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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[1]. 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[2,3], maximal violations of Bell inequalities[4–7] and the teleportation fidelity[8,9] 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[10–25]. 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. 10. In ref. 20 the authors constructed a set of very simple invariants which are less than the ones constructed in ref. 10. 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. 20 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. 20 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:

$$\rho=\frac{1}{4}\left(I_2\otimes I_2+\sum_{i=1}^{3}T_1^i\sigma_i\otimes I_2+\sum_{j=1}^{3}T_2^jI_2\otimes\sigma_j+\sum_{i,j=1}^{3}T_{12}^{ij}\sigma_i\otimes\sigma_j\right),$$

where I is the 2×2 identity matrix, σ_i, $i=1, 2, 3$, are Pauli matrices and $T_1^i=\mathrm{tr}(\rho(\sigma_i\otimes I))$ etc. Two two-qubit states ρ and

$$\hat{\rho}=\frac{1}{4}\left(I_2\otimes I_2+\sum_{i=1}^{3}\hat{T}_1^i\sigma_i\otimes I_2+\sum_{j=1}^{3}\hat{T}_2^jI_2\otimes\sigma_j+\sum_{i,j=1}^{3}\hat{T}_{12}^{ij}\sigma_i\otimes\sigma_j\right)$$

are called LU equivalent if there are some $U_i\in U(2)$, $i=1, 2$, such that $\hat{\rho}=(U_1\otimes U_2)\rho(U_1^\dagger\otimes U_2^\dagger)$. 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 $O=(o_{kl})\in SO(3)$, such that $U\sigma_kU^\dagger=\sum_{l=1}^{3}o_{kl}\,\sigma_l$. Therefore, ρ and $\hat{\rho}$ are LU equivalent if and only if there are some $O_i\in SO(3)$, $i=1$, 2, such that

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$$\begin{aligned}&\hat{T}_1 = O_1 T_1, \qquad \hat{T}_2 = O_2 T_2,\\ &\hat{T}_{12} = O_1 T_{12} O_2^t.\end{aligned} \tag{1}$$

One has two sets of vectors,

$$\begin{aligned} S_1 &= \{T_1,\ T_{12}T_2,\ T_{12}T_{12}^t T_1,\ T_{12}T_{12}^t T_{12}T_2,\ \cdots\},\\ S_2 &= \{T_2,\ T_{12}^t T_1,\ T_{12}^t T_{12}T_2,\ T_{12}^t T_{12}T_{12}^t T_1,\ \cdots\}.\end{aligned} \tag{2}$$

For convenience, we denote $S_1 = \{\mu_i | i = 1, 2, \cdots\}$, $S_2 = \{\nu_i | i = 1, 2, \cdots\}$, i.e., $\mu_1 = T_1$, $\mu_2 = T_{12}T_2$, $\mu_3 = T_{12}T_{12}^t T_1$ and so on. The vectors μ_i (ν_i) are transformed into $O_1\mu_i$ ($O_2\nu_i$) under local unitary transformations. Otherwise, local unitary transformation can transform $\mu_i \times \mu_j$ to $O_1(\mu_i \times \mu_j)$ and $\nu_i \times \nu_j$ to $O_2(\nu_i \times \nu_j)$. Hence it is direct to verify that the inner products $\langle \mu_i, \mu_j\rangle$, $\langle \nu_i, \nu_j\rangle$, $i, j = 1, 2, \cdots$, and $(\mu_i, \mu_j, \mu_k) \equiv \langle \mu_i, \mu_j \times \mu_k\rangle$, $(\nu_i, \nu_j, \nu_k) \equiv \langle \nu_i, \nu_j \times \nu_k\rangle$, $i, j, k = 1, 2, \cdots$, are invariants under local unitary transformations. Moreover, from the transformation $T_{12} \to O_1 T_{12} O_2^t$, we have that $\mathrm{tr}(T_{12}T_{12}^t)^\alpha$, $\alpha = 1, 2, \cdots$, and det T_{12} are also LU invariants.

For a set of 3-dimensional real vectors $S = \{\mu_i | i = 1, 2, \cdots\}$, we denote $\dim\langle S\rangle$ 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 $S = \{\mu_i | i = 1, 2, \cdots\}$ and $\hat{S} = \{\hat{\mu}_i | i = 1, 2, \cdots\}$, if the inner products $\langle \mu_i, \mu_j\rangle = \langle \hat{\mu}_i, \hat{\mu}_j\rangle$, then the following conclusions are true: (i) $\dim\langle S\rangle = \dim\langle \hat{S}\rangle$; (ii) The corresponding subsets of S and $\hat{S}$ have the same linear relations; (iii) There exist $O \in O(3)$ such that $\hat{\mu}_i = O\mu_i$. Furthermore, using $(\mu_i, \mu_j, \mu_k) = (\hat{\mu}_i, \hat{\mu}_j, \hat{\mu}_k)$, we can get that $O \in SO(3)$. If $\dim\langle S\rangle = 3$, then O is unique. For $\dim\langle S\rangle < 3$, $(\mu_i, \mu_j, \mu_k) = (\hat{\mu}_i, \hat{\mu}_j, \hat{\mu}_k) = 0$, and there is at least one $O \in SO(3)$ such that $\hat{\mu}_i = O\mu_i$.

