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Practical full and partial separability criteria for multipartite pure states based on the coefficient matrix method

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Abstract

We give the concept, construction and some basic properties of coefficient matrices of a multipartite qudit pure state. Then based on them, we obtain necessary and sufficient full and partial separability criteria for multipartite qudit pure states. These criteria are very practical, operational and convenient.

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1. Introduction

A multipartite qudit (i.e. a unit of quantum information in a d-level quantum system where d is arbitrary) system consists of two or more subsystems that may have different dimensions from one another. Therefore, it is the most general object that we investigate in quantum computation and quantum information [1]. Every main result in this paper is about a multipartite qudit system. A pure state $|\psi\rangle$ of a bipartite quantum system consisting of subsystems A with dimension d_A and B with dimension d_B can be written as $|\psi\rangle = \sum_{ij} c_{ij}|i_A\rangle|j_B\rangle$ where $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$ are the arbitrary orthonormal bases of A and B respectively. Then we can construct a $d_A \times d_B$ matrix C_A by arranging all the coefficients c_{ij}'s as $(C_A)_{ij} = c_{ij}$. On the other hand, we can also construct a $d_B \times d_A$ matrix C_B by arranging all the coefficients c_{ij}'s as $(C_B)_{ji} = c_{ij}$ which is just the transpose of C_A. We call either of C_A and C_B a *coefficient matrix*. Thus we can construct two coefficient matrices according to the coefficients of a bipartite pure state. For an n-partite quantum system in the case $n \geqslant 3$, the situation becomes different as we will argue in section 2. For example, for a tripartite pure state, we can construct six coefficient matrices. Generally speaking, for an n-partite pure state, we can construct $2^n - 2$ coefficient matrices.

Some authors in their findings on multipartite quantum systems have used the technique of coefficient matrices [2–7]. Most of them concern topics about multipartite entanglement or separability. Entanglement lies at the very heart of quantum information theory [8], but subjects of fully characterizing it whether qualitatively or quantitatively remain open [9]. Thus entanglement has become the central issue in the debate on multipartite quantum systems. Therefore, as mathematical tools for investigating multipartite quantum systems, coefficient matrices are mainly applied to discuss entanglement problems. For example, by considering three coefficient matrices of a four-qubit pure state, the authors of [3] showed that there is no four-qubit pure state whose two-qubit reduced density matrices are all maximally mixed and further proposed the four-qubit Higuchi–Sudbery state:

$$|M_4\rangle = \frac{1}{\sqrt{6}}[|0011\rangle + |1100\rangle + \omega(|1010\rangle + |0101\rangle) + \omega^2(|1001\rangle + |0110\rangle)] \tag{1.1}$$

where $\omega = \mathrm{e}^{2\pi \mathrm{i}/3}$, which is conjectured to have the maximal average entanglement as a system of two pairs of qubits [10, 11]. In [5, 6], Lamata *et al* offered an inductive criterion to classify multipartite entanglement under stochastic local operations and classical communication (SLOCC) [12, 13] based on the analysis of the right singular subspaces of the coefficient matrices of the state. Li *et al* [7] gave some necessary and sufficient conditions of separability for pure states of n-partite quantum systems with the same subsystem dimension in terms of n coefficient matrices of one state. However, it seems that there is little relatively detailed introduction to coefficient matrices in the literature. Because the coefficient matrix method is very operational, practical and convenient, we expect that it will have further and more extensive applications on investigating multipartite quantum systems. Thus, it is necessary to deal with it.

The rest of this paper is organized as follows. In section 2, we introduce the concept and construction of coefficient matrices of a multipartite qudit pure state in detail by deducing the equation $\rho = CC^*$ step by step that associates a reduced density matrix with its corresponding coefficient matrix, and subsequently we give some basic properties of coefficient matrices. In section 3, we give some practical necessary and sufficient full and partial separability criteria for multipartite qudit pure states based on the coefficient matrix method. We close with some concluding remarks in section 4.

2. The construction and basic properties of coefficient matrices for a multipartite qudit pure state

We begin with some notations. Throughout this paper the symbol '$*$' stands for the Hermitian adjoint operation and 'T' stands for transposition. Suppose a multipartite qudit system with state space H whose dimension is d consists of n subsystems with respective state space H_t whose dimension is d_t where $t = 1, 2, \ldots, n$. Then we have $H = H_1 \otimes H_2 \otimes \cdots \otimes H_n$ and $d = d_1 d_2 \cdots d_n$. Let $|\psi\rangle$ be a pure state on H and let $\{|i_t\rangle\} \equiv \{|0\rangle_t, |1\rangle_t, \ldots, |d_t - 1\rangle_t\}$ be an arbitrary orthonormal basis of H_t. Thus $|\psi\rangle$ can be expressed as

$$|\psi\rangle = \sum_{i_1=0}^{d_1-1} \sum_{i_2=0}^{d_2-1} \cdots \sum_{i_n=0}^{d_n-1} c_{i_1 i_2 \cdots i_n} |i_1\rangle |i_2\rangle \cdots |i_n\rangle = \sum_{i_1 i_2 \cdots i_n} c_{i_1 i_2 \cdots i_n} |i_1 i_2 \cdots i_n\rangle \tag{2.1}$$

where $c_{i_1 i_2 \cdots i_n}$'s are the coefficients of $|\psi\rangle$ satisfying the normalization condition $\sum_{i_1 i_2 \cdots i_n} |c_{i_1 i_2 \cdots i_n}|^2 = 1$. Let $\rho = |\psi\rangle\langle\psi|$ represent the density operator of the pure state $|\psi\rangle$ on H. Additionally, we note the string $i_1 i_2 \cdots i_n$. When the dimensions d_t of H_t may differ from one another for all $t = 1, 2, \ldots, n$, i_t takes d_t values: $0, 1, \ldots, d_t - 1$. In this situation, similar to an n-bit binary integer in the special case $d_t = 2$ for all

$t = 1, 2, \ldots, n$, the string $i_1 i_2 \cdots i_n$ is also a numerical representation called a *mixed radix number* [14]. Mixed radix numeral systems are the generalization of ordinary fixed radix numeral systems. More precisely, the mixed radix number $i_1 i_2 \cdots i_n$ represents the decimal integer $i_1 \times d_2 d_3 \cdots d_n + i_2 \times d_3 d_4 \cdots d_n + \cdots + i_{n-1} \times d_n + i_n$. In the sequential discussion, we will use this kind of mixed radix strings to denote the row and column indices of some matrices.

