambda_2^2 + 2(\cos\phi)\lambda_1\lambda_2^2\lambda_4 + \lambda_2^4 + 3\lambda_2^2\lambda_4^2 - \lambda_2^2 + \lambda_4^4 - \lambda_4^2 + \frac{1}{4} = 0 \tag{64}$$

Case 1. $\lambda_2 = 0$. Eq. (64) becomes $\lambda_4^4 - \lambda_4^2 + \frac{1}{4} = 0$. Then, obtain

$$\lambda_4 = \frac{1}{\sqrt{2}}. \tag{65}$$

Thus, obtain

$$|\zeta\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\phi}|100\rangle + \frac{1}{\sqrt{2}}|111\rangle, \tag{66}$$

where $\lambda_1 \neq 0$. One can verify that $|\zeta\rangle$ has a unique SD, i.e., itself.

Case 2. $\lambda_2 \neq 0$. We next show that Eq. (64) does not have a solution for λ_1 whenever $\lambda_2 \neq 0$.

To solve λ_1 from Eq. (64), let the discriminant

$$\begin{aligned}\Delta &= (2(\cos\phi)\lambda_2^2\lambda_4)^2 - 4\lambda_2^2(\lambda_2^4 + 3\lambda_2^2\lambda_4^2 - \lambda_2^2 + \lambda_4^4 - \lambda_4^2 + \frac{1}{4}) \\ &= \lambda_2^2\left(4\lambda_2^2 - 4\lambda_2^4 + 4\lambda_4^2 - 4\lambda_4^4 - 12\lambda_2^2\lambda_4^2 + 4\lambda_2^2\lambda_4^2\cos^2\phi - 1\right). \end{aligned} \tag{67}$$

Case 2.1. $\cos^2\phi = 1$. Eq. (67) becomes

$$\begin{aligned} \Delta &= \lambda_2^2\left(4\lambda_2^2 - 4\lambda_2^4 + 4\lambda_4^2 - 4\lambda_4^4 - 12\lambda_2^2\lambda_4^2 + 4\lambda_2^2\lambda_4^2 - 1\right) \\ &= -\lambda_2^2\left(2\lambda_2^2 + 2\lambda_4^2 - 1\right)^2. \end{aligned} \tag{68}$$

Let $\Delta = 0$ in Eq. (68). Then, obtain $2\lambda_2^2 + 2\lambda_4^2 = 1$. From Eq. (64), obtain

$$\lambda_1 = -(\cos\phi)\lambda_4 = \lambda_4, \tag{69}$$

where $\phi = \pi$.

From $\sum_{i=0}^4 \lambda_i^2 = 1$, $2\lambda_2^2 + 2\lambda_4^2 = 1$, and $\lambda_1 = \lambda_4$, obtain

$$\lambda_0^2 = 1 - (\lambda_1^2 + 2\lambda_2^2 + \lambda_4^2) = 1 - (2\lambda_2^2 + 2\lambda_4^2) = 0. \tag{70}$$

It is impossible for $\lambda_0 = 0$ because $\lambda_0\lambda_4 \neq 0$ for GHZ SLOCC class.

Case 2.2. $\cos^2\phi < 1$. Eq. (67) becomes

$$\begin{aligned} \Delta &= \lambda_2^2\left(4\lambda_2^2 - 4\lambda_2^4 + 4\lambda_4^2 - 4\lambda_4^4 - 12\lambda_2^2\lambda_4^2 + 4\lambda_2^2\lambda_4^2\cos^2\phi - 1\right) \\ &< \lambda_2^2\left(4\lambda_2^2 - 4\lambda_2^4 + 4\lambda_4^2 - 4\lambda_4^4 - 12\lambda_2^2\lambda_4^2 + 4\lambda_2^2\lambda_4^2 - 1\right) \\ &= -\lambda_2^2\left(2\lambda_2^2 + 2\lambda_4^2 - 1\right)^2. \end{aligned} \tag{71}$$

Clearly, $\Delta < 0$ for the subcase. Therefore, Eq. (64) does not have a solution for λ_1 for the subcase.