Next we clarify the independent invariants in S_1 and S_2. From the definition of μ_i, ν_i, we have

$$\langle \mu_i, \mu_j\rangle = \begin{cases} T_1^t (T_{12}T_{12}^t)^{a_{ij}} T_1, & \text{if } i, j \text{ are odd}\\ T_2^t (T_{12}^t T_{12})^{a_{ij}} T_2, & \text{if } i, j \text{ are even}\\ T_1^t (T_{12}T_{12}^t)^{b_{ij}} T_{12}T_2, & \text{if } i + j \text{ is odd}\end{cases}$$

$$\langle \nu_i, \nu_j\rangle = \begin{cases} T_2^t (T_{12}^t T_{12})^{a_{ij}} T_2, & \text{if } i, j \text{ are odd}\\ T_2^1 (T_{12}T_{12}^t)^{a_{ij}} T_1, & \text{if } i, j \text{ are even}\\ T_1^t (T_{12}T_{12}^t)^{b_{ij}} T_{12}T_2, & \text{if } i + j \text{ is odd}\end{cases}$$

where $a_{ij} = (i + j - 2)/2$, $b_{ij} = (i + j - 3)/2$. From Hamilton-Cayley theorem, when a_{ij}, $b_{ij} \geq 3$, the invariants $\langle \mu_i, \mu_j\rangle$ and $\langle \nu_i, \nu_j\rangle$ can be linearly represented by $\langle \mu_p, \mu_q\rangle$, $\langle \nu_p, \nu_q\rangle$, a_{pq}, $b_{pq} < 3$. Therefore there are only 9 linearly independent invariants: $\langle \mu_i, \mu_i\rangle$, $\langle \nu_i, \nu_i\rangle$, $i = 1, 2, 3$, and $\langle \mu_1, \mu_j\rangle$, $j = 2, 4, 6$. We denote them as $L=$ $L = \{\langle \mu_i, \mu_i\rangle, \langle \nu_i, \nu_i\rangle, \langle \mu_1, \mu_j\rangle | i = 1, 2, 3, j = 2, 4, 6\}$.

For 2-qubit states ρ and $\hat{\rho}$, if $\dim\langle S_1\rangle = \dim\langle \hat{S}_1\rangle = 3$, we need one more invariant $(\mu_{r_0}, \mu_{s_0}, \mu_{t_0})$ to guarantee that there is an $O_1 \in SO(3)$ such that $O_1\mu_i = \hat{\mu}_i$, for any i. Here μ_{r_0}, μ_{s_0} and μ_{t_0} are arbitrary three linear independent vectors in S_1. If $\dim\langle S_1\rangle = \dim\langle \hat{S}_1\rangle < 3$, then the invariants in L are enough to guarantee the existence of O_1. Similar conclusions are true for S_2 and $\hat{S}_2$.

Let μ_{r_0}, μ_{s_0} and μ_{t_0} (ν_{r_0}, ν_{s_0} and ν_{t_0}) denote arbitrary three linear independent vectors in S_1 (S_2) if $\dim\langle S_1\rangle = 3$ ($\dim\langle S_2\rangle = 3$). For the case that at least one of $\dim\langle S_1\rangle$ and $\dim\langle S_2\rangle$ 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* $(\mu_{r_0}, \mu_{s_0}, \mu_{t_0})$ and/or $(\nu_{r_0}, \nu_{s_0}, \nu_{t_0})$ if $\dim\langle S_1\rangle = 3$ and/or $\dim\langle S_2\rangle = 3$.

See Methods for the proof of Theorem 1.

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

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

See Methods for the proof of Lemma 1.

For the completeness of the set of invariants, we also need an extra invariant $\mathbf{I} = \varepsilon_{ijk}\varepsilon_{lmn} T_1^i T_2^l T_{12}^{jm} T_{12}^{kn}$, here ε_{ijk} and ε_{lmn} are Levi-Cevita symbol. Now we discuss the case of $\dim S_i = \dim \hat{S}_i < 3$, $i = 1, 2$.

Theorem 2 *Two 2-qubit states with* $\dim S_i = \dim \hat{S}_i < 3$, $i = 1, 2$ *are local unitary equivalent if and only if they* have the same values of the invariants in L, and the invariants $\mathrm{tr}(T_{12}T_{12}^t)^\alpha$, $\alpha = 1, 2$, det T_{12} and $\boldsymbol{I}$.

See Methods for the proof of Theorem 2.

From Theorem 1 and 2 we see that for the case at least one of $\langle S_i\rangle$ 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 $(\mu_{r_0}, \mu_{s_0}, \mu_{t_0})$ and/or $(\nu_{r_0}, \nu_{s_0}, \nu_{t_0})$. If both the dimensions of $\langle S_1\rangle$ and $\langle S_2\rangle$ are less than 3, then $(\mu_{r_0}, \mu_{s_0}, \mu_{t_0}) = (\nu_{r_0}, \nu_{s_0}, \nu_{t_0}) = 0$. To determine the LU equivalence, we need invariants from L, I, $\mathrm{tr}(T_{12}T_{12}^t)^\alpha$, $\alpha = 1, 2$, and det T_{12}.

Hence we need at most 13 independent invariants. In ref. 20, the authors considered only the generic case of $\dim\langle S_i\rangle = 3$, $i = 1$ and 2, in which the important invariants $(\mu_{r_0}, \mu_{s_0}, \mu_{t_0})$ and $(\nu_{r_0}, \nu_{s_0}, \nu_{t_0})$ are missed. By adding these missed invariants, we have remedied the error in ref. 20 and, moreover, generalized the method to the case of $\dim\langle S_i\rangle = 3$ for $i = 1$ or 2.