Now we will calculate the reduced density operator $\rho_{\bar{s}} = \mathrm{tr}_s(\rho)$ by tracing out the sth subsystem H_s where $s \in \{1, 2, \ldots, n\}$. The bar symbol '−' over the letter 's' in the subscript of $\rho_{\bar{s}}$ can be understood as 'complement'. Hence '$\bar{s}$' means the rest system of the entire system H after the sth subsystem H_s is removed from it. By (2.1), we get

$$
\begin{aligned}
\rho_{\bar{s}} &= \mathrm{tr}_s(\rho) = \mathrm{tr}_s(|\psi\rangle\langle\psi|) \\
&= \mathrm{tr}_s\left(\sum_{i_1 i_2 \cdots i_n j_1 j_2 \cdots j_n} c_{i_1 i_2 \cdots i_n} c^*_{j_1 j_2 \cdots j_n} |i_1\rangle\langle j_1| \otimes |i_2\rangle\langle j_2| \otimes \cdots \otimes |i_s\rangle\langle j_s| \otimes \cdots \otimes |i_n\rangle\langle j_n|\right) \\
&= \sum_{i_1 i_2 \cdots i_n j_1 j_2 \cdots j_n} c_{i_1 i_2 \cdots i_n} c^*_{j_1 j_2 \cdots j_n} \langle j_s \mid i_s\rangle\, |i_1 i_2 \cdots i_{s-1} i_{s+1} \cdots i_n\rangle\, \langle j_1 j_2 \cdots j_{s-1} j_{s+1} \cdots j_n| \\
&= \sum_{i_1 i_2 \cdots i_n j_1 j_2 \cdots j_n} c_{i_1 i_2 \cdots i_n} c^*_{j_1 j_2 \cdots j_n} \langle i_s \mid j_s\rangle\, |i_1 i_2 \cdots i_{s-1} i_{s+1} \cdots i_n\rangle\, \langle j_1 j_2 \cdots j_{s-1} j_{s+1} \cdots j_n| \\
&= \sum_{i_1 i_2 \cdots i_n j_1 j_2 \cdots j_n} c_{i_1 i_2 \cdots i_n} c^*_{j_1 j_2 \cdots j_n} |i_1 i_2 \cdots i_{s-1} i_{s+1} \cdots i_n\rangle\, \langle i_s \mid j_s\rangle\, \langle j_1 j_2 \cdots j_{s-1} j_{s+1} \cdots j_n| \\
&= \sum_{i_1 i_2 \cdots i_n} c_{i_1 i_2 \cdots i_n} |i_1 i_2 \cdots i_{s-1} i_{s+1} \cdots i_n\rangle\langle i_s| \sum_{j_1 j_2 \cdots j_n} c^*_{j_1 j_2 \cdots j_n} |j_s\rangle\, \langle j_1 j_2 \cdots j_{s-1} j_{s+1} \cdots j_n| \\
&= C_{\bar{s}} C^*_{\bar{s}}
\end{aligned}
\tag{2.2}
$$

where we set

$$
C_{\bar{s}} = \sum_{i_1 i_2 \cdots i_n} c_{i_1 i_2 \cdots i_n} |i_1 i_2 \cdots i_{s-1} i_{s+1} \cdots i_n\rangle\langle i_s|. \tag{2.3}
$$

Therefore, we can obtain the matrix expression $\rho_{\bar{s}} = C_{\bar{s}} C^*_{\bar{s}}$ with respect to the basis $\{|i_1 i_2 \cdots i_n\rangle\}$ where the matrix $C_{\bar{s}}$ of size $d_1 d_2 \cdots d_{s-1} d_{s+1} \cdots d_n \times d_s$, whose entry in the $i_1 i_2 \cdots i_{s-1} i_{s+1} \cdots i_n$th row and the i_sth column is $c_{i_1 i_2 \cdots i_{s-1} i_s i_{s+1} \cdots i_n}$, is constructed as follows:

$$
C_{\bar{s}} = \begin{pmatrix}
c_{00\cdots000\cdots00} & c_{00\cdots010\cdots00} & \cdots & c_{00\cdots0 i_s 0\cdots00} & \cdots & c_{00\cdots0(d_s-1)0\cdots00} \\
c_{00\cdots000\cdots01} & c_{00\cdots010\cdots01} & \cdots & c_{00\cdots0 i_s 0\cdots01} & \cdots & c_{00\cdots0(d_s-1)0\cdots01} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
c_{i_1 i_2\cdots i_{s-1} 0 i_{s+1}\cdots i_{n-1} i_n} & c_{i_1 i_2\cdots i_{s-1} 1 i_{s+1}\cdots i_{n-1} i_n} & \cdots & c_{i_1 i_2\cdots i_{s-1} i_s i_{s+1}\cdots i_{n-1} i_n} & \cdots & c_{i_1 i_2\cdots i_{s-1}(d_s-1) i_{s+1}\cdots i_{n-1} i_n} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
c_{a_1 a_2\cdots a_{s-1} 0 a_{s+1}\cdots a_{n-1} a_n} & c_{a_1 a_2\cdots a_{s-1} 1 a_{s+1}\cdots a_{n-1} a_n} & \cdots & c_{a_1 a_2\cdots a_{s-1} i_s a_{s+1}\cdots a_{n-1} a_n} & \cdots & c_{a_1 a_2\cdots a_{s-1}(d_s-1) a_{s+1}\cdots a_{n-1} a_n}
\end{pmatrix}
\tag{2.4}
$$

where the digit $a_t = d_t - 1$ for $t = 1, 2, \ldots, n$ and $t \neq s$ in the subscripts of the elements in the last row of $C_{\bar{s}}$. Thus all the entries of $C_{\bar{s}}$ are exactly all the coefficients of $|\psi\rangle$.

The conclusion is as follows.

Proposition 2.1. *Suppose $|\psi\rangle$ is a pure state on an n-partite qudit system $H = H_1 \otimes H_2 \otimes \cdots \otimes H_n$. Then the reduced density matrix $\rho_{\bar{s}}$ by tracing out the sth subsystem H_s can be expressed as*

$$
\rho_{\bar{s}} = C_{\bar{s}} C^*_{\bar{s}} \tag{2.5}
$$

where $C_{\bar{s}}$ is a $d_1 d_2 \cdots d_{s-1} d_{s+1} \cdots d_n \times d_s$ matrix, all of whose entries are exactly all the coefficients $c_{i_1 i_2 \cdots i_n}$'s of $|\psi\rangle$ with respect to some arbitrary orthonormal product basis $\{|i_1 i_2 \cdots i_n\rangle\}$, as shown by (2.4). We call $C_{\bar{s}}$ the coefficient matrix of the reduced density matrix $\rho_{\bar{s}}$ or the coefficient matrix of system $\bar{s}$.