Thus, we show that if a state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_B) = S(\rho_C) = \ln 2$ while $S(\rho_A) < \ln 2$, then the state must be $|\zeta\rangle$. A calculation yields that $S(\rho_B) = S(\rho_C) = \ln 2$ for $|\zeta\rangle$. Since $\lambda_1 \neq 0$, $S(\rho_A) < \ln 2$ for $|\zeta\rangle$.

We can conclude (i). $|\zeta\rangle$ has a unique SD, i.e., itself,. (ii). The state in the form of $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_B) = S(\rho_C) = \ln 2$ while $S(\rho_A) < \ln 2$ if and only if the state is $|\zeta\rangle$. (iii). For any state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$, it has the maximal vNEE $S(\rho_B) = S(\rho_C) = \ln 2$ while $S(\rho_A) < \ln 2$ if and only if it has a unique SD $|\zeta\rangle$.

6.6 *The states having the maximal vNEE* $S(\rho_B) = \ln 2$ *while* $S(\rho_A) < \ln 2$ *and* $S(\rho_C) < \ln 2$ *have a unique SD*

Clearly, that $S(\rho_B) = \ln 2$ implies

$$\alpha_B = J_1 + J_3 + J_4 = 1/4 \tag{72}$$

From Eq. (72), obtain

$$\lambda_1^2\lambda_4^2 - 2\lambda_1\lambda_2\lambda_3\lambda_4\cos\phi + \lambda_2^2\lambda_3^2 + \lambda_0^2\lambda_3^2 + \lambda_0^2\lambda_4^2 - 1/4 = 0 \tag{73}$$

Note that $\sum_{i=0}^4 \lambda_i^2 = 1$. By substituting λ_0^2 with $(1 - (\lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2))$, from Eq. (73), obtain

$$\lambda_1^2\lambda_3^2 + 2(\cos\phi)\lambda_1\lambda_2\lambda_3\lambda_4 + \lambda_2^2\lambda_4^2 + \lambda_3^4 + 2\lambda_3^2\lambda_4^2 - \lambda_3^2 + \lambda_4^4 - \lambda_4^2 + \frac{1}{4} = 0 \tag{74}$$

Case 1 $\lambda_3 = 0$. Eq. (74) becomes

$$\lambda_2^2\lambda_4^2 + (\lambda_4^2 - 1/2)^2 = 0 \tag{75}$$

From Eq. (75), obtain $\lambda_2 = 0$ and $\lambda_4^2 = 1/2$ and

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\phi}|000\rangle + \frac{1}{\sqrt{2}}|111\rangle. \tag{76}$$

It is known that $S(\rho_B) = S(\rho_C) = \ln 2$ for the state in Eq. (76).
Case 2. $\lambda_3 \neq 0$.
Case 2.1. $\lambda_2 = 0$. Eq. (74) becomes

$$\lambda_4^4 + 2\lambda_3^2\lambda_4^2 - \lambda_4^2 + \lambda_1^2\lambda_3^2 + \lambda_3^4 - \lambda_3^2 + \frac{1}{4} = 0. \tag{77}$$

To solve λ_4^2 from Eq. (77), let the discriminant

$$\Delta = (2\lambda_3^2 - 1)^2 - 4(\lambda_1^2\lambda_3^2 + \lambda_3^4 - \lambda_3^2 + \frac{1}{4}) = -4\lambda_1^2\lambda_3^2. \tag{78}$$

Let $\Delta = 0$ in Eq. (78). Then, obtain $\lambda_1 = 0$. From Eq. (77), obtain $\lambda_4^2 = \frac{1}{2} - \lambda_3^2$. Then, $\lambda_0^2 = 1/2$. Thus, obtain

$$|\psi\rangle = \frac{1}{\sqrt{2}}|000\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle. \tag{79}$$

It is known that $S(\rho_A) = S(\rho_B) = \ln 2$ for the state in Eq. (79).
Case 2.2. $\lambda_2 \neq 0$. To solve λ_1 from Eq. (74), let the discriminant

$$\begin{aligned}\Delta &= (2(\cos\phi)\lambda_2\lambda_3\lambda_4)^2 - 4\lambda_3^2(\lambda_2^2\lambda_4^2 + \lambda_3^4 + 2\lambda_3^2\lambda_4^2 - \lambda_3^2 + \lambda_4^4 - \lambda_4^2 + \frac{1}{4}) \\ &= \lambda_3^2\left(4\lambda_3^2 + 4\lambda_4^2 - 4\lambda_3^4 - 4\lambda_4^4 - 4\lambda_2^2\lambda_4^2 - 8\lambda_3^2\lambda_4^2 + 4\lambda_2^2\lambda_4^2\cos^2\phi - 1\right).\end{aligned} \tag{80}$$

