On Local Unitary Equivalence of Two and Three-qubit States

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We study the local unitary equivalence for two and three-qubit mixed states by investigating the invariants under local unitary transformations. For two-qubit system, we prove that the determination of the local unitary equivalence of 2-qubits states only needs 14 or less invariants for arbitrary two-qubit states. Using the same method, we construct invariants for three-qubit mixed states. We prove that these invariants are sufficient to guarantee the LU equivalence of certain kind of three-qubit states. Also, we make a comparison with earlier works.

Nonlocality is one of the astonishing phenomena in quantum mechanics. It is not only important in philosophical considerations of the nature of quantum theory, but also the key ingredient in quantum computation and communications such as cryptography. From the point of view of nonlocality, two states are completely equivalent if one can be transformed into the other by means of local unitary (LU) transformations. Many crucial properties such as the degree of entanglement, maximal violations of Bell inequalities and the teleportation fidelity remain invariant under LU transformations. For this reason, it has been a key problem to determine whether or not two states are LU equivalent.

There have been a plenty of results on invariants under LU transformations. However, one still does not have a complete set of such LU invariants which can operationally determine the LU equivalence of any two states both necessarily and sufficiently, except for 2-qubit states and some special 3-qubit states. For the 2-qubit state case, Makhlin presented a set of 18 polynomial LU invariants in ref. In ref. the authors constructed a set of very simple invariants which are less than the ones constructed in ref. Nevertheless, the conclusions are valid only for special (generic) two-qubit states and an error occurred in the proof. In this paper, we corrected the error in ref. by adding some missed invariants, and prove that the determination of the local unitary equivalence of 2-qubits states only needs 14 or less invariants for arbitrary two-qubit states. Moreover, we prove that the invariants in ref. plus some invariants from triple scalar products of certain vectors are complete for a kind of 3-qubit states.

Results

A general 2-qubit state can be expressed as:

$$\rho = \frac{1}{4} \left( I_2 \otimes I_2 + \sum_{i=1}^{3} T_i^I_1 \otimes \sigma_i + \sum_{j=1}^{3} T_j^J_2 \otimes \sigma_j + \sum_{i,j=1}^{3} T_{ij}^L \otimes \sigma_i \otimes \sigma_j \right),$$

where $I$ is the $2 \times 2$ identity matrix, $\sigma_i, i = 1, 2, 3$, are Pauli matrices and $T_i^I = \tr(\rho(\sigma_i \otimes I))$ etc. Two two-qubit states $\rho$ and

$$\tilde{\rho} = \frac{1}{4} \left( I_2 \otimes I_2 + \sum_{i=1}^{3} \tilde{T}_i^I \otimes \sigma_i + \sum_{j=1}^{3} \tilde{T}_j^J_2 \otimes \sigma_j + \sum_{i,j=1}^{3} \tilde{T}_{ij}^L \otimes \sigma_i \otimes \sigma_j \right)$$

are called LU equivalent if there are some $U_i \in U(2), i = 1, 2$, such that $\tilde{\rho} = (U_i \otimes U_j) \rho (U_i^\dagger \otimes U_j^\dagger)$. By using the well-known double-covering map $SU(2) \to SO(3)$, one has that for all $U \in SU(2)$, there is a matrix $O = (a_{ij}) \in SO(3)$, such that $U \sigma_i U^\dagger = \sum_{j=1}^{3} a_{ij} \sigma_j$. Therefore, $\rho$ and $\tilde{\rho}$ are LU equivalent if and only if there are some $O_i \in SO(3), i = 1, 2$, such that

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\[
\hat{T}_1 = O_1 T_v, \quad \hat{T}_2 = O_2 T_v, \\
\hat{T}_{12} = O_1 T_v O_2^T.
\]

(1)

One has two sets of vectors,

\[
S_i = \{ T_v, T_{12}, T_{12}^* T_v, T_{12} T_{12}^* T_v, \ldots \}, \\
S_j = \{ T_v, T_{12}^* T_v, T_{12}^* T_v T_{12}, T_{12} T_{12}^* T_v, \ldots \}.
\]

(2)

