Local Invariants for a Class of Mixed States

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Abstract

We investigate the equivalence of quantum states under local unitary transformations. A complete set of invariants under local unitary transformations is presented for a class of mixed states. It is shown that two states in this class are locally equivalent if and only if all these invariants have equal values for them.

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Quantum entangled states are playing very important roles in quantum information processing and quantum computation [1]. The properties of entanglement for multipartite quantum systems remain invariant under local unitary transformations on the subsystems. Hence the entanglement can be characterized by all the invariants under local unitary transformations. A complete set of invariants gives rise to the classification of the quantum states under local unitary transformations. Two quantum states are locally equivalent if and only if all these invariants have equal values for these states. In [2, 3], a generally non-operational method has been presented to compute all the invariants of local unitary transformations. In [4], the invariants for general two-qubit systems are studied and a complete set of 18 polynomial invariants is presented. In [5] the invariants for three qubits states are also discussed. In [6] a complete set of invariants for generic density matrices with full rank has been presented.

In the present paper we investigate the invariants for arbitrary (finite-) dimensional bipartite quantum systems. We present a complete set of invariants for a class of quantum
mixed states and show that two of these density matrices are locally equivalent if and only if all these invariants have equal values for these density matrices.

1 Invariants for a class of states with arbitrary rank

Let us consider a general mixed state $\rho$ in a bi-partite $n \times n$ system $H \otimes H$ ($n \geq 2$), with a given orthonormal basis $\{|1>,...,|n>\}$ of $H$. $\rho$ has the eigen-decomposition

$$\rho = \sum_{l=0}^{N} \mu_l |\xi_l> <\xi_l|,$$

where the rank of $\rho$ is $r(\rho) = N + 1$ ($N \geq 1$), $\mu_l$ are eigenvalues with the eigenvectors $|\xi_l> = \sum_{ij} \xi_{ij}^{(l)} |ij>$ (and $|\xi_l> <\xi_l|$ denotes, as usual, the projector onto $|\xi_l>$), $\xi_{ij}^{(l)} \in \mathbb{C}$. Let $A_l$ denote the matrix with entries $\xi_{ij}^{(l)}$. We call a matrix “multiplicity free” if each of its singular values has multiplicity one. Let $\mathcal{F}$ denote the class of states $\rho$ for which $A_0$ is multiplicity free. We shall find a complete set of local invariants for the class $\mathcal{F}$, such that any pair of states belong to $\mathcal{F}$ are equivalent under local unitary transformations if and only if they have the same values of these invariants.

Let $(\psi_1,...,\psi_n)$, $(\eta_1,...,\eta_n)$ be orthonormal bases such that $A_0 = \sum_i \lambda_i |\psi_i> <\eta_i|$ is the singular value decomposition of $A_0$, where $\lambda_1 > ... > \lambda_n$ denote the singular values arranged in the decreasing order. Let $b_{ij}^{(l)} := <\psi_i|A_l\eta_j>$ for $l = 1, 2, ..., N$, and for positive integers $k, r \geq 1$, and multi-indices $\check{l} = (i_1,...i_{k+1})$, (with $i_p$’s all distinct), $\check{m} = (j_1,...j_{r+1})$ (with $j_q$’s all distinct), where $i_p, j_q \in \{1,...,n\}$ $\forall p,q$, $\check{l} = (l_1,...,l_k)$, $\check{m} = (m_1,...,m_r)$ $(l_t, m_s \in \{1,...,N\})$ with $i_1 = j_1$, $i_{k+1} = j_{r+1}$, and such that $(\check{l}, \check{m}) \neq (\check{m}, \check{m})$, we define

$$I^\rho(\check{l}, \check{m}) := \frac{b_{i_1j_1}^{(l_1)}...b_{i_kb_{k+1}}^{(l_k)}}{b_{j_1j_2}^{(m_1)}...b_{j_mj_{r+1}}^{(m_r)}}$$

whenever the denominator in the above formula is nonzero. Let $\Sigma^\rho$ be the set of $(\check{l}, \check{m})$ such that $I^\rho(\check{l}, \check{m})$ is well defined.

The following theorem is an immediate consequence of Lemma 6, Lemma 7 and the remark 5.