Currently, we continue to calculate the reduced density matrix by tracing out *two* subsystems, say H_s and H_r, i.e. $\rho_{\overline{sr}} = \mathrm{tr}_{sr}(\rho)$. Here, without loss of generality, we set $s < r \in \{1, 2, \ldots, n\}$, and '$\overline{sr}$' means the rest system of the entire system H after the sth subsystem H_s and the rth subsystem H_r are removed from it. We get

$$\begin{aligned}
\rho_{\overline{sr}} &= \mathrm{tr}_{sr}(\rho) = \mathrm{tr}_{sr}(|\psi\rangle\langle\psi|) \\
&= \sum_{i_1 i_2 \cdots i_n j_1 j_2 \cdots j_n} c_{i_1 i_2 \cdots i_n} c^*_{j_1 j_2 \cdots j_n} \langle j_s \mid i_s\rangle \langle j_r \mid i_r\rangle |i_1 \cdots i_{s-1} i_{s+1} \cdots i_{r-1} i_{r+1} \cdots i_n\rangle \\
&\quad \times \langle j_1 \cdots j_{s-1} j_{s+1} \cdots j_{r-1} j_{r+1} \cdots j_n| \\
&= \sum_{i_1 i_2 \cdots i_n j_1 j_2 \cdots j_n} c_{i_1 i_2 \cdots i_n} c^*_{j_1 j_2 \cdots j_n} |i_1 \cdots i_{s-1} i_{s+1} \cdots i_{r-1} i_{r+1} \cdots i_n\rangle \langle i_s i_r \mid j_s j_r\rangle \\
&\quad \times \langle j_1 \cdots j_{s-1} j_{s+1} \cdots j_{r-1} j_{r+1} \cdots j_n| \\
&= \sum_{i_1 i_2 \cdots i_n} c_{i_1 i_2 \cdots i_n} |i_1 \cdots i_{s-1} i_{s+1} \cdots i_{r-1} i_{r+1} \cdots i_n\rangle \langle i_s i_r| \\
&\quad \times \sum_{j_1 j_2 \cdots j_n} c^*_{j_1 j_2 \cdots j_n} |j_s j_r\rangle \langle j_1 \cdots j_{s-1} j_{s+1} \cdots j_{r-1} j_{r+1} \cdots j_n| \\
&= C_{\overline{sr}} C^*_{\overline{sr}}
\end{aligned} \tag{2.6}$$

where we set

$$C_{\overline{sr}} = \sum_{i_1 i_2 \cdots i_n} c_{i_1 i_2 \cdots i_n} |i_1 \cdots i_{s-1} i_{s+1} \cdots i_{r-1} i_{r+1} \cdots i_n\rangle \langle i_s i_r|. \tag{2.7}$$

Therefore, we can obtain the matrix expression $\rho_{\overline{sr}} = C_{\overline{sr}} C^*_{\overline{sr}}$ with respect to the basis $\{|i_1 i_2 \cdots i_n\rangle\}$ where the matrix $C_{\overline{sr}}$ of size $d_1 d_2 \cdots d_{s-1} d_{s+1} \cdots d_{r-1} d_{r+1} \cdots d_n \times d_s d_r$, whose entry in the $i_1 i_2 \cdots i_{s-1} i_{s+1} \cdots i_{r-1} i_{r+1} \cdots i_n$th row and $i_s i_r$th column is $c_{i_1 i_2 \cdots i_{s-1} i_s i_{s+1} \cdots i_{r-1} i_r i_{r+1} \cdots i_n}$, is constructed as follows:

$$C_{\overline{sr}} = \begin{pmatrix}
c_{00\cdots0\cdots0\cdots00} & c_{00\cdots0\cdots1\cdots00} & \cdots & c_{00\cdots i_s\cdots i_r\cdots00} & \cdots & c_{00\cdots(d_s-1)\cdots(d_r-1)\cdots00} \\
c_{00\cdots0\cdots0\cdots01} & c_{00\cdots0\cdots1\cdots01} & \cdots & c_{00\cdots i_s\cdots i_r\cdots01} & \cdots & c_{00\cdots(d_s-1)\cdots(d_r-1)\cdots01} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
c_{i_1 i_2\cdots0\cdots0\cdots i_{n-1} i_n} & c_{i_1 i_2\cdots0\cdots1\cdots i_{n-1} i_n} & \cdots & c_{i_1 i_2\cdots i_s\cdots i_r\cdots i_{n-1} i_n} & \cdots & c_{i_1 i_2\cdots(d_s-1)\cdots(d_r-1)\cdots i_{n-1} i_n} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
c_{a_1 a_2\cdots0\cdots0\cdots a_{n-1} a_n} & c_{a_1 a_2\cdots0\cdots1\cdots a_{n-1} a_n} & \cdots & c_{a_1 a_2\cdots i_s\cdots i_r\cdots a_{n-1} a_n} & \cdots & c_{a_1 a_2\cdots(d_s-1)\cdots(d_r-1)\cdots a_{n-1} a_n}
\end{pmatrix} \tag{2.8}$$

where the digit $a_t = d_t - 1$ for $t = 1, 2, \ldots, n$ and $t \neq s, r$ in the subscripts of the elements in the last row of $C_{\overline{sr}}$. Thus, like $C_{\bar{s}}$, all the entries of $C_{\overline{sr}}$ are exactly all the coefficients of $|\psi\rangle$.

The conclusion is as follows.

Proposition 2.2. *Suppose $|\psi\rangle$ is a pure state on an n-partite qudit system $H = H_1 \otimes H_2 \otimes \cdots \otimes H_n$. Then the reduced density matrix $\rho_{\overline{sr}}$ by tracing out the sth and the rth subsystem H_s and H_r can be expressed as*

$$\rho_{\overline{sr}} = C_{\overline{sr}} C^*_{\overline{sr}} \tag{2.9}$$

where $C_{\overline{sr}}$ is a $d_1d_2\cdots d_{s-1}d_{s+1}\cdots d_{r-1}d_{r+1}\cdots d_n \times d_sd_r$ matrix, all of whose entries are exactly all the coefficients $c_{i_1i_2\cdots i_n}$'s of $|\psi\rangle$ with respect to some arbitrary orthonormal product basis $\{|i_1i_2\cdots i_n\rangle\}$, as shown by (2.8). We call $C_{\overline{sr}}$ the coefficient matrix of the reduced density matrix $\rho_{\overline{sr}}$ or the coefficient matrix of system $\overline{sr}$.

Along the same line above and by induction, we can calculate the reduced density operator after tracing out *any* number of subsystems and draw the similar conclusion. In other words, we have the similar and generalized result for an *arbitrary* reduced density matrix of an n-partite qudit pure state. Suppose ρ_P is the reduced density matrix of an arbitrary nontrivial *partition* (i.e. subset) $P \subseteq \{H_1, H_2, \ldots, H_n\}$ by tracing out its nontrivial complement partition $\bar{P} = \{H_1, H_2, \ldots, H_n\} - P$. If we set $I_P = \{t : H_t \in P\} = \{t_1, t_2, \ldots, t_m\}$ where $t_1 < t_2 < \cdots < t_m$ and $I_{\bar{P}} = \{t : H_t \in \bar{P}\} = \{t'_1, t'_2, \ldots, t'_l\}$ where $t'_1 < t'_2 < \cdots < t'_l$ as the nonempty index sets of partition P and partition $\bar{P}$, respectively, $d_P = \prod_{t\in I_P} d_t$ is the dimension of partition P and $d_{\bar{P}} = \prod_{t\in I_{\bar{P}}} d_t$ is the dimension of partition $\bar{P}$. In addition, we set the mixed radix number $i_{t_1}i_{t_2}\cdots i_{t_m} = i_P$ and the mixed radix number $i_{t'_1}i_{t'_2}\cdots i_{t'_l} = i_{\bar{P}}$. Similar to (2.2) and (2.6), it holds that $\rho_P = C_PC_P^*$ where we set

$$C_P = \sum_{i_1i_2\cdots i_n} c_{i_1i_2\cdots i_n}|i_{t_1}i_{t_2}\cdots i_{t_m}\rangle\langle i_{t'_1}i_{t'_2}\cdots i_{t'_l}| = \sum_{i_1i_2\cdots i_n} c_{i_1i_2\cdots i_n}|i_P\rangle\langle i_{\bar{P}}|. \tag{2.10}$$