For convenience, we denote \(S_1 = \{ \mu_i \mid i = 1, 2, \ldots \} \), \(S_2 = \{ \nu_j \mid j = 1, 2, \ldots \} \), i.e., \(\mu_1 = T_v, \mu_2 = T_{12} T_v, \mu_3 = T_{12}^* T_v \) and so on. The vectors \(\mu_i, (\nu_j)\) are transformed into \(O_1 \mu_i, (O_2 \nu_j)\) under local unitary transformations. Otherwise, local unitary transformation can transform \(\mu_i \times \nu_j\) to \(O_1 (\mu_i \times \nu_j)\) and \(O_2 (\nu_i \times \nu_j)\). Hence it is direct to verify that the inner products \(\langle \mu_i, \nu_j \rangle\) are invariants under local unitary transformations. Moreover, from the transformation \(T_{12} \rightarrow O_1 T_{12} O_2^T\), we have that \(\text{tr}(T_{12} T_{12}^*)^\alpha, \alpha = 1, 2, \ldots, \) and \(\text{det} T_{12}\) are also LU invariants.

For a set of \(3\)-dimensional real vectors \(S = \{ \mu_i \mid i = 1, 2, \ldots \}\), we denote \(\text{dim}(S)\) the dimension of the real linear space spanned by \(\{ \mu_i \}\), i.e., the number of linearly independent vectors of \(\{ \mu_i \}\). As the vectors in \(S_1\) and \(S_2\) are three-dimensional, there are at most \(3\) linearly independent vectors in each vector sets \(S_1\) and \(S_2\).

First note that, given two sets of \(3\)-dimensional real vectors \(S = \{ \mu_i \mid i = 1, 2, \ldots \}\) and \(\tilde{S} = \{ \tilde{\mu}_i \mid i = 1, 2, \ldots \}\), if the inner products \(\langle \mu_i, \mu_j \rangle\) and \(\langle \nu_i, \nu_j \rangle\) can be linearly represented by \(\langle \mu_\alpha, \mu_\beta \rangle\), \(\langle \nu_\alpha, \nu_\beta \rangle\), \(a_{\alpha \beta}, b_{\alpha \beta} < 3\). Therefore there are only \(9\) linearly independent invariants: \(\langle \mu_i, \mu_j \rangle\), \(\langle \nu_i, \nu_j \rangle\), \(i, j = 1, 2, 3\), and \(\langle \mu_i, \nu_j \rangle, j = 2, 4, 6\). We denote them as \(L = L = \{ (\mu_i, \mu_j), (\nu_i, \nu_j), (\mu_i, \nu_j) \mid i = 1, 2, 3, j = 2, 4, 6 \}\).

For \(2\)-qubit states \(\rho\) and \(\tilde{\rho}\), if \(\text{dim}(S_1) = \text{dim}(\tilde{S}_1) = 3\), we need one more invariant \(\langle \mu_6, \mu_6, \mu_6 \rangle\) to guarantee that there is an \(O_1 \in \text{SO}(3)\) such that \(\rho = \tilde{\rho}\). Here \(\mu_6, \mu_6, \mu_6\) are arbitrary three linear independent vectors in \(S_1\). If \(\text{dim}(S_1) = \text{dim}(\tilde{S}_1) < 3\), then the invariants in \(L\) are enough to guarantee the existence of \(O_1\). Similar conclusions are true for \(S_2\) and \(\tilde{S}_2\).

Let \(\mu_{6a}, \mu_{6b}, \mu_{6c}\) denote arbitrary three linear independent vectors in \(S_1\) if \(\text{dim}(S_1) = 3\). For the case that at least one of \(\text{dim}(S_1)\) and \(\text{dim}(S_2)\) is \(3\), we have

**Theorem 1**

Two \(2\)-qubit states are LU equivalent if and only if they have same values of the invariants in \(L\), the invariant \(\langle \mu_{6a}, \mu_{6b}, \mu_{6c} \rangle\) and/or \(\langle \nu_{6a}, \nu_{6b}, \nu_{6c} \rangle\) if \(\text{dim}(S_1) = 3\) and/or \(\text{dim}(S_2) = 3\).

See Methods for the proof of Theorem 1.

For the case both \(\text{dim}(S_1) < 3\) and \(\text{dim}(S_2) < 3\), we also have \(O_2 T_{12}^* \mu_1 = \tilde{T}_{12}^* O_2 \mu_1\) for some \(O_2 \in \text{SO}(3)\). But this does not necessarily give rise to \(\tilde{T}_{12} = O_1 T_{12} O_2^T\). In order to discuss these cases, we need the following result.