Case 2.2.1. $\cos^2\phi = 1$. Eq. (80) becomes

$$\Delta = -\lambda_3^2\left(2\lambda_3^2 + 2\lambda_4^2 - 1\right)^2. \tag{81}$$

Let $\Delta = 0$ in Eq. (81). Then, obtain $2\lambda_3^2 + 2\lambda_4^2 - 1 = 0$ and $\lambda_1 = \frac{-2(\cos\phi)\lambda_2\lambda_3\lambda_4}{2\lambda_3^2} = \frac{\lambda_2\lambda_4}{\lambda_3}$ from Eq. (74), where $\cos\phi = -1$. Then, $\lambda_0^2 = \frac{\lambda_3^2 - \lambda_2^2}{2\lambda_3^2}$ from $\lambda_0^2 + \lambda_1^2 + \lambda_2^2 = 1/2$. Under that $2\lambda_3^2 + 2\lambda_4^2 = 1$, $\lambda_3 > \lambda_2$, and $\lambda_i \neq 0$, $i = 2, 3$, obtain

$$|\pi\rangle = \lambda_0|000\rangle - \frac{\lambda_2\lambda_4}{\lambda_3}|100\rangle + \lambda_2|101\rangle + \lambda_3|101\rangle + \lambda_4|111\rangle. \tag{82}$$

One can verify $S(\rho_B) = \ln 2$ for $|\pi\rangle$ in Eq. (82). Since $\lambda_2\lambda_3 \neq 0$, $S(\rho_C) < \ln 2$ (ref. the state $|\zeta\rangle$) and $S(\rho_A) < \ln 2$ (ref. the state $|\varpi\rangle$). One can also check that $|\pi\rangle$ has a unique SD, i.e., itself.
Case 2.2.2. $\cos^2\phi < 1$. From Eq. (80),

$$\begin{aligned}\Delta &= \lambda_3^2\left(4\lambda_3^2 + 4\lambda_4^2 - 4\lambda_3^4 - 4\lambda_4^4 - 4\lambda_2^2\lambda_4^2 - 8\lambda_3^2\lambda_4^2 + 4\lambda_2^2\lambda_4^2\cos^2\phi - 1\right) \\ &< \lambda_3^2\left(4\lambda_3^2 + 4\lambda_4^2 - 4\lambda_3^4 - 4\lambda_4^4 - 4\lambda_2^2\lambda_4^2 - 8\lambda_3^2\lambda_4^2 + 4\lambda_2^2\lambda_4^2 - 1\right) \\ &= -\lambda_3^2\left(2\lambda_3^2 + 2\lambda_4^2 - 1\right)^2.\end{aligned} \tag{83}$$

Clearly, $\Delta < 0$ for the subcase. Therefore, Eq. (74) does not have a solution for λ_1 for the subcase.

Thus, we show that if a state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_B) = \ln 2$ while $S(\rho_A) < \ln 2$ and $S(\rho_C) < \ln 2$, then the state must be $|\pi\rangle$.

Similarly, we can conclude (i). $|\pi\rangle$ has a unique SD, i.e., itself. (ii). The state in the form of $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_B) = \ln 2$ while $S(\rho_A) < \ln 2$ and $S(\rho_C) < \ln 2$ if and only if the state is $|\pi\rangle$. (iii). For any state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$, it has the maximal vNEE $S(\rho_B) = \ln 2$ while $S(\rho_A) < \ln 2$ and $S(\rho_C) < \ln 2$ if and only if it has a unique SD $|\pi\rangle$.