As an example, let we consider the states ρ and $\hat{\rho}$ with $T_1 = (1, 1, 1)^t$ and $\hat{T}_1 = (1, 1, -1)^t$, respectively. $T_2 = \hat{T}_2$ and $T_{12}T_{12}^t = \hat{T}_{12}\hat{T}_{12}^t$ are diagonal with different nonzero elements on diagonal line. Hence $\dim\langle S_1\rangle = \dim\langle \hat{S}_1\rangle = 3$. In this case the invariants from ref. 20 have the same values for ρ and $\hat{\rho}$. Nevertheless, taking $\mu_{r_0} = T_1$, $\mu_{s_0} = T_1T_{12}T_{12}^t$ and $\mu_{t_0} = T_1(T_{12}T_{12}^t)^2$, and correspondingly, $\hat{\mu}_{r_0} = \hat{T}_1$, $\hat{\mu}_{s_0} = \hat{T}_1\hat{T}_{12}\hat{T}_{12}^t$, and $\hat{\mu}_{t_0} = \hat{T}_1(\hat{T}_{12}\hat{T}_{12}^t)^2$, we find that the triple scalar invariant we added are different for ρ and $\hat{\rho}$, $(\mu_{r_0}, \mu_{s_0}, \mu_{t_0}) = -(\hat{\mu}_{r_0}, \hat{\mu}_{s_0}, \hat{\mu}_{t_0}) \neq 0$. Therefore, ρ and $\hat{\rho}$ are not locally equivalent.

The expression of a complete set of LU invariants depends on the form of the invariants. Different constructions of LU invariants may give different numbers of the invariants in the complete set, and may have different advantages. Obviously the eigenvalues of a density matrix are LU invariants. Based on the eigenstate decompositions 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: $\mathbf{I}$, $(\mu_{r_0}, \mu_{s_0}, \mu_{t_0})$, $(\nu_{r_0}, \nu_{s_0}, \nu_{t_0})$ and $\det T_{12} = \det \hat{T}_{12}$ 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 state space. Generally such orbits are not manifolds, but varieties. For example, the set of pure states is a symplectic variety[26]. For general mixed states, the situation is much more complicated[27]. 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 ρ can be written as:

$$\begin{aligned}\rho \;=\; \frac{1}{8}\Bigg(& I_2 \otimes I_2 \otimes I_2 + \sum_{i=1}^{3} T_1^i \sigma_i \otimes I_2 \otimes I_2 + \sum_{j=1}^{3} T_2^j I_2 \otimes \sigma_j \otimes I_2 + \sum_{k=1}^{3} T_3^k I_2 \otimes I_2 \otimes \sigma_k \\ & + \sum_{i,j=1}^{3} T_{12}^{ij}\sigma_i \otimes \sigma_j \otimes I_2 + \sum_{i,k=1}^{3} T_{13}^{ik}\sigma_i \otimes I_2 \otimes \sigma_k + \sum_{j,k=1}^{3} T_{12}^{jk} I_2 \otimes \sigma_j \otimes \sigma_k \\ & + \sum_{i,j,k=1}^{3} T_{123}^{ijk}\sigma_i \otimes \sigma_j \otimes \sigma_k \Bigg).\end{aligned}$$

One has the coefficient vectors T_1, T_2, T_3, coefficient matrices T_{12}, T_{23}, T_{13} and coefficient tensor T_{123}. Now, ρ and $\hat{\rho}$ are LU equivalent if and only if there are $O_i \in SO(3)$, $i = 1, 2, 3$, such that $\hat{T}_i = O_iT_i$, $\hat{T}_{ij} = O_i \otimes O_jT_{ij}$, $\hat{T}_{123} = O_1 \otimes O_2 \otimes O_3T_{123}$. For simplicity we denote $t_{ijk} \equiv T_{123}^{ijk}$ and

$$\begin{aligned}T_{1|23} &= \begin{pmatrix} t_{111} & t_{112} & t_{113} & t_{121} & t_{122} & t_{123} & t_{131} & t_{132} & t_{133} \\ t_{211} & t_{212} & t_{213} & t_{221} & t_{222} & t_{223} & t_{231} & t_{232} & t_{233} \\ t_{311} & t_{312} & t_{313} & t_{321} & t_{322} & t_{323} & t_{331} & t_{332} & t_{333} \end{pmatrix}, \\ T_{2|13} &= \begin{pmatrix} t_{111} & t_{112} & t_{113} & t_{211} & t_{212} & t_{213} & t_{311} & t_{312} & t_{313} \\ t_{121} & t_{122} & t_{123} & t_{221} & t_{222} & t_{223} & t_{321} & t_{322} & t_{323} \\ t_{131} & t_{132} & t_{133} & t_{231} & t_{232} & t_{233} & t_{331} & t_{332} & t_{333} \end{pmatrix}, \\ T_{3|12} &= \begin{pmatrix} t_{111} & t_{121} & t_{131} & t_{211} & t_{221} & t_{231} & t_{311} & t_{321} & t_{331} \\ t_{112} & t_{122} & t_{132} & t_{212} & t_{222} & t_{232} & t_{312} & t_{322} & t_{332} \\ t_{113} & t_{123} & t_{133} & t_{213} & t_{223} & t_{233} & t_{313} & t_{323} & t_{333} \end{pmatrix}.\end{aligned}$$