**Lemma 1**

For two-qubit states \(\rho\) and \(\tilde{\rho}\), if \(\text{tr}(T_{12} T_{12}^*)^\alpha = \text{tr}(\tilde{T}_{12} \tilde{T}_{12}^*)^\alpha, \alpha = 1, 2\) and \(\text{det} T_{12} = \text{det} \tilde{T}_{12}\), then \(\tilde{T}_{12} = O_1 T_{12} O_2^T\) for some \(O_1, O_2 \in \text{SO}(3)\).

See Methods for the proof of Lemma 1.

For the completeness of the set of invariants, we also need an extra invariant \(I = \varepsilon_{ijk} \varepsilon_{lmn} T_{12}^{ij} T_{12}^{lm} T_{12}^{mn}\), here \(\varepsilon_{ijk}\) and \(\varepsilon_{lmn}\) are Levi-Cevita symbol. Now we discuss the case of \(\text{dim}(S_1) = \text{dim}(\tilde{S}_1) < 3, i = 1, 2\).

**Theorem 2**

Two \(2\)-qubit states with \(\text{dim}(S_1) = \text{dim}(\tilde{S}_1) < 3, i = 1, 2\) are local unitary equivalent if and only if they have the same values of the invariants in \(L\), and the invariants \(\text{tr}(T_{12} T_{12}^*)^\alpha, \alpha = 1, 2\) and \(\text{det} T_{12}\). See Methods for the proof of Theorem 2.

From Theorem 1 and 2 we see that for the case at least one of \(S_1\) has dimension three, we only need 11 or 10 invariants to determine the local unitary equivalence of two \(2\)-qubit states: namely, 9 invariants from \(L\), and \(\langle \mu_{6a}, \mu_{6b}, \mu_{6c} \rangle\) and/or \(\langle \nu_{6a}, \nu_{6b}, \nu_{6c} \rangle\). If both the dimensions of \(S_1\) and \(S_2\) are less than 3, then \(\langle \mu_{6a}, \mu_{6b}, \mu_{6c} \rangle = \langle \nu_{6a}, \nu_{6b}, \nu_{6c} \rangle = 0\). To determine the LU equivalence, we need invariants from \(L, I, \text{tr}(T_{12} T_{12}^*)^\alpha, \alpha = 1, 2\), and \(\text{det} T_{12}\).
Hence we need at most 13 independent invariants. In ref. 20, the authors considered only the generic case of \( \dim(S_3) = 3 \), \( i = 1 \) and \( 2 \), in which the important invariants \( (\mu_1, \mu_2, \mu_3) \) and \( (\nu_1, \nu_2, \nu_3) \) are missed. By adding these missed invariants, we have remedied the error in ref. 20 and, moreover, generalized the method to the case of \( \dim(S_3) = 3 \) for \( i = 1 \) or \( 2 \).

As an example, let us consider the states \( \rho \) and \( \tilde{\rho} \) with \( T_i = (1, 1, 1) \) and \( \tilde{T}_i = (1, 1, -1) \), respectively. \( T_2 = \tilde{T}_2 \) and \( T_{12} = \tilde{T}_{12} \) are diagonal with different nonzero elements on diagonal line. Hence \( \dim(S_3) = \dim(S_3) = 3 \). In this case the invariants from ref. 20 have the same values for \( \sigma \) and \( \tilde{\sigma} \). Nevertheless, taking \( \mu_0 = T_0, \mu_\nu = T_1T_1, \mu_\nu = T(T_2T_2)^2 \) and correspondingly \( \tilde{\mu}_0 = \tilde{T}_0, \tilde{\mu}_\nu = \tilde{T}_1\tilde{T}_1, \tilde{\mu}_\nu = \tilde{T}(\tilde{T}_2\tilde{T}_2)^2 \), we find that the triple scalar invariant we added are different for \( \rho \) and \( \tilde{\rho} \), \( (\mu_0, \mu_\nu, \mu_\nu) = (\tilde{\mu}_0, \tilde{\mu}_\nu, \tilde{\mu}_\nu) = 0 \). Therefore, \( \rho \) and \( \tilde{\rho} \) are not locally equivalent.