**Theorem 1** Two quantum states in $\mathcal{F}$ with the same rank and eigenvalues $\mu_l$, $l = 0,...,N$, are equivalent under local unitary transformations if and only if they have the same values of the following invariants:

1) Matrices $(B_l)_{ij} = |<\psi_i, A_l\eta_j>|$, $i,j = 1,...,n$, $l = 1,...,N$,

2) Vector $C = (<\psi_1, A_0\eta_1>,...,<\psi_n, A_0\eta_n>)$,

3) Vectors $D_l = (<\psi_1, A_l\eta_1>,...,<\psi_{n-1}, A_l\eta_{n-1}>)$, $l = 1,...,N$,

4) $I^\rho$ with the domain $\Sigma^\rho$. 


Proof: It is clear that the quantities above are local invariant. Let us prove that these invariants are complete for the class $F$. Suppose that $\rho$ and $\rho'$ are two states in the class $F$ such that they have the same values of these invariants. Let $\rho = \sum_{i=0}^{N} \mu_i |\xi_i > < \xi_i|$ and $\rho' = \sum_{i=0}^{N} \mu_i |\xi'_i > < \xi'_i|$ be the eigen-decomposition of the two states, and let $A_l = (a^{(l)}_{ij})$, $A'_l = (a'^{(l)}_{ij})$ be $n \times n$ complex matrices associated with the decomposition of $\xi_i$ and $\xi'_i$ respectively, that is, $\xi_i = \sum_{i} a^{(l)}_{ij} |ij >$, and $\xi'_i = \sum_{i} a'^{(l)}_{ij} |ij >$. By assumption, $A_0$ and $A'_0$ are multiplicity-free, with the singular-value decomposition

$$A_0 = \sum_i \lambda_i |\psi_i > < \eta_i|,$$  

$$A'_0 = \sum_i \lambda'_i |\psi'_i > < \eta'_i|,$$

with the singular values arranged in the decreasing order. Since $\lambda_i = < \psi_i, A_0 \eta_i >$ and $\lambda'_i = < \psi'_i, A'_0 \eta'_i >$, it follows that $\lambda_i = \lambda'_i$ for all $i$. Set $(B_l)_{ij} = < \psi_i, A_l \eta_j >$, $(B'_l)_{ij} = < \psi'_i, A'_l \eta'_j >$ for $l = 0, 1, ..., N$. It is easy to see from the equalities of the invariants labeled by 3) and 1) in (2) respectively. Thus, by Lemma 7 of Appendix, we conclude that there exist unitary matrices $U$ and $V$ such that $UA_lV^* = A'_l$ for $l = 0, 1, ..., N$. Clearly, we have, $\xi'_i = \sum_{ij} a'^{(l)}_{ij} |ij > = \sum_{ij} \sum_{kl} u_{ik} a_{kl} \bar{\pi}_{jl} |ij > = \sum_{kl} a_{kl} (\sum_{i} u_{ik} |i >) \otimes (\sum_{j} \bar{\pi}_{jl} |j >) = (U \otimes \bar{V}) \xi_i$, where $U = (w_{ij})$, $V = (v_{ij})$, $\bar{V} = (\bar{v}_{ij})$. Thus, $\rho' = (U \otimes \bar{V})\rho(U \otimes \bar{V})^*$.

As an example we calculate all the invariants for the Werner state [7], $\rho_w = (1-p)I_{4 \times 4}/4 + p|\Psi_- > < \Psi_-|$, where $0 \leq p \leq 1$, $I_{4 \times 4}$ is the $4 \times 4$ identity matrix and $|\Psi_- > = \frac{1}{\sqrt{2}}(|01 > -|10 >)$.

Here, $N = 3$, $\mu_1 = \mu_2 = \mu_3 = \frac{1-p}{4}$, $\mu_4 = \frac{3p+1}{4}$. We have,

$$\xi_0 = |00 >, \quad \xi_1 = |11 >, \quad \xi_2 = \frac{1}{\sqrt{2}}(|01 > +|10 >), \quad \xi_3 = \frac{1}{\sqrt{2}}(|01 > -|10 >).$$

Hence $A_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $A_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, $A_2 = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$, $A_3 = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$. The orthonormal bases $\{\psi_1, \psi_2\}$ and $\{\eta_1, \eta_2\}$ can be chosen to be the canonical basis $\{|0 >, |1 >\}$.