6.7 The states having the maximal vNEE $S(\rho_C) = \ln 2$ *while* $S(\rho_A) < \ln 2$ *and* $S(\rho_B) < \ln 2$ *have a unique SD*

Proof. Clearly, that $S(\rho_C) = \ln 2$ implies

$$\alpha_C = J_1 + J_2 + J_4 = 1/4 \tag{84}$$

From Eq. (84), obtain

$$\lambda_1^2\lambda_4^2 - 2\lambda_1\lambda_2\lambda_3\lambda_4 \cos\phi + \lambda_2^2\lambda_3^2 + \lambda_0^2\lambda_2^2 + \lambda_0^2\lambda_4^2 - 1/4 = 0 \tag{85}$$

Note that $\sum_{i=0}^4 \lambda_i^2 = 1$. Substituting λ_0^2 with $(1 - (\lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2))$ in Eq. (85), obtain

$$\lambda_1^2\lambda_2^2 + 2(\cos\phi)\lambda_1\lambda_2\lambda_3\lambda_4 + \lambda_2^4 + 2\lambda_2^2\lambda_4^2 - \lambda_2^2 + \lambda_3^2\lambda_4^2 + \lambda_4^4 - \lambda_4^2 + \frac{1}{4} = 0 \tag{86}$$

Case 1. $\lambda_2 = 0$.

Eq. (86) becomes

$$\lambda_3^2\lambda_4^2 + (\lambda_4^2 - 1/2)^2 = 0 \tag{87}$$

Then, $\lambda_3 = 0$ and $\lambda_4^2 = 1/2$ from Eq. (87). Thus,

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\phi}|000\rangle + \frac{1}{\sqrt{2}}|111\rangle. \tag{88}$$

It is known that $S(\rho_B) = S(\rho_C) = \ln 2$ for the state in Eq. (88).

Case 2. $\lambda_2 \neq 0$.

Case 2.1. $\lambda_3 = 0$. Eq. (86) becomes

$$\lambda_4^4 + 2\lambda_2^2\lambda_4^2 - \lambda_4^2 + \lambda_1^2\lambda_2^2 + \lambda_2^4 - \lambda_2^2 + \frac{1}{4} = 0 \tag{89}$$

To solve λ_4^2 from Eq. (89), let the discriminant

$$\Delta = (2\lambda_2^2 - 1)^2 - 4(\lambda_1^2\lambda_2^2 + \lambda_2^4 - \lambda_2^2 + \frac{1}{4}) = -4\lambda_1^2\lambda_2^2. \tag{90}$$

Let $\Delta = 0$ in Eq. (90). Then, obtain $\lambda_1 = 0$. From Eq. (89), $\lambda_4^2 = \frac{1}{2} - \lambda_2^2$. Then, $\lambda_0 = 1/\sqrt{2}$. Thus, obtain

$$|\psi\rangle = \frac{1}{\sqrt{2}}|000\rangle + \lambda_2|101\rangle + \lambda_4|111\rangle. \tag{91}$$

It is known that $S(\rho_A) = S(\rho_C) = \ln 2$ for the state in Eq. (91).

Case 2.2. $\lambda_3 \neq 0$. To solve λ_1 from Eq. (86), let the discriminant Δ for λ_1

$$\begin{aligned}\Delta &= (2(\cos\phi)\lambda_2\lambda_3\lambda_4)^2 - 4\lambda_2^2(\lambda_2^4 + 2\lambda_2^2\lambda_4^2 - \lambda_2^2 + \lambda_3^2\lambda_4^2 + \lambda_4^4 - \lambda_4^2 + \frac{1}{4}) \\ &= \lambda_2^2\left(4\lambda_2^2 - 4\lambda_2^4 + 4\lambda_4^2 - 4\lambda_4^4 - 8\lambda_2^2\lambda_4^2 - 4\lambda_3^2\lambda_4^2 + 4\lambda_3^2\lambda_4^2\cos^2\phi - 1\right) \qquad (92)\end{aligned}$$

Case 2.2.1. $\cos^2\phi = 1$. Eq. (92) becomes

$$\begin{aligned}\Delta &= \lambda_2^2\left(4\lambda_2^2 - 4\lambda_2^4 + 4\lambda_4^2 - 4\lambda_4^4 - 8\lambda_2^2\lambda_4^2 - 4\lambda_3^2\lambda_4^2 + 4\lambda_3^2\lambda_4^2 - 1\right) \\ &= -\lambda_2^2\left(2\lambda_2^2 + 2\lambda_4^2 - 1\right)^2. \qquad (93)\end{aligned}$$