Also, we write $\mathcal{T}_1 = T_{1|23}T_{1|23}^t$, $\mathcal{T}_2 = T_{2|13}T_{2|13}^t$, $\mathcal{T}_3 = T_{3|12}T_{3|12}^t$ and $\mathcal{T}_{23} = T_{1|23}^tT_{1|23}$, $\mathcal{T}_{13} = T_{2|13}^tT_{2|13}$, $\mathcal{T}_{12} = T_{3|12}^tT_{3|12}$. Similar to to the two-qubit case, one has three sets of vectors,

$$\begin{aligned}S_1 &= \left\{\mathcal{T}_1^{r-1}T_1, \mathcal{T}_1^{r-1}T_{12} **, \mathcal{T}_1^{r-1}T_{13} **, \mathcal{T}_1^{r-1}T_{1|23} **\right\}, \\ S_2 &= \left\{\mathcal{T}_2^{r-1}T_2, \mathcal{T}_2^{r-1}T_{12}^t **, \mathcal{T}_2^{r-1}T_{23} **, \mathcal{T}_2^{r-1}T_{2|13} **\right\}, \\ S_3 &= \left\{\mathcal{T}_3^{r-1}T_3, \mathcal{T}_3^{r-1}T_{13}^t **, \mathcal{T}_3^{r-1}T_{23}^t **, \mathcal{T}_3^{r-1}T_{3|12} **\right\},\end{aligned}$$

where $r = 1, 2, 3$ and ** represents all the suitable vectors constructed from T_{ij}, $T_{i|jk}$, $\mathcal{T}_i$ and T_i such that the vectors in S_i are transformed into O_iS_i under LU transformations. For instance, we have $T_{12}^tS_1 \subset S_2$, $T_{13}^tS_1 \subset S_3$, $T_{1|23}S_2 \otimes S_3 \subset S_1$ and so on, where for $S_2 = \{\nu_i | i = 1, 2, \cdots\}$ and $S_3 = \{\omega_j | j = 1, 2, \cdots\}$, we have denoted $S_2 \otimes S_3 = \{\nu_i \otimes \omega_j | i, j = 1, 2, \cdots\}$ etc. Because the vectors in S_i are all 3-dimensional, we have

$\dim\langle S_i\rangle \leq 3$. 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 $\dim\langle S_i\rangle = 3$ for $i = 1, 2, 3$.

Theorem 3 *Given two 3-qubit states ρ and $\hat{\rho}$*, if $\langle X_i, X_j\rangle = \langle\hat{X}_i, \hat{X}_j\rangle$, $(X_i, X_j, X_k) = (\hat{X}_i, \hat{X}_j, \hat{X}_k)$ for $X = \mu, \nu, \omega$ *and* $i, j, k = 1, 2, \cdots$, and $\dim\langle S_i\rangle = \dim\langle\hat{S}_i\rangle = 3$ for at least two $i \in 1, 2, 3$, then ρ and $\hat{\rho}$ are LU equivalent.

See Methods for the proof of Theorem 3.

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

$$\mathrm{tr}(\mathcal{T}_i^r) = \mathrm{tr}(\hat{\mathcal{T}}_i^r), \quad T_i^t\mathcal{T}_i^{r-1}T_i = \hat{T}_i^t\hat{\mathcal{T}}_i^{r-1}\hat{T}_i, \quad r, i = 1, 2, 3, \tag{3}$$

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

$$P_i\mathcal{T}_iP_i^t = \begin{pmatrix} t_{i1} & & \\ & t_{i2} & \\ & & t_{i3} \end{pmatrix} = \hat{P}_i\hat{\mathcal{T}}_i\hat{P}_i^t, \quad P_iT_i = \hat{P}_i\hat{T}_i = \begin{pmatrix} a_{i1} \\ a_{i2} \\ a_{i3} \end{pmatrix}. \tag{4}$$

Denote

$$Y_i \equiv \begin{pmatrix} a_{i1} & a_{i2} & a_{i3} \\ t_{i1}a_{i1} & t_{i2}a_{i2} & t_{i3}a_{i3} \\ t_{i1}^2a_{i1} & t_{i2}^2a_{i2} & t_{i3}^2a_{i3} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ t_{i1} & t_{i2} & t_{i3} \\ t_{i1}^2 & t_{i2}^2 & t_{i3}^2 \end{pmatrix}\begin{pmatrix} a_{i1} & & \\ & a_{i2} & \\ & & a_{i3} \end{pmatrix} \equiv \Lambda_i\Theta_i.$$