Thus, $(B_l)_{ij} = | < \psi_i, A_l \eta_j > | = |(A_l)_{ij}|$ in this case. The invariants are:
1) $B_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, $B_2 = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$, $B_3 = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$;
2) $C = (1, 0)$;
3) $D_l = 0$, $l = 1, 2, 3$;
4) $\Sigma^o = \{(i_1, i_2), (j_1, j_2), (l_1, m_1)\}$; $l_1, m_1 \in \{2, 3\}$, $i_p, j_q \in \{1, 2\}$, $i_1 \neq i_2, j_1 \neq j_2, (i_1, i_2, l_1) \neq (j_1, j_2, m_1)$, which can be explicitly written as:

$$\{(i_1, 2), (1, 2), (2, 3)\}; \{(i_1, 2), (1, 2), (3, 2)\}; \{(i_1, 2), (2, 1), (2, 3)\}; \{(i_1, 2), (2, 1), (3, 2)\}; \{(i_2, 1), (1, 2), (2, 3)\}; \{(i_2, 1), (2, 1), (2, 3)\}; \{(i_2, 1), (1, 2), (3, 2)\}; \{(i_2, 1), (2, 1), (3, 2)\}.$$ 

The values of $I^o$ on the above elements (in the same order) are $1, 1, 1, -1, 1, 1, 1, -1, -1, -1, -1$. 

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Remark 2 The class of states $\mathcal{F}$ for which our result works is indeed a large one. In fact, $\mathcal{F} \cap \mathcal{F}_k$ is dense (in norm) in $\mathcal{F}_k$, where $\mathcal{F}_k$ denotes the set of $n \times n$ bipartite states of rank $k+1$, $k \geq 0$. Consider any state $\rho \in \mathcal{F}_k$, with the eigen-decomposition $\rho = \sum_{i=0}^{k} \mu_i |\xi_i\rangle \langle \xi_i|$, with $\xi_i = \sum_{ij} a_{ij}^i |i\rangle |j\rangle$ and suppose that $A_0 := (a_{ij}^i)_{i,j=1}^{n}$ is not necessarily multiplicity-free. We claim that for any $\epsilon > 0$, we can choose $n \times n$ multiplicity-free matrix $A_0' = (a_{ij}^i')$ such that $|a_{ij} - a_{ij}'| \leq \epsilon \forall i, j$. Indeed, if $A_0 = \sum_i \lambda_i |\psi_i\rangle \langle \psi_i|$, with $\lambda_i$'s may not be all distinct, we can choose $\lambda_i$'s which are distinct among themselves, with $|\lambda_i - \lambda_i'| \leq \epsilon$ for all $i$. $A_0'$ can be taken to be the matrix $\sum_i \lambda_i' |\psi_i\rangle \langle \psi_i|$, where $\lambda_0' = \sum_{ij} a_{ij}' |ij\rangle$. Clearly, any two states $\rho$ and $\rho'$ are locally equivalent. Thus, $\rho' \in \mathcal{F}_k \cap \mathcal{F}$ and $\|\rho - \rho\| \leq 2n^3 \epsilon$.

2 The invariants for another class of rank two states

We now consider another class of states which are rank two states on $\mathbb{C}^n \times \mathbb{C}^n$ such that the matrices $A_0, A_1$ are of the following form:

$$A_0 = pP + (1-p)(1-P), \quad A_1 = qQ + (1-q)(1-Q),$$

(3)

where $0 < p, q < 1$ and $P, Q$ are projection operators. We denote this class of states by $\mathcal{G}$.

Theorem 3 The following is a complete set of local invariants for the states in class $\mathcal{G}$:

$$\begin{align*}
Tr(\rho^2), \quad Tr(A_0^k), \quad Tr(A_1^k); \\
Tr[((2P-1)(2Q-1))^k], \quad Tr[((2P-1)E_{\pm})^k], \quad k = 1, ..., n,
\end{align*}$$

(4)

where $E_{\pm}$ denotes the projection onto the eigenspace of $(2P-1)(2Q-1)$ corresponding to the eigenvalue $\pm 1$.