Therefore, we can obtain the matrix expression $\rho_P = C_PC_P^*$ with respect to the basis $\{|i_1i_2\cdots i_n\rangle\}$ where the matrix C_P of size $d_P \times d_{\bar{P}}$, whose entry $c_{i_P,i_{\bar{P}}}$ in the i_Pth row and the $i_{\bar{P}}$th column where $0 \leqslant i_P \leqslant d_P - 1$, $0 \leqslant i_{\overline{P}} \leqslant d_{\bar{P}} - 1$ is the coefficient $c_{i_1i_2\cdots i_n}$ of $|\psi\rangle$ such that $i_{t_1}i_{t_2}\cdots i_{t_m} = i_P$ and $i_{t'_1}i_{t'_2}\cdots i_{t'_l} = i_{\bar{P}}$, is constructed as follows:

$$C_P = \begin{pmatrix} c_{0,0} & c_{0,1} & \cdots & c_{0,i_{\bar{P}}} & \cdots & c_{0,(d_{\bar{P}}-1)} \\ c_{1,0} & c_{1,1} & \cdots & c_{1,i_{\bar{P}}} & \cdots & c_{1,(d_{\bar{P}}-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ c_{i_P,0} & c_{i_P,1} & \cdots & c_{i_P,i_{\bar{P}}} & \cdots & c_{i_P,(d_{\bar{P}}-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ c_{(d_P-1),0} & c_{(d_P-1),1} & \cdots & c_{(d_P-1),i_{\bar{P}}} & \cdots & c_{(d_P-1),(d_{\bar{P}}-1)} \end{pmatrix}. \tag{2.11}$$

Thus, like $C_{\bar{s}}$ and $C_{\overline{sr}}$, all the entries of C_P are exactly all the coefficients of $|\psi\rangle$.

The conclusion is as follows.

Theorem 2.1. *Suppose $|\psi\rangle$ is a pure state on an n-partite qudit system $H = H_1 \otimes H_2 \otimes\cdots\otimes H_n$. Then the reduced density matrix ρ_P of an arbitrary nontrivial partition P by tracing out its nontrivial complement partition $\bar{P}$ can be expressed as*

$$\rho_P = C_PC_P^* \tag{2.12}$$

where C_P is a $d_P \times d_{\bar{P}}$ matrix, all of whose entries are exactly all the coefficients $c_{i_1i_2\cdots i_n}$'s of $|\psi\rangle$ with respect to some arbitrary orthonormal product basis $\{|i_1i_2\cdots i_n\rangle\}$, as shown by (2.11). We call C_P the coefficient matrix of the reduced density matrix ρ_P or the coefficient matrix of partition P.

For example, suppose $\{H_1, H_2, H_3, H_4, H_5\}$ is a five-qubit system having pure state $|\psi\rangle$. Then by theorem 2.1, the coefficient matrix $C_{\{H_1,H_3\}}$ of the reduced density matrix $\rho_{\{H_1,H_3\}}$ of partition $\{H_1, H_3\}$ is a 4×8 matrix satisfying $\rho_{\{H_1,H_3\}} = C_{\{H_1,H_3\}}C^*_{\{H_1,H_3\}}$ and the entry $c_{10,101}$ of $C_{\{H_1,H_3\}}$ with binary row index 10 (or alternatively 2 in decimal representation) and binary column index 101 (or alternatively 5 in decimal representation) is the coefficient c_{11001} of $|\psi\rangle$. Other entries of $C_{\{H_1,H_3\}}$ can be determined similarly and finally we can get

$$C_{\{H_1,H_3\}} = \begin{pmatrix} c_{00,000} & c_{00,001} & c_{00,010} & c_{00,011} & c_{00,100} & c_{00,101} & c_{00,110} & c_{00,111} \\ c_{01,000} & c_{01,001} & c_{01,010} & c_{01,011} & c_{01,100} & c_{01,101} & c_{01,110} & c_{01,111} \\ c_{10,000} & c_{10,001} & c_{10,010} & c_{10,011} & c_{10,100} & c_{10,101} & c_{10,110} & c_{10,111} \\ c_{11,000} & c_{11,001} & c_{11,010} & c_{11,011} & c_{11,100} & c_{11,101} & c_{11,110} & c_{11,111} \end{pmatrix}$$
$$= \begin{pmatrix} c_{00000} & c_{00001} & c_{00010} & c_{00011} & c_{01000} & c_{01001} & c_{01010} & c_{01011} \\ c_{00100} & c_{00101} & c_{00110} & c_{00111} & c_{01100} & c_{01101} & c_{01110} & c_{01111} \\ c_{10000} & c_{10001} & c_{10010} & c_{10011} & c_{11000} & c_{11001} & c_{11010} & c_{11011} \\ c_{10100} & c_{10101} & c_{10110} & c_{10111} & c_{11100} & c_{11101} & c_{11110} & c_{11111} \end{pmatrix}.$$

In addition, we have two more concrete examples. Suppose $\{H_1, H_2, H_3\}$ is a three-qubit system which has six nontrivial partitions: $\{H_1\}, \{H_2\}, \{H_3\}, \{H_1, H_2\}, \{H_1, H_3\}$ and $\{H_2, H_3\}$. We use $C_1, C_2, C_3, C_{12}, C_{13}$ and C_{23} to denote the corresponding six coefficient matrices of these partitions, respectively. For the case of the GHZ (Greenberger–Horne–Zeilinger) state [15] $|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$, the coefficients $c_{000} = c_{111} = 1/\sqrt{2}$ and other coefficients are all zeros. Thus we can obtain the six coefficient matrices by (2.11) as follows:

$$C_1 = C_2 = C_3 = \begin{pmatrix} 1/\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/\sqrt{2} \end{pmatrix},$$
$$C_{12} = C_{13} = C_{23} = \begin{pmatrix} 1/\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1/\sqrt{2} \end{pmatrix}. \tag{2.13}$$