The results in ref. 11 concluded that ρ and $\hat{\rho}$ are local unitary equivalent if and only if the invariants in Theorem 3, together with the invariants $\mathrm{tr}(\mathcal{T}_i^r)$, $r, i = 1, 2, 3$ for the case of $\det \Lambda_i\Theta_i \neq 0$, $i = 1, 2, 3$. Obviously, if $\det \Lambda_i\Theta_i \neq 0$, P_iT_i, $P_i\mathcal{T}_iT_i$ and $P_i\mathcal{T}_i^2T_i$ are linear independent, so all $\dim\langle S_i\rangle = 3$. But $\dim\langle S_i\rangle = 3$ does not necessarily imply $\det \Lambda_i\Theta_i \neq 0$. Here we only need that two of the $\dim\langle S_i\rangle$ 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 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. 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 $\dim\langle S_1\rangle = \dim\langle\hat{S}_1\rangle = 3$. From the construction of S_1 and S_2, we have that $\nu_{i+1} = T_{12}^t\mu_i$, $\hat{\nu}_{i+1} = \hat{T}_{12}^t\hat{\mu}_i$, $i = 1, 2, \cdots$. Then $O_2T_{12}^t\mu_i = O_2\nu_{i+1} = \hat{\nu}_{i+1} = \hat{T}_{12}^t\hat{\mu}_i = \hat{T}_{12}^tO_1\mu_i$, $i = 1, 2, \cdots$. Since μ_{r_0}, μ_{s_0} and μ_{t_0} are linearly independent, $\det(\mu_{r_0}\ \mu_{s_0}\ \mu_{t_0}) \neq 0$, where $(\mu_{r_0}\ \mu_{s_0}\ \mu_{t_0})$ denotes the 3×3 matrix given by the three column vectors μ_{r_0}, μ_{s_0} and μ_{t_0}. From $O_2T_{12}^t(\mu_{r_0}\ \mu_{s_0}\ \mu_{t_0}) = \hat{T}_{12}^tO_1(\mu_{r_0}\ \mu_{s_0}\ \mu_{t_0})$, we get $O_2T_{12}^t = \hat{T}_{12}^tO_1$. Then $\hat{T}_{12} = O_1T_{12}O_2^t$. The same result can be obtained from $\dim\langle S_2\rangle = \dim\langle\hat{S}_2\rangle = 3$. ■

Proof of Lemma 1 From $\mathrm{tr}(T_{12}T_{12}^t)^\alpha = \mathrm{tr}(\hat{T}_{12}\hat{T}_{12}^t)^\alpha$, $\alpha = 1, 2$ and $\det T_{12} = \det \hat{T}_{12}$, one has that T_{12} and $\hat{T}_{12}$ have the same singular values. According to the singular value decomposition, there are $P_i, \hat{P}_i \in O(3)$, $i = 1, 2$, such that $P_1T_{12}P_2^t = \hat{P}_1\hat{T}_{12}\hat{P}_2^t = diag(t_1, t_2, t_3)$, where t_1, t_2 and t_3 are the singular values. Set $O_1 = \hat{P}_1^tP_1$, $O_2 = \hat{P}_2^tP_2 \in O(3)$, we have $\hat{T}_{12} = O_1T_{12}O_2^t$. From $\det T_{12} = \det \hat{T}_{12}$, we have that $\det O_1 = \det O_2 = \pm 1$. If $\det O_1 = \det O_2 = -1$, we may change P_i to $-P_i$ to have $O_i \in SO(3)$. ■

Proof of Theorem 2 We only need to prove the "only if" part, i.e., to find $O_1, O_2 \in SO(3)$ such that $\hat{T}_{12} = O_1T_{12}O_2^t$, $\hat{T}_1 = O_1T_1$, and $\hat{T}_2 = O_2T_2$ for two 2-qubit states ρ and $\hat{\rho}$. From Lemma 1, we have $P_i, \hat{P}_i \in O(3)$, such that $\hat{P}_i^tP_i \in SO(3)$ and

$$P_1T_{12}P_2^t = \hat{P}_1\hat{T}_{12}\hat{P}_2^t = \mathrm{diag}(t_1, t_2, t_3). \tag{5}$$

Hence

$$P_1T_{12}T_{12}^tP_1^t = \hat{P}_1\hat{T}_{12}\hat{T}_{12}^t\hat{P}_1^t = P_2T_{12}^tT_{12}P_2^t = \hat{P}_2\hat{T}_{12}^t\hat{T}_{12}\hat{P}_2^t = \mathrm{diag}(t_1^2, t_2^2, t_3^2).$$

Let $D = \mathrm{diag}(t_1, t_2, t_3)$, then $P_1S_1 = \{P_1T_1, DP_2T_2, D^2P_1T_1, D^3P_2T_2, D^4P_1T_1, \cdots\}$, $P_2S_2 = \{P_2T_2, DP_1T_1, D^2P_2T_2, D^3P_1T_1, D^4P_2T_2, \cdots\}$, we have $\langle P_1\mu_i, P_1\mu_j\rangle = \langle\mu_i, \mu_j\rangle = \langle\hat{\mu}_i, \hat{\mu}_j\rangle = \langle\hat{P}_1\hat{\mu}_i, \hat{P}_1\hat{\mu}_j\rangle$, and $\langle P_2\nu_i, P_2\nu_j\rangle = \langle\hat{P}_2\hat{\nu}_i, \hat{P}_2\hat{\nu}_j\rangle$. Denote $P_1T_1 = (a_1\ \ b_1\ \ c_1)^t$, $P_2T_2 = (a_2\ \ b_2\ \ c_2)^t$. By using $\langle P_1\mu_1, P_1\mu_j\rangle = \langle\hat{P}_1\hat{\mu}_1, \hat{P}_1\hat{\mu}_j\rangle$, $j = 1, 3, 5$, i.e. $\langle P_1T_1, D^rP_1T_1\rangle = \langle\hat{P}_1\hat{T}_1, D^r\hat{P}_1\hat{T}_1\rangle$, $r = 0, 2, 4$, we get

$$t_1^j a_1^2 + t_2^j b_1^2 + t_3^j c_1^2 = t_1^j \hat{a}_1^2 + t_2^j \hat{b}_1^2 + t_3^j \hat{c}_1^2, \quad j = 0, 2, 4. \tag{6}$$