Proof : Clearly, the above quantities are local invariants. We show that they are complete. Let $\rho'$ be another state in $\mathcal{G}$, with $p', q', P'$ and $Q'$ instead of $p, q, P$ and $Q$ respectively. Since $\rho$ has two eigenvalues and $Tr(\rho) = 1$, the eigenvalues are determined by $Tr(\rho^2)$. Similarly, $Tr(A_0^k)$ and $Tr(A_1^k)$ completely determine $p$ and $q$. Thus, $p = p'$ and $q = q'$. Furthermore, by Lemma 8, the equality of the traces $Tr[((2P-1)(2Q-1))^k], Tr[((2P-1)E_{\pm})^k], \quad k = 1, ..., n_i$, with their primed counterparts implies that we can find unitary matrix $U$ such that $UPU^* = P'$, $UQU^* = Q'$. This proves that $\rho$ and $\rho'$ are locally equivalent. □

This Theorem applies to a class of $d$-computable states [9], with a slight modification as follows. Consider a fixed local unitary operator $W = T_1 \otimes T_2$, and let $\mathcal{G}_W$ denote the set of states $\rho$ such that $W \rho W^* \in \mathcal{G}$. Clearly, any two states $\rho$ and $\rho'$ in $\mathcal{G}_W$ are locally equivalent if and only if $W \rho W^*$ and $W \rho' W^*$ in $\mathcal{G}$ are locally equivalent too, which can be determined by computing the invariants (4).
For example, we consider a pure state on $\mathbb{C}^4 \times \mathbb{C}^4$, $|\psi\rangle = \sum_{i,j=1}^{4} a_{ij} |ij\rangle$, $a_{ij} \in \mathbb{C}$, $\sum_{i,j=1}^{4} a_{ij} a_{ij}^* = 1$. Suppose that the matrix $A = (a_{ij})$ has the form

$$A = \begin{pmatrix} 0 & 0 & a_1 & b_1 \\ 0 & 0 & b_1 & d_1 \\ a_1 & b_1 & 0 & 0 \\ b_1 & d_1 & 0 & 0 \end{pmatrix},$$

(5)

$a_1, b_1, d_1 \in \mathbb{C}$, satisfying $a_1, d_1 \geq 0$, $a_1 d_1 \geq |b_1|^2$. In this case, $|\psi\rangle$ is a $d$-computable state and its entanglement of formation is a monotonically increasing function of the generalized concurrence $d = 4(a_1 d_1 - |b_1|^2)$. The entanglement of formation for any mixed states with decompositions on $d$-computable states can be calculated analytically. Let $|\psi'\rangle = \sum_{i,j=1}^{4} a'_{ij} |ij\rangle$ be another pure state with $A' = (a'_{ij})$ of the form (5) and $<\psi'|\psi> = 0$. Then

$$\rho = \mu |\psi><\psi| + (1 - \mu) |\psi'><\psi'|$$

is an entangled rank two density matrix. Set $T = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$ and $W = T \otimes I_4$. As the matrices $A, A'$ are of the form $TB$, where $B$ is a nonnegative matrix with at most two different eigenvalues with degeneracy two, $\rho \in G_W$, and the invariants (4) determine the equivalence of two mixed states of the form (6) under local unitary transformations.

3 Remarks and conclusions

We have investigated the equivalence of quantum bipartite states under local unitary transformations. For the states $\rho$ for which $A_0$ is multiplicity free, as well as for the states $\rho$ which are of rank two on $\mathbb{C}^n \times \mathbb{C}^n$ such that each of the matrices $A_0$ and $A_1$ is a nonnegative matrix having at most two different eigenvalues, a complete set of invariants under local unitary transformations is presented. Two of these states are locally equivalent if and only if all these invariants have equal values for them.

The results can be generalized to the multipartite case. For instance, we can consider a tripartite state $\rho_{ABC}$ with subsystems, say, $A, B$ and $C$ as bipartite states $\rho_{A|BC}$, $\rho_{AB|C}$ or $\rho_{AC|B}$. If the conditions in our theorems are satisfied for one of the bipartite decompositions, say $\rho_{A|BC}$, we can judge whether two such tripartite states are equivalent or not under local unitary transformations, in this bipartite decomposition. If they are, we consider further $\rho_{BC} = Tr_A(\rho_{A|BC})$, which is again a bipartite state and can be judged by using our theorems, if the related conditions are satisfied. In this way the equivalence for a class of multipartite states can also be studied according to our theorems.
4 APPENDIX