Let $\Delta = 0$ in Eq. (93). Then, obtain $2\lambda_2^2 + 2\lambda_4^2 - 1 = 0$. From Eq. (86), obtain $\lambda_1 = \frac{-2(\cos\phi)\lambda_2\lambda_3\lambda_4}{2\lambda_2^2} = \frac{\lambda_3\lambda_4}{\lambda_2}$, where $\cos\phi = -1$. Then, $\lambda_0^2 = \frac{1}{2\lambda_2^2}\left(\lambda_2^2 - \lambda_3^2\right)$. So, under that $\lambda_2 > \lambda_3$, $2\lambda_2^2 + 2\lambda_4^2 = 1$, $\lambda_i \neq 0$, $i = 2, 3$, obtain

$$|\varkappa\rangle = \lambda_0|000\rangle - \frac{\lambda_3\lambda_4}{\lambda_2}|100\rangle + \lambda_2|101\rangle + \lambda_3|101\rangle + \lambda_4|111\rangle. \qquad (94)$$

One can verify that $S(\rho_C) = \ln 2$ for $|\varkappa\rangle$ in Eq. (94). Since $\lambda_2\lambda_3 \neq 0$, $S(\rho_A) < \ln 2$ (ref. the state $|\xi\rangle$) and $S(\rho_B) < \ln 2$ (ref. the state $|\zeta\rangle$). One can also check that $|\varkappa\rangle$ has a unique SD, i.e., itself.

Case 2.2.2. $\cos^2\phi < 1$. Eq. (92) becomes

$$\begin{aligned}\Delta &= \lambda_2^2\left(4\lambda_2^2 - 4\lambda_2^4 + 4\lambda_4^2 - 4\lambda_4^4 - 8\lambda_2^2\lambda_4^2 - 4\lambda_3^2\lambda_4^2 + 4\lambda_3^2\lambda_4^2\cos^2\phi - 1\right) \\ &< \lambda_2^2\left(4\lambda_2^2 - 4\lambda_2^4 + 4\lambda_4^2 - 4\lambda_4^4 - 8\lambda_2^2\lambda_4^2 - 4\lambda_3^2\lambda_4^2 + 4\lambda_3^2\lambda_4^2 - 1\right) \\ &= -\lambda_2^2\left(2\lambda_2^2 + 2\lambda_4^2 - 1\right)^2 \qquad (95)\end{aligned}$$

Clearly, $\Delta < 0$ for the subcase. Therefore, Eq. (86) does not have a solution for λ_1 for the subcase.

Thus, we show that if a state of the form $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_C) = \ln 2$ while $S(\rho_A) < \ln 2$ and $S(\rho_B) < \ln 2$, then the state must be $|\varkappa\rangle$.

Similarly, we can conclude (i). $|\varkappa\rangle$ has a unique SD, i.e., itself. (ii). The state in the form of $(\lambda_0, \lambda_1 e^{i\chi}, \lambda_2, \lambda_3, \lambda_4)$ has the maximal vNEE $S(\rho_C) = \ln 2$ while $S(\rho_A) < \ln 2$ and $S(\rho_B) < \ln 2$ if and only if the state is $|\varkappa\rangle$. (iii). For any state $|\psi\rangle = \sum_{i,j,k} c_{ijk}|ijk\rangle$, it has the maximal vNEE $S(\rho_C) = \ln 2$ while $S(\rho_A) < \ln 2$ and $S(\rho_B) < \ln 2$ if and only if it has a unique SD $|\varkappa\rangle$.

7 Summary

It is not hard to understand the uniqueness of SD for three qubits for the five SLOCC classes except for the GHZ SLOCC class. In this paper, we propose a necessary and sufficient condition for the uniqueness of SD for three qubits for the GHZ SLOCC class. By the condition, one can determine whether a three-qubit state has one or two SDs without actually performing the Schmidt decomposition.

We also explore the relation between the uniqueness of SD and the maximal vNEE. To this end, we prove that any state having the maximal vNEE $S(\rho_x) = \ln 2$, $x = A, B$, or C must have a unique SD. Therefore, we should not choose a state having two SDs for its maximal vNEE for quantum information theory.