Similarly, using $\langle P_2\nu_1, P_2\nu_j\rangle = \langle \hat{P}_2\hat{\nu}_1, \hat{P}_2\hat{\nu}_j\rangle$, $j = 1, 3, 5$, and $\langle P_1\mu_1, P_1\mu_j\rangle = \langle \hat{P}_1\hat{\mu}_1, \hat{P}_1\hat{\mu}_j\rangle$, $j = 2, 4{,}6$, we obtain

$$t_1^j a_2^2 + t_2^j b_2^2 + t_3^j c_2^2 = t_1^j \hat{a}_2^2 + t_2^j \hat{b}_2^2 + t_3^j \hat{c}_2^2, \quad j = 0, 2, 4. \tag{7}$$

$$t_1^j a_1 a_2 + t_2^j b_1 b_2 + t_3^j c_1 c_2 = t_1^j \hat{a}_1\hat{a}_2 + t_2^j \hat{b}_1\hat{b}_2 + t_3^j \hat{c}_1\hat{c}_2, \quad j = 1, 3, 5. \tag{8}$$

1. If t_1, t_2, t_3 are all not equal, from (6) and (7) we can conclude that $\alpha_i = \pm\hat{\alpha}_i$ for $\alpha = a, b, c$ and $i = 1, 2$.

(i) If $t_i \neq 0$, $i = 1, 2, 3$, from (8) we get $\alpha_1\alpha_2 = \hat{\alpha}_1\hat{\alpha}_2$ for $\alpha = a, b, c$. Now if $\alpha_1\alpha_2 \neq 0$, then we have $\alpha_1 = \hat{\alpha}_1 \Leftrightarrow \alpha_2 = \hat{\alpha}_2$. If $\alpha_1\alpha_2 = 0$, suppose $\alpha_1 = 0$, then we have $\hat{\alpha}_1 = 0$. If $\alpha_2 = \hat{\alpha}_2$, we also can write $\alpha_1 = \hat{\alpha}_1$. Let $R = \mathrm{diag}\{e_1, e_2, e_3\}$, where e_i take values $+1$ or -1, such that $RP_1T_1 = \hat{P}_1\hat{T}_1$. Then one must have $RP_2T_2 = \hat{P}_2\hat{T}_2$. Note that the equality (5) is also true if one replaces P_i by RP_i. Let $O_1 = \hat{P}_1^t RP_1$, $O_2 = \hat{P}_2^t RP_2$. We have $\hat{T}_i = O_iT_i$ for $i = 1{,}2$, and $\hat{T}_{12} = O_1T_{12}O_2^t$. To assure that O_i be special, we have $\det R = 1$. Firstly, from $\dim\langle P_iS_i\rangle = \dim\langle S_i\rangle < 3$, we have that P_iT_i, $D^2P_iT_i$, $D^4P_iT_i$ are linearly dependent. Then there is at least one $\alpha_i^0 \in \{a_i, b_i, c_i\}$ that is zero. Hence if P_1T_1 and $D^2P_1T_1$ are linearly independent, we have that DP_2T_2 can be linearly represented by P_1T_1 and $D^2P_1T_2$. Using $t_1t_2t_3 \neq 0$ and supposing $a_1 = 0$, we get that a_2 is also zero. Now e_1 in R can be chosen to be 1 or -1 freely. We can choose e_1 to assure that $\det R = 1$. Similarly, for the case that P_2T_2 and DP_2T_2 are linear independent, we can also find R which has determinate one. Lastly, if P_iT_i and $D^2P_iT_i$ 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 $\alpha_1 = \alpha_2 = 0$, such that $\det R = 1$.

(ii) If there exists a $t_i = 0$, say, $t_3 = 0$, then we have $\alpha_1\alpha_2 = \hat{\alpha}_1\hat{\alpha}_2$ for $\alpha = a, b$ from (8). And the invariant **I** can assure that $c_1c_2 = \hat{c}_1\hat{c}_2$. From the discussion above, we have the conclusion.

2. If there are two different values of t_1, t_2, t_3, suppose $t_1 = t_2 \neq t_3$. 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 $t_i \neq 0$, $i = 1{,}2{,}3$, from (8) we get $a_1a_2 + b_1b_2 = \hat{a}_1\hat{a}_2 + \hat{b}_1\hat{b}_2$, $c_1c_2 = \hat{c}_1\hat{c}_2$. Then there exists a matrix $M \in O(2)$ such that $M\begin{pmatrix} a_i \\ b_i \end{pmatrix} = \begin{pmatrix} \hat{a}_i \\ \hat{b}_i \end{pmatrix}$, $i = 1, 2$. And there is an $e = 1$ or -1 such that $ec_i = \hat{c}_i$ for $i = 1, 2$. Therefore letting $R = \begin{pmatrix} M & \\ & e \end{pmatrix}$, one has $RPT_1 = \hat{P}\hat{T}_1$ and $RQT_2 = \hat{Q}\hat{T}_2$ again. For the speciality of R, from the dimension of $\langle S_i\rangle$, we have $\det\begin{pmatrix} a_1 & a_2 \\ b_1 & b_2 \end{pmatrix} = 0$ or $c_1 = c_2 = 0$. Hence, we can choose suitable M or e to make sure that R is special.