Lemma 4 Let $B_l = (b_{ij}^{(l)})$, $C_l = (c_{ij}^{(l)})$ be $n \times n$ matrices with complex entries, $l = 1, \ldots, N$, where $n$ and $N$ are positive integers. Then there exist complex numbers $u_i$, $i = 1, \ldots, n$, with $|u_i| = 1$, $\forall i$ and $c_{ij}^{(l)} = \frac{u_i}{u_j} b_{ij}^{(l)}$ for all $i, j = 1, \ldots, n$, $l = 1, \ldots, N$ if and only if the following conditions hold :

(I) $b_{ii}^{(l)} = c_{ii}^{(l)} \forall i, l$,

(II) $|b_{ij}^{(l)}| = |c_{ij}^{(l)}| \forall i, j, l$,

(III) For all choices of $l_1, \ldots, l_k, m_1, \ldots, m_r \in \{1, 2, \ldots, N\}$ ($k, r \geq 1$), $i_1, \ldots, i_{k+1}, j_1, \ldots, j_{r+1} \in \{1, 2, \ldots, n\}$ with $i_1 = j_1$, $i_{k+1} = j_{r+1}$,

$$b_{i_1i_2}^{(l_1)} b_{i_2i_3}^{(l_2)} \ldots b_{i_ki_{k+1}}^{(l_k)} c_{i_{k+1}j_1}^{(m_1)} \ldots c_{i_{r+1}j_{r+1}}^{(m_r)} = c_{i_1i_2}^{(l_1)} c_{i_2i_3}^{(l_2)} \ldots c_{i_{k+1}j_1}^{(m_1)} b_{i_1i_2}^{(l_2)} \ldots b_{i_{r+1}j_{r+1}}^{(m_r)}$$

Proof : The proof of the necessity of the conditions (I), (II), (III) is trivial. We prove the sufficiency of these conditions. Assume that (I), (II), (III) are satisfied. We define a relation $\sim$ on the set $\{1, 2, \ldots, n\}$ as follows. Let us set $i \sim j$ for all $i$, and for $i, j$ different, let us say $i \rightarrow j$ if there exist $i_1, \ldots, i_{k+1}$ ($k \geq 1$) with $i_1 = i$, $i_{k+1} = j$ and $l_1, \ldots, l_k$ such that $b_{i_1i_2}^{(l_1)}, b_{i_2i_3}^{(l_2)}, \ldots, b_{i_{k+1}}^{(l_k)}$ are all nonzero (by (II) this is equivalent to saying that similar quantities with $b$ replaced by $c$ are all nonzero). We set $i \sim j$ (for different $i, j$) if $i \rightarrow j$ and $j \rightarrow i$. It is easy to verify that $\sim$ is an equivalence relation. Let $\{1, 2, \ldots, n\} = E_1 \cup \ldots \cup E_p$ ($p \geq 1$) be the decomposition into equivalence classes. Choose and fix any $i_1^*, \ldots, i_p^*$ from $E_1, \ldots, E_p$ respectively. Set $u_i = 1$ for $i \in \{i_1^*, \ldots, i_p^*\}$. For any other $i$, say $i \in E_t$ ($1 \leq t \leq p$), but $i \neq i_t^*$, we define

$$u_i := \frac{c_{i_1i_2}^{(l_1)} \ldots c_{i_{k+1}}^{(l_k)}}{b_{i_1i_2}^{(l_1)} \ldots b_{i_{k+1}}^{(l_k)}},$$

where $i_1 = i, i_2, \ldots, i_k, i_{k+1} = i_t^*, l_1, \ldots, l_k$ are chosen such that $b_{i_1i_2}^{(l_1)}, \ldots, b_{i_{k+1}}^{(l_k)}$ are nonzero, which exist as $i \sim i_t^*$. $u_i$ is well defined by (III). Indeed, if any other such “path” $i' = i, i'_2, \ldots, i'_{r+1} = i_t^*, l'_1, \ldots, l'_r$ is used, we have by (III)

$$\frac{c_{i_1i_2}^{(l_1)} \ldots c_{i_{k+1}}^{(l_k)}}{b_{i_1i_2}^{(l_1)} \ldots b_{i_{k+1}}^{(l_k)}} = \frac{c_{i'_1i'_2}^{(l'_1)} \ldots c_{i'_{r+1}}^{(l'_r)}}{b_{i'_1i'_2}^{(l'_1)} \ldots b_{i'_{r+1}}^{(l'_r)}},$$

which shows that $u_i$ remains the same if the primed sequence is used. Note also that by (II), we have $|u_i| = 1$ for all $i$.