The expression of a complete set of LU invariants depends on the form of the invariants. Different constructions of density matrices, in ref. 12 complete set of LU invariants are presented for arbitrary dimensional bipartite states. Nevertheless, such kind of construction of invariants results in problems when the density matrices are degenerate, i.e. different eigenstates have the same eigenvalues. The 18 LU invariants constructed in ref. 10 are based on the Bloch representations of 2-qubit states and has no such problem as in ref. 12. However, these 18 invariants are complete but more than necessary in the sense that the number of independent invariants can be reduced by suitable constructions of the invariants. The LU invariants constructed in ref. 20 are also in terms of Bloch representations. Such constructed invariants work for both non-degenerate and degenerate states. Nevertheless, the invariants \( I, (k, \nu, \mu, \nu), (\nu_1, \nu_2, \nu_3) \) and \( \det T_{ij} = \det \tilde{T}_{ij} \) make the corresponding theorems incorrect even for generic cases studied in ref. 20. By adding these invariants, our set of invariants work for arbitrary 2-qubit states. In fact, a set of complete LU invariants characterizes completely the LU orbits in the quantum logical space. Generally such orbits are not manifolds, but varieties. For example, the set of pure states is a symplectic variety28. For general mixed states, the situation is much more complicated25. Our results would highlight the analysis on the structures of LU orbits.

Now we come to discuss the case of three-qubit system. A three-qubit state \( \rho \) can be written as:

\[
\rho = \frac{1}{8} \left\{ I_2 \otimes I_2 \otimes I_2 + \sum_{i=1}^{3} T_{ij}^\rho \otimes I_2 \otimes I_2 + \sum_{j=1}^{3} T_{ij}^\rho \otimes I_2 \otimes I_2 + \sum_{k=1}^{3} T_{ijk}^\rho \otimes I_2 \otimes I_2 \right\}
\]

One has the coefficient matrices \( T_{ij}, T_{ij}, T_{ij} \) and coefficient tensor \( T_{ijk} \). Now, \( \rho \) and \( \tilde{\rho} \) are LU equivalent if and only if there are \( O_i \in SO(3), i = 1, 2, 3 \), such that \( T_i = \tilde{O}_i T_0 \). For simplicity we denote \( t_{ij}^{\rho} \equiv T_{ij}^{\rho} \) and

\[
T_{123} = \begin{bmatrix}
  t_{111} & t_{112} & t_{113} & t_{121} & t_{122} & t_{123} & t_{131} & t_{132} & t_{133} \\
  t_{211} & t_{212} & t_{213} & t_{221} & t_{222} & t_{223} & t_{231} & t_{232} & t_{233} \\
  t_{311} & t_{312} & t_{313} & t_{321} & t_{322} & t_{323} & t_{331} & t_{332} & t_{333}
\end{bmatrix}
\]

\[
T_{213} = \begin{bmatrix}
  t_{111} & t_{112} & t_{113} & t_{121} & t_{122} & t_{123} & t_{131} & t_{132} & t_{133} \\
  t_{211} & t_{212} & t_{213} & t_{221} & t_{222} & t_{223} & t_{231} & t_{232} & t_{233} \\
  t_{311} & t_{312} & t_{313} & t_{321} & t_{322} & t_{323} & t_{331} & t_{332} & t_{333}
\end{bmatrix}
\]

\[
T_{312} = \begin{bmatrix}
  t_{111} & t_{112} & t_{113} & t_{121} & t_{122} & t_{123} & t_{131} & t_{132} & t_{133} \\
  t_{211} & t_{212} & t_{213} & t_{221} & t_{222} & t_{223} & t_{231} & t_{232} & t_{233} \\
  t_{311} & t_{312} & t_{313} & t_{321} & t_{322} & t_{323} & t_{331} & t_{332} & t_{333}
\end{bmatrix}
\]

Also, we write \( T_i = T_{123}T_{ij}, T_2 = T_{213}T_{ij}, T_3 = T_{312}T_{ij} \) and \( T_{23} = T_{123}T_{ij}, T_{13} = T_{123}T_{ij}, T_{12} = T_{123}T_{ij} \). Similar to the two-qubit case, one has three sets of vectors,

\[
S_1 = \left\{ T_1^{-r}T_0, T_1^{r}T_1^{-1}T_2^{*}, T_1^{-r}T_2^{*}, T_1^{-r}T_3^{*}, T_1^{-r}T_{123}^{*} \right\}
\]

\[
S_2 = \left\{ T_2^{-r}T_2, T_2^{-r}T_1^{*}, T_2^{-r}T_3^{*}, T_2^{-r}T_{123}^{*} \right\}
\]

\[
S_3 = \left\{ T_3^{-r}T_3, T_3^{-r}T_1^{*}, T_3^{-r}T_2^{*}, T_3^{-r}T_{123}^{*} \right\}
\]