(ii) If $t_1 = t_2 = 0$, we only have $c_1c_2 = \hat{c}_1\hat{c}_2$. We can get $M_i \in O(2)$ such that $M_i\begin{pmatrix} a_i \\ b_i \end{pmatrix} = \begin{pmatrix} \hat{a}_i \\ \hat{b}_i \end{pmatrix}$, $i = 1, 2$, and $R_i = \begin{pmatrix} M_i & \\ & e \end{pmatrix}$ to get the result similarly. We can choose suitable M_i for the speciality of R_i.

(iii) If $t_3 = 0$, then one has R_1, R_2 with the same M but different e to prove the theorem. The speciality for R_i is similar to the case of $t_i \neq 0$.

3. If $t_1 = t_2 = t_3 \neq 0$, 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 $i = 1, 2$, and $a_1a_2 + b_1b_2 + c_1c_2 = \hat{a}_1\hat{a}_2 + \hat{b}_1\hat{b}_2 + \hat{c}_1\hat{c}_2$. Then we have $R \in SO(3)$ such that $RP_1T_1 = \hat{P}_1\hat{T}_1$ and $RP_2T_2 = \hat{Q}_2\hat{T}_2$. Replacing P_i by RP_i in (5) we get the result.

4. If $t_1 = t_2 = t_3 = 0$, 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 $RP_iT_i = \hat{P}_i\hat{T}_i$, $i = 1, 2$. Replacing P_i by RP_i in (5) one gets the result. ■

Proof of Theorem 3 For 3-qubit states ρ and $\hat{\rho}$, they are LU equivalent if and only if there are $O_i \in SO(3)$, $i = 1, 2, 3$, such that $\hat{T}_i = O_iT_i$, $\hat{T}_{ij} = O_iT_{ij}O_j^t$ and $\hat{T}_{123} = O_1 \otimes O_2 \otimes O_3T_{123}$. Suppose $\dim\langle S_i\rangle = \dim\langle \hat{S}_i\rangle = 3$, for $i = 1, 2$. By using the given invariants, we have $O_i \in SO(3)$ such that $\hat{\mu}_i = O_1\mu_i$, $\hat{\nu}_i = O_2\nu_i$ and $\hat{\omega}_i = O_3\omega_i$ for $i = 1, 2, \cdots$, as well as, $\hat{T}_{12}^t\hat{\mu}_i = O_2T_{12}^t\mu_i$, $\hat{T}_{13}^t\hat{\mu}_i = O_3T_{13}^t\mu_i$, $\hat{T}_{23}^t\hat{\nu}_i = O_3T_{23}^t\nu_i$ and $\hat{T}_{3|12}\hat{\mu}_i \otimes \hat{\nu}_j = O_3T_{3|12}\mu_i \otimes \nu_j$ for $i, j = 1, 2, \cdots$. Suppose μ_{i_1}, μ_{i_2} and μ_{i_3} are linear independent. Then $O_2T_{12}^t(\mu_{i_1}\ \mu_{i_2}\ \mu_{i_3}) = \hat{T}_{12}^t(\hat{\mu}_{i_1}\ \hat{\mu}_{i_2}\ \hat{\mu}_{i_3}) = \hat{T}_{12}^tO_1(\mu_{i_1}\ \mu_{i_2}\ \mu_{i_3})$. Hence we get $O_2T_{12}^t = \hat{T}_{12}^tO_1$, i.e. $\hat{T}_{12} = O_1T_{12}O_2^t$. Similarly, we have $\hat{T}_{13} = O_1T_{13}O_2^t$, $\hat{T}_{23} = O_2T_{23}O_3^t$. From $\hat{T}_{3|12}\hat{\mu}_i \otimes \hat{\nu}_j = O_3T_{3|12}\mu_i \otimes \nu_j$, $i, j = 1, 2, \cdots$, we have

$$\hat{T}_{3|12}O_1 \otimes O_2(\mu_{i_1}\ \mu_{i_2}\ \mu_{i_3}) \otimes (\nu_{j_1}\ \nu_{j_2}\ \nu_{j_3}) = O_3T_{3|12}(\mu_{i_1}\ \mu_{i_2}\ \mu_{i_3}) \otimes (\nu_{j_1}\ \nu_{j_2}\ \nu_{j_3}),$$

where ν_{j_1}, ν_{j_2}, ν_{j_3} are linear independent vectors in S_2. Using the linear independence of μ_{i_1}, μ_{i_2}, μ_{i_3} and ν_{j_1}, ν_{j_2}, ν_{j_3}, we get $\hat{T}_{3|12}O_1 \otimes O_2 = O_3T_{3|12}$ or $\hat{T}_{3|12} = O_3T_{3|12}O_1^t \otimes O_2^t$ which is equivalent to $\hat{T}_{123} = O_1 \otimes O_2 \otimes O_3T_{123}$. ■