With this definition of the $u_i$,’s we claim that

$$c_{ij}^{(l)} = \frac{u_i}{u_j} b_{ij}^{(l)} \quad (7)$$

for all $l, i, j$. For $i = j$, (7) follows from (I). In case $b_{ij}^{(l)} = 0$, the relation (7) follows from (II). The only nontrivial case to prove arises when $b_{ij}^{(l)}$ (and hence also $c_{ij}^{(l)}$) is nonzero for $i \neq j$. 


Thus, $i, j$ can be assumed to belong to the same equivalence class, say $E_t$. If $j = i^*_t$, we can take $k = 1$, with $i_1 = i$, $i_2 = j$ in the definition of $u_i$, and the relation (7) follows. Otherwise, i.e. if $j \neq i^*_t$, we choose sequences $i_1 = i$, $i_2, \ldots, i_{k+1} = i^*_t$, $l_1, \ldots, l_k$ for the definition of $u_i$, and $j_1 = j$, $j_2, \ldots, j_{r+1} = i^*_t$, $m_1, \ldots, m_r$ for the definition of $u_j$, so that
\[
\frac{u_i b_{ij}^{(l)}}{u_j c_{ij}^{(l)}} = \frac{b_{ij}^{(l)} b_{j1}^{(m_1)} \cdots b_{jr}^{(m_r)} c_{ij}^{(l)} c_{j1}^{(m_1)} \cdots c_{jr}^{(m_r)}}{b_{ij}^{(l)} b_{j1}^{(l)} \cdots b_{jr}^{(l)} c_{ij}^{(l)} c_{j1}^{(l)} \cdots c_{jr}^{(l)}} = 1
\]
by (III). This completes the proof of the Lemma. \hfill \Box

**Remark 5** In the statement of the above Lemma, it is easy to see that in the condition (III) it is enough to consider distinct $i_1, i_2, \ldots, i_{k+1}$ and distinct $j_1, \ldots, j_{r+1}$, as $b_{ii}^{(l)} = c_{ii}^{(l)}$ for all $i, l$.

Now we state and prove a result which is a slight variation of Lemma 4, which suits our purpose.

**Lemma 6** Let $B_l = (b_{ij}^{(l)})$, $C_l = (c_{ij}^{(l)})$ be as in Lemma 4, with $n \geq 2$. Then there exist complex numbers $u_i, i = 1, \ldots, n$, $v_n$ with $|u_i| = 1$, $\forall, i$, $|v_n| = 1$, such that $c_{ij}^{(l)} = \frac{u_i b_{ij}^{(l)}}{u_j c_{ij}^{(l)}}$, $\forall i, j, l = 1, \ldots, n$ and $l = 1, \ldots, N$ if and only if the following conditions hold:

I) $b_{ii}^{(l)} = c_{ii}^{(l)}$ $\forall i = 1, \ldots, n - 1$, $l = 1, \ldots, N$;

II) $|b_{ij}^{(l)}| = |c_{ij}^{(l)}|$ $\forall i, j = 1, \ldots, n$, $l = 1, \ldots, N$;

III) For all choices of $l_1, \ldots, l_k, m_1, \ldots, m_r \in \{1, 2, \ldots, N\}$ ($k, r \geq 1$), $i_1, \ldots, i_{k+1}, j_1, \ldots, j_{r+1} \in \{1, 2, \ldots, n\}$ with $i_1 = j_1, i_{k+1} = j_{r+1}$, and with the restriction that $(i_1, \ldots, i_{k+1})$ are all distinct and so are $(j_1, \ldots, j_{r+1})$, one has
\[
b_{i_1 i_2}^{(l_1)} b_{i_2 i_3}^{(l_2)} \cdots b_{i_{k+1} i_1}^{(l_k)} c_{j_1 j_2}^{(m_1)} \cdots c_{j_{r+1} j_{r+1}}^{(m_r)} = c_{i_1 i_2}^{(l_1)} c_{i_2 i_3}^{(l_2)} \cdots c_{i_{k+1} i_1}^{(l_k)} b_{j_1 j_2}^{(m_1)} \cdots b_{j_{r+1} j_{r+1}}^{(m_r)}.
\]