where \( r = 1, 2, 3 \) and \( * \) represents all the suitable vectors constructed from \( T_i \). \( T_{123} \) and \( T_{ij} \) such that the vectors in \( S_1 \) are transformed into \( OS_1 \) under LU transformations. For instance, we have \( T_{123}S_1 \subset S_2 \), \( T_{123}S_2 \subset S_2 \), \( T_{123}S_3 \subset S_3 \), and so on, where for \( S_1 = \{ |i| = 1, 2, \cdots \} \) and \( S_3 = \{ |j| = 1, 2, \cdots \} \), we have denoted \( S_2 \otimes S_1 = \{ |i| \otimes |j|, i = 1, 2, \cdots \} \). Because the vectors in \( S_1 \) are all 3-dimensional, we have...
dim($S_i$) ≤ 3. The inner products $\langle \mu_i, \mu_j \rangle$, $\langle \nu_i, \nu_j \rangle$ and $\langle \omega_i, \omega_j \rangle$, $i, j = 1, 2, \cdots$, are all invariants under LU transformations. Using the method in ref. 20, we now prove that these invariants together with the additional ones in theorem 3 are sufficient to guarantee the LU equivalence of certain kind of three-qubit states with at least two of dim($S_i$) = 3 for $i = 1, 2, 3$.

**Theorem 3** Given two 3-qubit states $\rho$ and $\hat{\rho}$, if $(X_i, Y_i) = (\hat{X}_i, \hat{X}_i)$, $(X_i, Y_i, Z_i) = (\hat{X}_i, \hat{X}_i, \hat{X}_i)$ for $X = \mu, \nu, \omega$ and $i, j = 1, 2, \cdots$, and dim($S_i$) = dim($\hat{S}_i$) = 3 for at least two $i = 1, 2, 3$, then $\rho$ and $\hat{\rho}$ are LU equivalent.

See Methods for the proof of Theorem 3.

If at most one of dim($S_i$) is 3, things become more complicated. Now we give a comparison with the results in ref. 11. For 3-qubit states $\rho$ and $\hat{\rho}$, if

$$\text{tr}(T^i) = \text{tr}(\hat{T}^i), \quad T^i T_i^{r-1} = T_i^{r-1} \hat{T}^i, \quad r = 1, 2, 3,$$

then there are $P_r, \hat{P}_r \in O(3)$ such that

$$P_r T^i P_i^r = \begin{pmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix}, \quad P_r \hat{T}^i = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}.$$

Denote

$$Y_r = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \end{pmatrix} = \Lambda_r \Theta_r.$$

The results in ref. 11 concluded that $\rho$ and $\hat{\rho}$ are local unitary equivalent if and only if the invariants in Theorem 3, together with the invariants $\text{tr}(T_r^i)$, $r = 1, 2, 3$, for the case of $\det \Lambda_r \Theta_r \equiv 0$, $i = 1, 2, 3$. Obviously, if $\det \Lambda_r \Theta_r \equiv 0$, $P_r T^i_r$, $P_r \hat{T}^i_r$ and $P_r \hat{T}^i_r T_r^i$ are linear independent, so all dim($S_i$) = 3. But dim($S_i$) does not necessarily imply $\det \Lambda_r \Theta_r \equiv 0$. Here we only need that two of the dim($S_i$) are 3. So we give the sufficient conditions for local unitary equivalence of more states than the ones given in ref. 11.

**Conclusion**

We study the local unitary equivalence for two and three-qubit mixed states by investigating the invariants under local unitary transformations. We corrected the error in ref. 20 by adding some missing invariants, and prove that the determination of the local unitary equivalence of 2-qubits states only needs 14 or less invariants for arbitrary two-qubit states. Moreover, we prove that the invariants in ref. 20 plus some invariants from triple scalar products of certain vectors are complete for a kind of 3-qubit states. Comparing with the results in ref. 11, it has been shown that we judge the LU equivalence for a larger class of 3-qubit states.