Similarly, for the case of the W state [13] $|W\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$, the coefficients $c_{001} = c_{010} = c_{100} = 1/\sqrt{3}$ and other coefficients are all zeros. Thus the six coefficient matrices are as follows:

$$C_1 = C_2 = C_3 = \begin{pmatrix} 0 & 1/\sqrt{3} & 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & 0 & 0 & 0 \end{pmatrix},$$
$$C_{12} = C_{13} = C_{23} = \begin{pmatrix} 0 & 1/\sqrt{3} \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & 0 \\ 0 & 0 \end{pmatrix}. \tag{2.14}$$

Formula (2.12) is a practical and convenient way to compute the reduced density matrices of a multipartite quantum system having a pure state and thus can substitute for tracing out operations. For example, if we use $\rho_1, \rho_2, \rho_3, \rho_{12}, \rho_{13}$ and ρ_{23} to denote the six reduced density matrices of the six nontrivial partitions of a three-qubit system having the W state, respectively, by (2.12) and (2.14) we will obtain

$$\rho_1 = \rho_2 = \rho_3 = C_1C_1^* = C_2C_2^* = C_3C_3^* = \begin{pmatrix} 0 & 1/\sqrt{3} & 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} 0 & 1/\sqrt{3} \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 2/3 & 0 \\ 0 & 1/3 \end{pmatrix} \tag{2.15}$$

and

$$\rho_{12} = \rho_{13} = \rho_{23} = C_{12}C_{12}^* = C_{13}C_{13}^* = C_{23}C_{23}^* = \begin{pmatrix} 0 & 1/\sqrt{3} \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & 0 \\ 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 0 & 1/\sqrt{3} & 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1/3 & 0 & 0 & 0 \\ 0 & 1/3 & 1/3 & 0 \\ 0 & 1/3 & 1/3 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2.16}$$

According to purification [1], which connects mixed states with pure states, *any* density matrix can be viewed as a reduced density matrix after tracing out the corresponding reference system. We can, therefore, get the following more general result by theorem 2.1.

Corollary 2.1. *For any density matrix ρ on a Hilbert space V with dimension d, there always exists a matrix C such that*

$$\rho = CC^* \tag{2.17}$$

in which C is a matrix of size $d \times d_r$ where $d_r \geqslant rank(\rho)$ is the dimension of the reference system corresponding to some purification $|\psi\rangle$ of ρ, all of whose entries are exactly all the coefficients of $|\psi\rangle$ with respect to some arbitrary orthonormal product basis. The matrix C can be arranged according to (2.11). We call C the coefficient matrix of the density matrix ρ or the coefficient matrix of space V.

For convenience and without confusion, when we use the term ‘coefficient matrix’ in the subsequent discussion, we will not mention which reduced density matrix or partition of some multipartite qudit system having a pure state this coefficient matrix corresponds to but let it implicit in contexts. Similarly, all matrices and coefficients of pure states are with respect to the given orthonormal product bases that will also be implicit in contexts later unless we emphasize otherwise specifically.

Now we give some basic properties of coefficient matrices.

Property 2.1. *For a pure state of an n-partite qudit system,*

(1) there are totally $2^n - 2$ coefficient matrices (of nontrivial partitions);

(2) all coefficient matrices have the same entries at the top-left corners which are $c_{00\cdots0}$’s (n zeros in the subscript) as well as the same entries at the bottom-right corners which are $c_{(d_1-1)(d_2-1)\cdots(d_n-1)}$’s (the subscript is not a product of (d_t-1)’s, $t = 1, 2, \ldots, n$, but a permutation of them);

(3) the coefficient matrix of a partition P is the transpose of that of its complement partition $\bar{P}$:

$$C_P = C_{\bar{P}}^T; \tag{2.18}$$

(4) there are totally $2^{n-1} - 1$ pairs of coefficient matrices, each of which, i.e. $\{C_P, C_{\bar{P}}\}$, consists of the coefficient matrix of some partition and that of its complement partition that are one another’s transposes;

(5) coefficient matrices are basis dependent and accurately there exists a right unitary relation between two corresponding coefficient matrices with respect to two bases, i.e. if we use C_P and C'_P to denote the coefficient matrix of a partition P with respect to basis B and basis B' respectively (here the basis we refer to is the arbitrary one with respect to which

the pure state of the n-partite qudit system is expressed as shown by (2.1)), then there exists a $d_{\bar{P}} \times d_{\bar{P}}$ *unitary matrix U such that*

$$C'_P = C_P U; \tag{2.19}$$

(6) *although coefficient matrices are basis dependent, their ranks are not. More precisely, if we use* C_P *and* C'_P *to denote the coefficient matrix of a partition P with respect to basis B and basis B′ respectively, it always holds that*

$$\text{rank}(C'_P) = \text{rank}(C_P) = \text{rank}(\rho_P) \tag{2.20}$$

where ρ_P *is the reduced density operator of partition P.*

Proof. Properties (1)–(4) are easy to verify by (2.11). Here we will only prove (5) and (6).
(5) All entries of a coefficient matrix are exactly all the coefficients of a pure state that are basis dependent. Therefore coefficient matrices are basis dependent. By (2.12), we can get

$$C'_P C'^*_P = C_P C^*_P = \rho_P. \tag{2.21}$$

Hence C'_P and C_P have the same singular values. If we arrange their singular values in decreasing order and choose the same left singular vectors (the left singular vectors of a matrix A are the eigenvectors corresponding to the non-zero eigenvalues of AA^*) for them so that their right singular vectors (the right singular vectors of a matrix A are the eigenvectors corresponding to the non-zero eigenvalues of A^*A) may be determined correspondingly, we can obtain their respective singular value decompositions as follows:

$$C_P = \sum_k s_k |k_P\rangle\langle k_{\bar{P}}| \tag{2.22}$$

$$C'_P = \sum_k s_k |k_P\rangle\langle k'_{\bar{P}}| \tag{2.23}$$

where nonnegative s_k's are singular values, the orthonormal $|k_P\rangle$'s are left singular vectors and the orthonormal $|k_{\bar{P}}\rangle$'s and the orthonormal $|k'_{\bar{P}}\rangle$'s are the right singular vectors of C_P and C'_P, respectively. By extending $|k_{\bar{P}}\rangle$'s and $|k'_{\bar{P}}\rangle$'s to orthonormal bases $|K_{\bar{P}}\rangle$'s and $|K'_{\bar{P}}\rangle$'s, respectively, we can construct a $d_{\bar{P}} \times d_{\bar{P}}$ unitary matrix $U = \sum_K |K_{\bar{P}}\rangle\langle K'_{\bar{P}}|$ such that $C'_P = C_P U$.
(6) According to (2.21) and the result $\text{rank}(M) = \text{rank}(MM^*)$, where M is any matrix, in matrix theory [16], it follows that $\text{rank}(C'_P) = \text{rank}(C_P) = \text{rank}(\rho_P)$. □

We can see that (2.13) (for the GHZ state) and (2.14) (for the W state) are two concrete examples for properties (1)–(4). Equation (2.19) in property (5) shows explicitly the relation between two corresponding coefficient matrices with respect to two bases. Property (6) tells us that the rank of a coefficient matrix is basis independent. Thus it seems reasonable to assume that the ranks of coefficient matrices *reflect* some essential qualities of a multipartite pure state. Hence we can use the ranks of coefficient matrices to *characterize* these qualities. We will illustrate this in section 3 shortly. Therefore, in general case, we do not care about the choice of basis.