Let $N, n \geq 1$ be positive integers, and $A_0, A_1, \ldots, A_N; A'_0, A'_1, \ldots, A'_N$ be $n \times n$ positive matrices, $n \geq 2$. Let $(\lambda_1, \ldots, \lambda_n)$ be the singular values of $A_0$, and $(\lambda'_1, \ldots, \lambda'_n)$ be those of $A'_0$. Assume furthermore that $(\lambda_1, \ldots, \lambda_n)$ are all distinct, say, $\lambda_1 > \ldots > \lambda_n$, and similarly $\lambda'_1 > \ldots > \lambda'_n$. Let $(\psi_1, \ldots, \psi_n)$, $(\eta_1, \ldots, \eta_n)$ be two orthonormal bases for $C^n$ such that the singular value decomposition of $A_0$ is given by
\[
A_0 = \sum_i \lambda_i |\psi_i><\eta_i|.
\]

Similarly, let $(\psi'_1, \ldots, \psi'_n)$ and $(\eta'_1, \ldots, \eta'_n)$ are the orthonormal bases corresponding to the singular value decomposition of $A'_0$. Let matrices $B_l, C_l, l = 1, \ldots, N$ be defined by $(B_l)_{ij} = b_{ij}^{(l)}$, $(C_l)_{ij} = c_{ij}^{(l)}$, where $b_{ij}^{(l)} = <\psi_i, A_l \eta_j>$, $c_{ij}^{(l)} = <\psi'_i, A'_l \eta'_j>$. We have:
Lemma 7 There exist two unitary matrices $U, V$ such that $UA_lV^* = A'_l$ for all $l = 0, 1, ..., N$ if and only if $\lambda_i = \lambda'_i \forall i$ and the conditions (I), (II) and (III) in the statement of Lemma 6 are satisfied for the choices of $b^{(l)}_{ij}, c^{(l)}_{ij}$'s as above.

Proof: Let $V_1, V_2, V'_1, V'_2$ be unitary matrices such that $V_1A_0V^*_2 = D_0 := diag(\lambda_1, ..., \lambda_n)$ and $V'_1A'_0V'^*_2 = D'_0 := diag(\lambda'_1, ..., \lambda'_n)$. Clearly, $V_1A_lV^*_2 = B_l$, $V'_1A'_lV'^*_2 = C_l$ for $l = 1, ..., N$.

Proof of the “if” part: Here, $D_0 = D'_0 = D$, say. By Lemma 6, we can find $u_i, i = 1, ..., n$, $v_n$ with $|u_i| = 1, |v_n| = 1$, and $c^{(l)}_{ij} = \frac{u_i b^{(l)}_{ij}}{v_j}$ $\forall i, j = 1, ..., n, l = 0, ..., N$, with $v_j = u_j$ for $j = 1, ..., n - 1$. In other words, $C_l = W_lB_lW^*_2, l = 1, ..., N$, where $W_l$ is the unitary given by $W_l := diag(u_1, ..., u_n)$ and similarly, $W_2 := diag(u_1, ..., u_{n-1}, v_n)$. We take $U := V'_1W_1V_1$, $V = V'_2W_2V_2$, and it is easy to verify that $UA_lV^* = A'_l$ for $l = 0, 1, ..., N$.