**Methods**

**Proof of Theorem 1** Suppose dim($S_i$) = dim($\hat{S}_i$) = 3. From the construction of $S_i$ and $\hat{S}_i$, we have that $V_{\alpha+1} = T^{1\mu}_{\alpha+1}$, $\tilde{V}_{\alpha+1} = \tilde{T}^{1\mu}_{\alpha+1}$, $\alpha = 1, 2, \cdots$. Then $O_rT^1_{\mu+1} = O_r\tilde{T}^1_{\mu+1}$, $\alpha = 1, 2, \cdots$. Since $\nu_{\mu+1} = T^{1\mu}_{\mu+1}$, $\nu_{\mu+1} = \tilde{T}^{1\mu}_{\mu+1}$, $\alpha = 1, 2, \cdots$, and since $\nu_{\mu+1}$, $\nu_{\mu+1}$ are linearly independent, $\det(\mu_{\mu+1}, \mu_{\mu+1}) \neq 0$, where $\mu_{\mu+1}, \mu_{\mu+1}$ denotes the 3 × 3 matrix given by the three column vectors $\nu_{\mu+1}$, $\nu_{\mu+1}$, $\nu_{\mu+1}$. From $O_rT^1_{\mu+1} = O_r\tilde{T}^1_{\mu+1}$, we get $O_r \tilde{T}^1_{\mu+1} = \tilde{T}^1_{\mu+1}$. Then $\tilde{T}^1_{\mu+1} = \tilde{T}^1_{\mu+1}$. The same result can be obtained from dim($\hat{S}_i$) = dim($\hat{S}_i$) = 3.

**Proof of Lemma 1** From $\text{tr}(T^1_{\mu+1} T^1_{\mu+1}) = \text{tr}(\tilde{T}^1_{\mu+1} \tilde{T}^1_{\mu+1})$, $\alpha = 1, 2$ and $\det T_{\mu+1} = \det \tilde{T}^1_{\mu+1}$, one has that $T_{\mu+1}$ and $\tilde{T}^1_{\mu+1}$ have the same singular values. According to the singular value decomposition, there are $P_r, \hat{P}_r \in O(3), i = 1, 2, 1, 2$, such that $P_r T^1_{\mu+1} P_i^r = \hat{P}_r \tilde{T}^1_{\mu+1} \hat{P}_i^r = \text{diag}(t_{11}, t_{12}, t_{13})$, where $t_{11}$, $t_{12}$ and $t_{13}$ are the singular values. Set $O_1 = \hat{P}_r P_r$, $O_2 = \hat{P}_r \hat{P}_r \in O(3)$, we have $T_{\mu+1} = O_1 T_{\mu+1} O_1^t$. From $\det T_{\mu+1} = \det T_{\mu+1}^t$, we have that $\det O_1 = \det O_2 = \pm 1$. If $\det O_1 = \det O_2 = -1$, we may change $P_r$ to $-P_r$ to have $O_1 \in SO(3)$.

**Proof of Theorem 2** We only need to prove the ”only if” part, i.e., to find $O_2$, $O_2 \in SO(3)$ such that $T_{\mu+1} = O_2 T_{\mu+1}^t$ for two 3-qubit states $\rho$ and $\hat{\rho}$. From Lemma 1, we have $P_r, \hat{P}_r \in O(3)$, such that $P_r \hat{P}_r \in SO(3)$ and

$$P_r T^1_{\mu+1} P_i^r = \hat{P}_r \tilde{T}^1_{\mu+1} \hat{P}_i^r = \text{diag}(t_{11}, t_{12}, t_{13}).$$

Hence

$$P_r T^1_{\mu+1} T^1_{\mu+1} = \hat{P}_r \tilde{T}^1_{\mu+1} \hat{T}^1_{\mu+1} = \text{diag}(t_{11}, t_{12}, t_{13}).$$

Let $D = \text{diag}(t_{11}, t_{12}, t_{13})$, then $P S_i = \{P_r T^1_{\mu+1} D_r P^T_{\mu+1} D^T r P^T_{\mu+1} D^T r P^T_{\mu+1} \cdots\}$, $P S_i = \{P_r T^1_{\mu+1} D_r P^T_{\mu+1} D^T r P^T_{\mu+1} D^T r P^T_{\mu+1} \cdots\}$. Denote $P T^1_{\mu+1} = (a_1, b_1, c_1)^T$, $P^T_{\mu+1} = (a_2, b_2, c_2)^T$. By using $P S_i = \{P_r T^1_{\mu+1} D_r P^T_{\mu+1} D^T r P^T_{\mu+1} D^T r P^T_{\mu+1} \cdots\}$, $j = 1, 3, 5, \cdots$, i.e. $(P T^1_{\mu+1} D^T r P^T_{\mu+1} D^T r P^T_{\mu+1} \cdots) = \{P r T^1_{\mu+1} D^T r P^T_{\mu+1} D^T r P^T_{\mu+1} \cdots\}$, we get...
If $\alpha_j = \pm \hat{\alpha}_i$ for $\alpha = a, b, c$ and $i = 1, 2$. 