3. Practical necessary and sufficient full and partial separability criteria for multipartite pure states based on the coefficient matrix method

Definition 3.1. *A pure state $|\psi\rangle$ of an n-partite qudit system $H = H_1 \otimes H_2 \otimes \cdots \otimes H_n$ is (fully) separable if*

$$|\psi\rangle = |\psi_1\rangle|\psi_2\rangle \cdots |\psi_n\rangle \tag{3.1}$$

where $|\psi_t\rangle \in H_t$, $t = 1, 2, \ldots, n$. An n-partite qudit pure state $|\psi\rangle$ is entangled if it is not separable.

Theorem 3.1. *Suppose an n-partite qudit pure state $|\psi\rangle$ has expression (2.1). Then the following statements are mutually equivalent:*

(A) $|\psi\rangle$ is (fully) separable;
(B) all $2^n - 2$ coefficient matrices are of rank 1;
(C) all n one-party subsystem coefficient matrices are of rank 1;
(D) all 2×2 minors of all $2^n - 2$ coefficient matrices are zeros;
(E) all 2×2 minors of all n one-party subsystem coefficient matrices are zeros;
(F)

$$c_{i_1 i_2 \cdots i_n} c_{j_1 j_2 \cdots j_n} = c_{k_1 k_2 \cdots k_n} c_{l_1 l_2 \cdots l_n} \tag{3.2}$$

where $i_1 i_2 \cdots i_n$, $j_1 j_2 \cdots j_n$, $k_1 k_2 \cdots k_n$ and $l_1 l_2 \cdots l_n$ are mutually different coefficient indices and $\{i_t, j_t\} = \{k_t, l_t\}$, $t = 1, 2, \ldots, n$.

In (F), the sets $\{i_t, j_t\}$ and $\{k_t, l_t\}$ permit the appearance of two identical elements like $\{0, 0\}$, $\{1, 1\}$. At the same time, they do not care about the order of elements. For example, $\{0, 1\}$ and $\{1, 0\}$ are viewed as the same set.

Proof.

(a) (A) *iff* (B)
Suppose C_P is the coefficient matrix of any partition P. By definition 3.1 and (2.20), we have

$$|\psi\rangle \text{is separable} \Leftrightarrow \text{the reduced state } \rho_P \text{ of any partition } P \text{ is a pure state}$$
$$\Leftrightarrow \text{rank}(\rho_P) = 1 \text{ for any partition } P \Leftrightarrow \text{rank}(C_P) = 1 \text{ for any partition } P.$$

(b) (A) *iff* (C)
The proof is similar to (a).

(c) (B) *iff* (D)
Since $\text{rank}(C_P) \geqslant 1$, by linear algebra (a matrix is of rank r if and only if there is one non-zero $r \times r$ minor in it and all $(r + 1) \times (r + 1)$ minors in it are zeros), we obtain (B) *iff* (D).

(d) (C) *iff* (E)
The proof is similar to (c).

(e) (D) *iff* (F)

First, we prove that four coefficients $c_{i_1 i_2 \cdots i_n}$, $c_{j_1 j_2 \cdots j_n}$, $c_{k_1 k_2 \cdots k_n}$ and $c_{l_1 l_2 \cdots l_n}$ whose different indices satisfy $\{i_t, j_t\} = \{k_t, l_t\}$ for $t = 1, 2, \ldots, n$ must form a 2×2 submatrix of some coefficient matrix. For any t, the equation $\{i_t, j_t\} = \{k_t, l_t\}$ is equivalent to

$$\begin{cases} i_t = k_t \\ j_t = l_t \end{cases} \quad \text{or} \quad \begin{cases} i_t = l_t \\ j_t = k_t \end{cases}.$$

According to these two cases, we can classify all t's or partition the set $I = \{1, 2, \ldots, n\}$ into two disjoint sets I_P and $I_{\bar{P}}$ as follows:

$$I_P = \left\{ t : \begin{cases} i_t = k_t \\ j_t = l_t \end{cases}, t \in I \right\} \qquad \text{and} \qquad I_{\bar{P}} = \left\{ t : \begin{cases} i_t = l_t \\ j_t = k_t \end{cases}, t \in I \right\}.$$

Although the t's in the particular situation $i_t = j_t = k_t = l_t$ may be included in both of the above two sets, for convenience we only classify them into I_P. Suppose that the partition corresponding to I_P is P with its coefficient matrix C_P. By theorem 2.1, we know that $c_{i_1 i_2 \cdots i_n}$ and $c_{k_1 k_2 \cdots k_n}$ are in the same row of C_P, $c_{j_1 j_2 \cdots j_n}$ and $c_{l_1 l_2 \cdots l_n}$ are in the same row of C_P, $c_{i_1 i_2 \cdots i_n}$ and $c_{l_1 l_2 \cdots l_n}$ are in the same column of C_P and $c_{j_1 j_2 \cdots j_n}$ and $c_{k_1 k_2 \cdots k_n}$ are in the same column of C_P. Since $i_1 i_2 \cdots i_n$, $j_1 j_2 \cdots j_n$, $k_1 k_2 \cdots k_n$ and $l_1 l_2 \cdots l_n$ are mutually different, the four coefficients $c_{i_1 i_2 \cdots i_n}$, $c_{j_1 j_2 \cdots j_n}$, $c_{k_1 k_2 \cdots k_n}$ and $c_{l_1 l_2 \cdots l_n}$ must form a 2×2 submatrix of C_P.

If all 2×2 minors of all $2^n - 2$ coefficient matrices are zeros, by the above result, the determinant of the 2×2 submatrix of C_P formed by any four coefficients $c_{i_1 i_2 \cdots i_n}$, $c_{j_1 j_2 \cdots j_n}$, $c_{k_1 k_2 \cdots k_n}$ and $c_{l_1 l_2 \cdots l_n}$ satisfying $\{i_t, j_t\} = \{k_t, l_t\}$ for $t = 1, 2, \ldots, n$ is zero, i.e. $c_{i_1 i_2 \cdots i_n} c_{j_1 j_2 \cdots j_n} = c_{k_1 k_2 \cdots k_n} c_{l_1 l_2 \cdots l_n}$.