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Appendix A . Calculating U^A

For each case for the values of α, β, γ, and τ in Eqs. (7, 8, 9, 10), we give a simple and symmetric U^A in Table A.1 which satisfies the equation $\det L_0^A = 0$. For cases 1-4, $U^A = I$ (the identity). For cases 5 and 6, $U^A = \sigma_x$ (the Pauli operator). We derive U^A for Case 7 below.

Case 7. $\alpha \neq 0$ and $\gamma \neq 0$.

For the case, when $u_{01}^A = 0$, then $u_{00}^A \neq 0$ and Eq. (11) reduces to that $\det L_0^A = \alpha(u_{00}^A)^2 \neq 0$. Similarly, when $u_{00}^A = 0$, then $u_{01}^A \neq 0$ and Eq. (11) reduces to that $\det L_0^A = \gamma(u_{01}^A)^2 \neq 0$. So, for the case, clearly $u_{01}^A u_{00}^A \neq 0$ to make $\det L_0^A = 0$. Let $t = \frac{u_{00}^A}{u_{01}^A}$. Then, $t \neq 0$ and Eq. (11) becomes

$$\alpha t^2 + \beta t + \gamma = 0.$$

Then, from $u_{00}^A = u_{01}^A t$ and via the properties of a unitary matrix, a straightforward and complicated calculation yields

$$U^A = \begin{pmatrix} \frac{t}{\sqrt{|t|^2+1}} & \frac{1}{\sqrt{|t|^2+1}} \\ \frac{1}{\sqrt{|t|^2+1}} & -\frac{t^*}{\sqrt{|t|^2+1}} \end{pmatrix}. \tag{A.1}$$

Case 7.1. $\beta = 0$.

Eq. (36) has two solutions:

$$t = \frac{\pm\sqrt{-\alpha\gamma}}{\alpha}, \tag{A.2}$$

from which we can obtain two solutions for U^A.

Case 7.2. $\beta \neq 0$ but $\tau = 0$.

Eq. (36) has one solution

$$t = -\frac{\beta}{2\alpha}, \tag{A.3}$$

from which we obtain a unique U^A.

Case 7.3. $\beta \neq 0$ but $\tau \neq 0$.

Eq. (36) has two solutions:

$$t = \frac{-\beta \pm \sqrt{\tau}}{2\alpha}, \tag{A.4}$$

from which we obtain two solutions for U^A.

Table A.1 lists the number of solutions for Eq. (11), which is also the number of solutions for U^A, in all cases.

Table A.1. The number of solutions for U^A

cases	α	γ	β	τ	num_sol	SLOCC classes	U^A
1	0	0	0	0	infinite	B-AC,C-AB,A-B-C	I
2	0	0	$\neq 0$	$\neq 0$	2	GHZ	I
3	0	$\neq 0$	0	0	1	W or A-BC	I
4	0	$\neq 0$	$\neq 0$	$\neq 0$	2	GHZ	I
5	$\neq 0$	0	0	0	1	W or A-BC	σ_x
6	$\neq 0$	0	$\neq 0$	$\neq 0$	2	GHZ	σ_x
7.1	$\neq 0$	$\neq 0$	0	$\neq 0$	2	GHZ	Eq.(A.1,A.2)
7.2	$\neq 0$	$\neq 0$	$\neq 0$	0	1	W or A-BC	Eq.(A.1,A.3)
7.3	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	2	GHZ	Eq.(A.1,A.4)

Appendix B . SVD for degenerate 2 by 2 matrices L_0^A

Let $M = L_0^A$ from Eq. (5).

Case 1. $M = 0$. We choose $U = V = I$. Clearly, $UMV = 0$.

Case 2. Just three entries of M vanish. In the following, ϕ is real and $r > 0$. Let $\Sigma = diag(r, 0)$, $U = \begin{pmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{pmatrix}$, and $U' = \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}$.

Case 2.1. $M = \begin{pmatrix} re^{i\phi} & 0 \\ 0 & 0 \end{pmatrix}$. Then, $UMI = \Sigma$.