(i) If $t_i = 0$, $i = 1, 2, 3$, from (8) we get $\alpha_i \alpha_2 = \hat{\alpha}_i \hat{\alpha}_2$ for $\alpha = a, b, c$. Now if $\alpha_i \alpha_2 \neq 0$, then we have $\alpha_i = \hat{\alpha}_i \Leftrightarrow \alpha_2 = \hat{\alpha}_2$. If $\alpha_i \alpha_2 = 0$, suppose $\alpha_i = 0$, then we have $\alpha_2 = 0$. If $\alpha_2 = \hat{\alpha}_2$, we also can write $\alpha_1 = \hat{\alpha}_1$. Let $R = \text{diag}(e_i, e_2, e_3)$, where $e_i$ take values $+1$ or $-1$, such that $\text{det}(R^2 P_i T_i) = \hat{P}_i T_i$. Then one must have $R^2 P_i T_i = \hat{P}_i T_i$. Note that the equality (3) is also true if one replaces $P_i$ by $R^2 P_i$. Let $O_i = \hat{P}_i T_i P_i$. Hence, $O_i T_i = \hat{P}_i T_i$ for $i = 1, 2, 3$. We have $\hat{T}_i = \hat{O}_i T_i$ for $i = 1, 2, 3$, and $\hat{T}_{ij} = \hat{O}_i T_i \hat{O}_j$ for $i \neq j$. To assure that $O_i$ be special, we have det $R = 1$. Firstly, from dim$(PS_i) = \dim(S_i) < 3$, we have that $P_i T_i, D^2 P_i T_i, D^4 P_i T_i$ are linearly dependent. Then there is at least one $\alpha_i \in \{a_i, b_i, c_i\}$ that is zero. Hence if $P_i T_i$ and $D^2 P_i T_i$ are linearly independent, we have that $D^4 P_i T_i$ can be linearly represented by $P_i T_i$ and $D^2 P_i T_i$. Using $t_2 t_3 = 0$ and supposing $a_i = 0$, we get that $a_i$ is also zero. Now $e_i \in R$ can be chosen to be $1$ or $-1$ freely. We can choose $e_i$ to assure that $R = 1$. Similarly, for the case that $P_i T_i$ and $D^2 P_i T_i$ are linear independent, we can also find $R$ which has determinate one. Lastly, if $P_i T_i$ and $D^2 P_i T_i$ are linear dependent, then there are at least two members are zero in $\{a_i, b_i, c_i\}$, $i = 1, 2$. Therefore, there is an $\alpha \in \{a, b, c\}$ satisfying $\alpha_i = \alpha_2 = 0$, such that det $R = 1$.

(ii) If there exists a $t_i = 0$, say $t_0 = 0$, then we have $\alpha_i \alpha_2 = \hat{\alpha}_i \hat{\alpha}_2$ for $\alpha = a, b$ from (8). And the invariant I can assure that $c \hat{\alpha}_2 = \hat{\alpha}_2$. From the discussion above, we have the conclusion.

2. If there are two different values of $t_i$, $t_j$, $t_k$, suppose $t_i = t_j = t_k$. Then from (6) and (7), we can get $a_i^2 + b_i^2 = \hat{a}_i^2 + \hat{b}_i^2$, $c_i = \pm \hat{c}_i$ for $i = 1, 2$.

(i) If $t_i = 0$, $i = 1, 2, 3$, from (8) we get $a_i c_i + b_i b_i = \hat{\alpha}_i \hat{c}_i + \hat{b}_i \hat{b}_i$, $c_i c_i = \hat{c}_i \hat{c}_i$. Then there exists a matrix $M \in (2)$ such that $M (a_i b_i) = (\hat{a}_i \hat{b}_i)$, $i = 1, 2$. And there is an $e = 1$ or $-1$ such that $e(c_i \hat{c}_i) = \hat{c}_i \hat{c}_i$ for $i = 1, 2$.

Therefore letting $R = \left(\begin{array}{c} M \end{array} \right)$, one has $R T_i = \hat{P}_i T_i$ and $R Q T_i = \hat{Q}_i T_i$ again. For the speciality of $R$, from the dimension of $(S_i)$, we have det $(a_i b_i) = 0$ or $c_i = \hat{c}_i = 0$. Hence, we can choose suitable $M$ or $e$ to make sure that $R$ is special.