Conversely, we can prove the four entries of any 2×2 minor of any coefficient matrix C_P must be four coefficients $c_{i_1 i_2 \cdots i_n}$, $c_{j_1 j_2 \cdots j_n}$, $c_{k_1 k_2 \cdots k_n}$ and $c_{l_1 l_2 \cdots l_n}$ satisfying $\{i_t, j_t\} = \{k_t, l_t\}$ for $t = 1, 2, \ldots, n$. By (2.11), any 2×2 minor D of any coefficient matrix C_P has the form

$$D = \begin{vmatrix} c_{i_P, i_{\bar{P}}} & c_{i_P, i'_{\bar{P}}} \\ c_{i'_P, i_{\bar{P}}} & c_{i'_P, i'_{\bar{P}}} \end{vmatrix}.$$

If we set $c_{i_P, i_{\bar{P}}} = c_{i_1 i_2 \cdots i_n}$, $c_{i'_P, i'_{\bar{P}}} = c_{j_1 j_2 \cdots j_n}$, $c_{i_P, i'_{\bar{P}}} = c_{k_1 k_2 \cdots k_n}$ and $c_{i'_P, i_{\bar{P}}} = c_{l_1 l_2 \cdots l_n}$ respectively, by theorem 2.1, we get

$$\begin{cases} i_t = k_t \\ j_t = l_t \end{cases} \text{for } t \in I_P = \{t : H_t \in P\} \quad \text{and} \quad \begin{cases} i_t = l_t \\ j_t = k_t \end{cases} \text{for } t \in I_{\bar{P}} = \{t : H_t \in \bar{P}\}.$$

Therefore $\{i_t, j_t\} = \{k_t, l_t\}$ for any $t \in \{1, 2, \ldots, n\}$.

If (3.2) holds, by the above result, we can obtain $c_{i_1 i_2 \cdots i_n} c_{j_1 j_2 \cdots j_n} = c_{k_1 k_2 \cdots k_n} c_{l_1 l_2 \cdots l_n}$, i.e. $c_{i_P, i_{\bar{P}}} c_{i'_P, i'_{\bar{P}}} = c_{i_P, i'_{\bar{P}}} c_{i'_P, i_{\bar{P}}}$. Thus $D = 0$ or equivalently all 2×2 minors of all $2^n - 2$ coefficient matrices are zeros. □

As criteria for separability of multipartite pure states, theorem 3.1 is very operational and convenient. For example, because all coefficient matrices in (2.13) and (2.14) are of rank 2, by criterion (B), we can ascertain that both the GHZ state and the W state are entangled pure states. Compared with criteria (B) and (C), criteria (D), (E) and (F) avoid computation of ranks of coefficient matrices and investigate the coefficients directly. For example, for the Higuchi–Sudbery state $|M_4\rangle$ (see (1.1)) of a four-qubit system $\{A, B, C, D\}$, the 2×2 minor

$$\begin{vmatrix} 0 & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} & 0 \end{vmatrix}$$

of the coefficient matrix

$$C_{AB} = \frac{1}{\sqrt{6}} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & \omega & \omega^2 & 0 \\ 0 & \omega^2 & \omega & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

is non-zero. Thus by criterion (D), the Higuchi–Sudbery state is an entangled pure state. Criterion (F) is a generalization of a corresponding result in [7]. Unlike criteria (D) and (E), it does not restrict the examined four coefficients in a 2×2 submatrix of a coefficient matrix, but rather with the condition $\{i_t, j_t\} = \{k_t, l_t\}$ for $t = 1, 2, \ldots, n$. For instance, the inseparability of the Higuchi–Sudbery state can also be determined if we investigate the four coefficients $c_{0001} = 0$, $c_{0101} = \frac{1}{\sqrt{6}}\omega$, $c_{1001} = \frac{1}{\sqrt{6}}\omega^2$ and $c_{1101} = 0$ which lie in the second column of C_{AB} (by the result in the proof '(D) $\Rightarrow$ (F)' of '(D) *iff* (F)', we can see that these four coefficients must form a 2×2 submatrix of the coefficient matrix C_{ACD}) and get $c_{0001}c_{1101} = 0 \neq c_{0101}c_{1001} = \omega^3/6 = 1/6$.

Theorem 3.1 gives us practical *full* separability criteria for multipartite pure states, but it is also important to discuss their *partial* separability with respect to given partitions. In this case, the coefficient matrix method still allows for practical criteria.

Definition 3.2. *A pure state $|\psi\rangle$ of n elementary qudit subsystems $H_1, H_2, \ldots, H_n$ is separable with respect to a given partition $\{I_1, \ldots, I_m\}$, where I_t's ($1 \leqslant t \leqslant m$, $2 \leqslant m \leqslant n$) are disjoint nonempty subsets of the index set $I = \{1, \ldots, n\}$ and $\bigcup_{t=1}^{m} I_t = I$, if*

$$|\psi\rangle = |\psi_{I_1}\rangle|\psi_{I_2}\rangle \cdots |\psi_{I_m}\rangle \tag{3.3}$$

where $|\psi_{I_t}\rangle \in H_{I_t}$, which denotes the tensor product of all elementary Hilbert spaces corresponding to the indices in I_t, $t = 1, 2, \ldots, m$. An n-partite qudit pure state $|\psi\rangle$ is entangled with respect to a given partition $\{I_1, \ldots, I_m\}$ if it is not separable with respect to this partition.

According to this definition, we can see that a multipartite pure state is called separable with respect to a given partition $\{I_1, \ldots, I_m\}$ if it is fully separable in the sense that it is regarded as a pure state of m parties $H_{I_1}, H_{I_2}, \ldots, H_{I_m}$. Thus we can use full separability criteria theorem 3.1 based on the coefficient matrix method to investigate the partial separability of a multipartite pure state. However, we should note that the coefficient matrices that we use are based on the orthonormal product basis of *n elementary* quantum subsystems rather than that of the m composite parties. Therefore we should adjust theorem 3.1 appropriately.

Theorem 3.2. *Suppose an n-partite qudit pure state $|\psi\rangle$ has expression (2.1). Then the following statements are mutually equivalent:*

- *(I) $|\psi\rangle$ is separable with respect to a given partition $\{I_1, \ldots, I_m\}$;*
- *(II) all $2^m - 2$ coefficient matrices corresponding to all $2^m - 2$ nontrivial unions of I_t's, $t = 1, 2, \ldots, m$ (i.e. $I_1, \ldots, I_1 \cup I_2, \ldots, I_2 \cup I_3 \cup \cdots \cup I_n$) are of rank 1;*
- *(III) all m coefficient matrices corresponding to all I_t's, $t = 1, 2, \ldots, m$, are of rank 1;*
- *(IV) all 2×2 minors of all $2^m - 2$ coefficient matrices corresponding to all $2^m - 2$ nontrivial unions of I_t's, $t = 1, 2, \ldots, m$, are zeros;*
- *(V) all 2×2 minors of all m coefficient matrices corresponding to all I_t's, $t = 1, 2, \ldots, m$, are zeros;*
- *(VI)*

$$c_{i_1 i_2 \cdots i_n} c_{j_1 j_2 \cdots j_n} = c_{k_1 k_2 \cdots k_n} c_{l_1 l_2 \cdots l_n} \tag{3.4}$$

where $i_1 i_2 \cdots i_n$, $j_1 j_2 \cdots j_n$, $k_1 k_2 \cdots k_n$ and $l_1 l_2 \cdots l_n$ are mutually different coefficient indices and $\left\{i_{I_t}, j_{I_t}\right\} = \left\{k_{I_t}, l_{I_t}\right\}$, $t = 1, 2, \ldots, m$, where $i_{I_t} = i_{s_1} i_{s_2} \cdots i_{s_q}$ if $I_t = \{s_1, s_2, \ldots, s_q\}$, $s_1 < s_2 < \cdots < s_q$ and j_{I_t}, k_{I_t} and l_{I_t} have the same meanings.