Proof of the “only if” part: Suppose now that there are unitary matrices $U, V$ such that $UA_lV^* = A'_l$ for $l = 0, 1, ..., N$. It follows from the assumption $UA_0V^* = A'_0$ that $D_0 = D'_0 = D$, say. We have $UA_0V^* = UV_1D'V^*_2 = V'_1D'V^*_2 = A'_0$, from which it follows that $W_1D = DW_2$, where $W_1 = V_1UV^*_1$, $W_2 = V'_2VV^*_2$. Thus, $W_1DD^*W_1^* = DW_2'W_2D^* = DD^*$. Since $D$ is diagonal with all entries distinct and nonnegative, $DD^* = D^2 = diag(\lambda_1^2, ..., \lambda_n^2)$. It follows that $W_1$ must also be diagonal, i.e. $W_1 = diag(u_1, ..., u_n)$ for some $u_1, ..., u_n$ with $|u_i| = 1$. Similarly, $W_2$ is diagonal, say $diag(v_1, ..., v_n)$. Furthermore, we have $W_1D = DW_2$, which implies that $\lambda_iu_i = \lambda_iv_i$ for all $i$, and as $\lambda_1, ..., \lambda_{n-1}$ are strictly positive numbers (only $\lambda_n$ can possibly be 0), we conclude that $u_i = v_i$ for $i = 1, ..., n - 1$. Obviously, $C_l = W_lB_lW^*_2$, from which the conditions (I), (II) and (III) of Lemma 6 follow. \square

Lemma 8 Let $(P, Q)$ and $(P', Q')$ be two pairs of projections in $n$-dimensional ($n \geq 1$) Hilbert space. There exits a unitary matrix $U$ such that $P' = UPU^*$ and $Q' = UQU^*$ if and only if the following conditions are satisfied:

\begin{equation}
\begin{align*}
(\text{I}) & \quad Tr[((2P - 1)(2Q - 1))^m] = Tr[((2P' - 1)(2Q' - 1))^m], \quad m = 1, ..., n; \\
(\text{II}) & \quad Tr[((2P - 1)E_{\pm})^m] = Tr[((2P' - 1)E'_{\pm})^m], \quad m = 1, ..., n, \\
\end{align*}
\end{equation}

where $E_{\pm}$ and $E'$ denote the projection onto the eigenspace of the eigenvalue 1 and $-1$ of the unitary matrix $(2P - 1)(2Q - 1)$ respectively. $E'_{\pm}$ are defined similarly, replacing $P$ and $Q$ by $P'$ and $Q'$.

Proof: The result can be proved by applying the characterization of a pair of projections obtained by Halmos [10] (see also [11] and the references therein for related discussion). We, however, present a proof in our finite-dimensional situation.

The “only if” part is trivial. So we suppose that the conditions (I) and (II) hold. Let $S = 2P - 1, V = (2P - 1)(2Q - 1)$, and $S' = 2P' - 1, V' = (2P' - 1)(2Q' - 1)$. $S$ and $S'$ are selfadjoint unitary matrices, $V$ and $V'$ are unitary ones. We also have $SVS = V^*$,
$S'V'S' = V''$. Note that by (I), the eigenvalues of $V$ and $V'$ are the same, and have the same multiplicities. Let $\Delta$ be the set of these eigenvalues, and $\Delta_+$ (resp. $\Delta_-$) be the set of eigenvalues with positive (resp. negative) imaginary parts. Furthermore, if we denote by $H_\lambda$ (resp. $H_\lambda'$) the eigenspace of $V$ (resp. of $V'$) corresponding to the eigenvalue $\lambda$ ($dim(H_\lambda) = dim(H_\lambda')$, as is already noted), then it is easy to verify that $SH_\lambda = H_{\lambda-1}$, and a similar fact is true for $S'$ and $H_\lambda'$. We want to define a unitary $U$ from $C^n = \bigoplus \lambda H_\lambda$ to $C^n = \bigoplus \lambda H_\lambda'$ such that $USU^* = S'$. For $\lambda \in \Delta_+$, choose any unitary $U_\lambda$ from $H_\lambda$ onto $H_\lambda'$ (this is possible as $H_\lambda$ and $H_\lambda'$ have the same dimension), and then for $\lambda \in \Delta_-$, i.e. $\lambda^{-1} \in \Delta_+$, choose $U_\lambda = S'|_{H_{\lambda^{-1}}'} = U_{\lambda^{-1}}S|_{H_\lambda}$. Finally, we need to define $U_{\pm 1}$, for which we shall make use of (II). By (II), $S|_{H_{\lambda+1}} = SE_+$ is unitarily equivalent to $S'E_+'$, so there exists a unitary $U_{+1}$ satisfying $U_{+1}S|_{H_{\lambda+1}}U_{+1}^* = S'E_+'$. Similarly, $U_{-1}$ can be defined. By construction, it is clear that $USU^* = S'$ and $UVU' = V'$, which is equivalent to having $UPU^* = P'$ and $UQU^* = Q'$.

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