(ii) If $t_i = t_j = 0$, we only have $c_i \hat{c}_i = \hat{c}_i \hat{c}_i$. We can get $M_i \in (2)$ such that $M_i (a_i b_i) = (\hat{a}_i \hat{b}_i)$, $i = 1, 2$, and $R_i = \left(\begin{array}{cc} M_i & \end{array} \right)$ to get the result similarly. We can choose suitable $M_i$ for the speciality of $R_i$.

(iii) If $t_i = 0$, then one has $R_i$, $R_i$ with the same $M$ but different $e$ to prove the theorem. The speciality for $R_i$ is similar to the case of $t_i = 0$.

3. If $t_i = t_j = t_k = 0$, from (6), (7) and (8), we get $a_i^2 + b_i^2 + c_i^2 = \hat{a}_i^2 + \hat{b}_i^2 + \hat{c}_i^2$ for $i = 1, 2, 3$.

Therefore we have $R \in SO(3)$ such that $R T_i = \hat{P}_i T_i$ and $R Q T_i = \hat{Q}_i T_i$. Replacing $P_i$ by $R P_i$ in (3) we get the result.

4. If $t_j = t_j = t_k = 0$, we have $a_i^2 + b_i^2 + c_i^2 = \hat{a}_i^2 + \hat{b}_i^2 + \hat{c}_i^2$ for $i = 1, 2$. Therefore one has $R \in SO(3)$ such that $R T_i = \hat{P}_i T_i$, $i = 1, 2$. Replacing $P_i$ by $R P_i$ in (3) one gets the result.

**Proof of Theorem 3** For 3-qubit states $\rho$ and $\hat{\rho}$, they are LU equivalent if and only if there are $O_i \in SO(3)$, $i = 1, 2, 3$, such that $\hat{T}_i = O_i T_i$, $\hat{T}_j = O_j T_j O_i$, and $\hat{T}_{ij} = O_i \otimes O_j \otimes O_{ij}$. Suppose $\dim(S_i) = \dim(S_i) = 3$, for $i = 1, 2, 3$. By using the given invariants, we have $O_i \in SO(3)$ such that $\mu_i = \hat{\mu}_i$, $\nu_i = \hat{\nu}_i$, and $\omega_i = \hat{\omega}_i$ for $i = 1, 2, \ldots$, as well as $\hat{T}_i \hat{T}_j = \hat{T}_j \hat{T}_i$, $\hat{T}_i \hat{T}_j = \hat{T}_j \hat{T}_i$, and $\hat{T}_{ij} \hat{T}_{kl} = \hat{T}_{ij} \hat{T}_{kl}$ for $i, j = 1, 2, \ldots$, $k, l = 1, 2, \ldots$, $i \neq j, k$. Suppose $\mu_i$, $\mu_i$ and $\mu_i$ are linear independent. Then $O_i \hat{T}_{ij} \hat{T}_{kl} = \hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl}$, $i = 1, 2, \ldots$, $k, l = 1, 2, \ldots$, $i \neq j, k$. Hence we get $O_i \hat{T}_{ij} \hat{T}_{kl} = \hat{O}_i \hat{T}_{ij} \hat{T}_{kl}$. Similarly, we have $\hat{T}_i = O_i \hat{T}_j O_i \hat{T}_j$. From $\hat{T}_{ij} \hat{T}_{kl} = \hat{T}_{ij} \hat{T}_{kl}$, $\hat{T}_{ij} \hat{T}_{kl} = \hat{T}_{ij} \hat{T}_{kl}$, $i = 1, 2, \ldots$, $k, l = 1, 2, \ldots$, $i \neq j, k$, we have $\hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl} = \hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl}$, $\hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl} = \hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl}$, where $\nu_i$, $\nu_i$, $\nu_i$ are linear independent vectors in $S_2$. Using the linear independence of $\mu_i$, $\mu_i$, $\mu_i$ and $\nu_i$, $\nu_i$, $\nu_i$, we get $\hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl} = \hat{T}_{ij} \hat{T}_{kl}$, $\hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl} \hat{T}_{ij} \hat{T}_{kl} = \hat{T}_{ij} \hat{T}_{kl}$, which is equivalent to $\hat{T}_{ij} \hat{T}_{kl} = \hat{T}_{ij} \hat{T}_{kl}$.
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Author Contributions

B.-Z.S., S.-M.F. and Z.-X.W. wrote the main manuscript text. All of the authors reviewed the manuscript.

Additional Information

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