Case 2.2. $M = \begin{pmatrix} 0 & re^{i\phi} \\ 0 & 0 \end{pmatrix}$. Then, $UM\sigma_x = \Sigma$.

Case 2.3. $M = \begin{pmatrix} 0 & 0 \\ re^{i\phi} & 0 \end{pmatrix}$. Then, $U'MI = \Sigma$.

Case 2.4. $M = \begin{pmatrix} 0 & 0 \\ 0 & re^{i\phi} \end{pmatrix}$. Then, $U'M\sigma_x = \Sigma$.

Case 3. Just two entries of M vanish. Let

$$\Pi = \begin{pmatrix} \frac{a^*}{\sqrt{aa^*+bb^*}} & \frac{b^*}{\sqrt{aa^*+bb^*}} \\ \frac{b^*}{\sqrt{aa^*+bb^*}} & -\frac{a\frac{b^*}{b}}{\sqrt{aa^*+bb^*}} \end{pmatrix}, \tag{B.1}$$

$$D = \begin{pmatrix} \sqrt{aa^*+bb^*} & 0 \\ 0 & 0 \end{pmatrix}. \tag{B.2}$$

Case 3.1. $M = \begin{pmatrix} a & b \\ 0 & 0 \end{pmatrix}$. Then, $\sigma_z M\Pi = D$.

Case 3.2. $M = \begin{pmatrix} 0 & 0 \\ a & b \end{pmatrix}$. Then, $\sigma_x M\Pi = D$.

Case 3.3. $M = \begin{pmatrix} a & 0 \\ b & 0 \end{pmatrix}$. Then, $\Pi M I = D$.

Case 3.4. $M = \begin{pmatrix} 0 & a \\ 0 & b \end{pmatrix}$. Then, $\Pi M\sigma_x = D$.

Case 4. All the four entries of M do not vanish.

Let $M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, where $abcd \neq 0$. Without loss of generality, we consider that $\frac{c}{a} = \frac{d}{b} = k$ and then $M = \begin{pmatrix} a & b \\ ka & kb \end{pmatrix}$.

Let

$$K = \begin{pmatrix} \frac{1}{\sqrt{(kk^*+1)}} & \frac{k^*}{\sqrt{kk^*+1}} \\ \frac{k}{\sqrt{kk^*+1}} & -\frac{1}{\sqrt{kk^*+1}} \end{pmatrix}, \tag{B.3}$$

then,

$$KM\Pi = \begin{pmatrix} \sqrt{aa^*+bb^*}\sqrt{kk^*+1} & 0 \\ 0 & 0 \end{pmatrix}. \tag{B.4}$$

Appendix C . All the states of the GHZ SLOCC class that have a unique SD

Via Theorem 1 and by calculating ϱ, we show that a state $\{\lambda_0, \lambda_1 e^{i\phi}, \lambda_2, \lambda_3, \lambda_4\}$ of GHZ SLOCC class has a unique SD if and only if it is of one of the following forms.

Form 1. When $\lambda_1 = 0$, a state has a unique SD if and only if its SD is of the form $\{\frac{1}{\sqrt{2}}, 0, \lambda_2, \lambda_3, \lambda_4\}$.

Form 2. When $\lambda_2 = 0$, a state has a unique SD if and only if its SD is of the form $\{\lambda_0, \lambda_1, 0, \lambda_3, \lambda_4\}$, where $2\lambda_0^2 + 2\lambda_1^2 = 1$.

Form 3. When $\lambda_3 = 0$, a state has a unique SD if and only if its SD is of the form $\{\lambda_0, \lambda_1, \lambda_2, 0, \lambda_4\}$, where $2\lambda_0^2 + 2\lambda_1^2 = 1$.

Form 4. When $\lambda_2 = \lambda_3 = 0$, a state has a unique SD if and only if its SD is of the form $\{\lambda_0, \lambda_1, 0, 0, \frac{1}{\sqrt{2}}\}$

Form 5. When $\lambda_1\lambda_2\lambda_3 \neq 0$, a state has a unique SD if and only if its SD satisfies $\cos\phi = \frac{\lambda_4\left(2\lambda_0^2+2\lambda_1^2-1\right)}{2\lambda_1\lambda_2\lambda_3}$.