References

1. Nielsen, M. A. & Chuang, I. L. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, England(2000).
2. Bennett, C. H., DiVincenzo, D. P., Smolin, J. A. & Wootters, W. K. Mixed-state entanglement and quantum error correction. *Phys. Rev. A* **54**, 3824 (1996); Bennett, C. H., Bernstein, H. J., Popescu, S. & Schumacher, B. Concentrating Partial Entanglement by Local Operations. *ibid*. **53**, 2046 (1996); Vedral, V., Plenio, M. B., Rippin, M. A. & Knight, P. L. Quantifying Entanglement. *Phys. Rev. Lett.* **78**, 2275 (1997).
3. Wootters, W. K. Entanglement of Formation of an Arbitrary State of Two Qubits. *Phys. Rev. Lett.* **80**, 2245 (1998).
4. Horodecki, R., Horodecki, P. & Horodecki, M. Violating Bell inequality by mixed spin-1/2 states: necessary and sufficient condition. *Phys. Lett. A* **200**, 340 (1995).
5. Werner, R. F. & Wolf, M. M. All-multipartite Bell-correlation inequalities for two dichotomic observables per site. *Phys. Rev. A* **64**, 032112 (2001).
6. Żukowski, M. & Brukner, Č. Bells Theorem for General N –Qubit States. *Phys. Rev. Lett.* **88**, 210401 (2002).
7. Li, M. & Fei, S. M. Bell inequalities for multipartite qubit quantum systems and their maximal violation. *Phys. Rev. A* **86**, 052119 (2012).
8. Horodecki, M., Horodecki, P. & Horodecki, R. General teleportation channel, singlet fraction, and quasidistillation. *Phys. Rev. A* **60**, 1888 (1999).
9. Albeverio, S., Fei, S. M. & Yang, W. L. Optimal teleportation based on bell measurements. *Phys. Rev. A* **66**, 012301 (2002).
10. Makhlin, Y. Nonlocal Properties of Two-Qubit Gates and Mixed States, and the Optimization of Quantum Computations. *Quant. Info. Proc.* **1**, 243 (2002).
11. Linden, N., Popescu, S. & Sudbery, A. Nonlocal Parameters for Multiparticle Density Matrices. *Phys. Rev. Lett.* **83**, 243 (1999); Sun, B. Z., Fei, S. M., Li-Jost, X. Q. & Wang, Z. X. A Note on Equivalence of Bipartite States under Local Unitary Transformations. *J. Phys. A* **39**, L43-L47 (2006).
12. Zhou, C. Q., Zhang, T. G., Fei, S. M., Jing, N. H. & Li-Jost, X. Q. Local unitary equivalence of arbitrary dimensional bipartite quantum states. *Phys. Rev. A* **86**, 010303(R) (2012).
13. Zhang, T. G., Zhao, M. J., Li, M., Fei, S. M. & Li-Jost, X. Q. Criterion of local unitary equivalence for multipartite states. *Phys. Rev. A* **88**, 042304 (2013).
14. Liu, B., Li, J. L., Li, X. & Qiao, C. F. Local Unitary Classification of Arbitrary Dimensional Multipartite Pure States. *Phys. Rev. Lett.* **108**, 050501 (2012).
15. Li, M., Zhang, T. G., Fei, S. M., Li-Jost, X. Q. & Jing, N. H. Local unitary equivalence of multiqubit mixed quantum states. *Phys. Rev. A* **89**, 062325 (2014).
16. Martins, A. M. Necessary and sufficient conditions for local unitary equivalence of multiqubit states. *Phys. Rev. A* **91**, 042308 (2015).
17. Li, J. L. & Qiao, C. F. Classification of arbitrary multipartite entangled states under local unitary equivalence. *J. Phys. A* **46**, 075301 (2013).
18. Jing, N. H., Li, M., Li-Jost, X. Q., Zhang, T. G. & Fei, S. M. SLOCC invariants for multipartite mixed states. *J. Phys. A* **47**, 215303 (2014).
19. Specht, W. Zur Theorie der Matrizen II, Jahresbericht Deutsch Math. Verein. *Jber. Deutsch Math. Verein.* **50**, 19 (1940).
20. Jing, N. H., Fei, S. M., Li, M., Li-Jost, X. Q. & Zhang, T. G. Local unitary invariants of generic multiqubit states. *Phys. Rev. A* **92**, 022306 (2015).
21. Albeverio, S., Fei, S. M., Parashar, P. & Yang, W. L. Nonlocal properties and local invariants for bipartite systems. *Phys. Rev. A* **68**, 010303 (2003).
22. Albeverio, S., Fei, S. M. & Goswami, D. Local Invariants for a Class of Mixed States. *Phys. Lett. A* **340**, 37 (2005).
23. Albeverio, S., Cattaneo, L., Fei, S. M. & Wang, X. H. Equivalence of Tripartite Quantum States under Local Unitary Transformations. *Int. J. Quant. Inform.* **3**, 603 (2005).
24. Kraus, B. Local Unitary Equivalence of Multipartite Pure States. *Phys. Rev. Lett.* **104**, 020504 (2010).
25. Kraus, B. Local unitary equivalence and entanglement of multipartite pure states. *Physical Review A* **82**(3) (2010).
26. Maciążek, T., Oszmaniec, M. & Sawicki, A. How many invariant polynomials are needed to decide local unitary equivalence of qubit states? *J. Math. Phys.* **54**, 092201 (2013); Sawicki, A. & Kuś, M. Geometry of the local equivalence of states. *J. Phys. A: Math. Theor*. 44, 495301 (2011).
27. King, R. C., Welsh, T. A. & Jarvis, P. D. The mixed two-qubit system and the structure of its ring of local invariants. *J. Phys. A.* **40**, 10083 (2007).

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Author Contributions

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Additional Information

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