In (VI), the sets $\left\{i_{I_t}, j_{I_t}\right\}$ and $\left\{k_{I_t}, l_{I_t}\right\}$ permit the appearance of two identical elements like $\{01, 01\}$, $\{101, 101\}$. At the same time, they do not care about the order of elements. For example, $\{011, 111\}$ and $\{111, 011\}$ are viewed as the same set.

Proof.

(i) (I) *iff* (II)

Suppose C_P is the coefficient matrix corresponding to any nontrivial union I_P of I_t's and P is the tensor product of all elementary Hilbert spaces corresponding to I_P. By definition 3.2 and (2.20), we have

$|\psi\rangle$ is separable with respect to a given partition $\{I_1, \cdots, I_m\} \Leftrightarrow$ the reduced state ρ_P corresponding to any nontrivial union I_P of I_t's is a pure state $\Leftrightarrow$ rank$(\rho_P) = 1$ for any nontrivial union $I_P \Leftrightarrow$ rank$(C_P) = 1$ for any nontrivial union I_P.

(ii) (I) *iff* (III)

The proof is similar to (i).

(iii) (II) *iff* (IV)

The proof is similar to (c) in the proof of theorem 3.1.

(iv) (III) *iff* (V)

The proof is similar to (c) in the proof of theorem 3.1.

(v) (IV) *iff* (VI)

First, along the similar line to (c) in the proof of theorem 3.1, we prove that four coefficients $c_{i_1i_2\cdots i_n}$, $c_{j_1j_2\cdots j_n}$, $c_{k_1k_2\cdots k_n}$ and $c_{l_1l_2\cdots l_n}$ whose different indices satisfy $\{i_{I_t}, j_{I_t}\} = \{k_{I_t}, l_{I_t}\}$ for $t = 1, 2, \ldots, m$ must form a 2×2 submatrix of the coefficient matrix C_P corresponding to some nontrivial union I_P of I_t's. For any t, the equation $\{i_{I_t}, j_{I_t}\} = \{k_{I_t}, l_{I_t}\}$ is equivalent to

$$\begin{cases} i_{I_t} = k_{I_t} \\ j_{I_t} = l_{I_t} \end{cases} \quad \text{or} \quad \begin{cases} i_{I_t} = l_{I_t} \\ j_{I_t} = k_{I_t} \end{cases}.$$

According to these two cases, we can partition the index set $I = \{1, 2, \ldots, n\}$ into two disjoint sets I_P and $I_{\bar{P}}$ as follows:

$$I_P = \bigcup_{t:\begin{cases} i_{I_t}=k_{I_t} \\ j_{I_t}=l_{I_t} \end{cases}} I_t \quad \text{and} \quad I_{\bar{P}} = \bigcup_{t:\begin{cases} i_{I_t}=l_{I_t} \\ j_{I_t}=k_{I_t} \end{cases}} I_t.$$

Here we classify only the t's in the particular situation $i_{I_t} = j_{I_t} = k_{I_t} = l_{I_t}$, which may be included in both the above two cases, into the case $\begin{cases} i_{I_t}=k_{I_t} \\ j_{I_t}=l_{I_t} \end{cases}$. Suppose that the tensor product of all elementary Hilbert spaces corresponding to I_P is P with its coefficient matrix C_P. By theorem 2.1, we know that $c_{i_1i_2\cdots i_n}$ and $c_{k_1k_2\cdots k_n}$ are in the same row of C_P, $c_{j_1j_2\cdots j_n}$ and $c_{l_1l_2\cdots l_n}$ are in the same row of C_P, $c_{i_1i_2\cdots i_n}$ and $c_{l_1l_2\cdots l_n}$ are in the same column of C_P and $c_{j_1j_2\cdots j_n}$ and $c_{k_1k_2\cdots k_n}$ are in the same column of C_P. Since $i_1i_2\cdots i_n$, $j_1j_2\cdots j_n$, $k_1k_2\cdots k_n$ and $l_1l_2\cdots l_n$ are mutually different, the four coefficients $c_{i_1i_2\cdots i_n}$, $c_{j_1j_2\cdots j_n}$, $c_{k_1k_2\cdots k_n}$ and $c_{l_1l_2\cdots l_n}$ must form a 2×2 submatrix of C_P.

It immediately follows from the above result that (IV) $\Rightarrow$ (VI).

Conversely, we can prove that the four entries of any 2×2 minor of the coefficient matrix C_P corresponding to any nontrivial union I_P of I_t's must be the four coefficients $c_{i_1i_2\cdots i_n}$, $c_{j_1j_2\cdots j_n}$, $c_{k_1k_2\cdots k_n}$ and $c_{l_1l_2\cdots l_n}$ satisfying $\{i_{I_t}, j_{I_t}\} = \{k_{I_t}, l_{I_t}\}$ for $t = 1, 2, \ldots, m$. By (2.11), any 2×2 minor D of the coefficient matrix C_P corresponding to any nontrivial union I_P of I_t's has the form

$$D = \begin{vmatrix} c_{i_P, i_{\bar{P}}} & c_{i_P, i'_{\bar{P}}} \\ c_{i'_P, i_{\bar{P}}} & c_{i'_P, i'_{\bar{P}}} \end{vmatrix}.$$

If we set $c_{i_P,i_{\bar{P}}} = c_{i_1i_2\cdots i_n}$, $c_{i'_P,i'_{\bar{P}}} = c_{j_1j_2\cdots j_n}$, $c_{i_P,i'_{\bar{P}}} = c_{k_1k_2\cdots k_n}$ and $c_{i'_P,i_{\bar{P}}} = c_{l_1l_2\cdots l_n}$ respectively, by theorem 2.1, we get

$$\begin{cases} i_{I_t} = k_{I_t} \\ j_{I_t} = l_{I_t} \end{cases} \quad \text{for} \quad I_t \subseteq I_P \quad \text{and} \quad \begin{cases} i_{I_t} = l_{I_t} \\ j_{I_t} = k_{I_t} \end{cases} \quad \text{for} \quad I_t \subseteq I_{\bar{P}}$$

where $I_{\bar{P}}$ is the complement of I_P. Therefore $\{i_{I_t}, j_{I_t}\} = \{k_{I_t}, l_{I_t}\}$ for any $t \in \{1, 2, \ldots, m\}$.

It immediately follows from the above result that (VI) $\Rightarrow$ (IV). □

We can see that theorem 3.2 corresponds to theorem 3.1 very well and it also gives us practical criteria for partial separability of multipartite pure states. For example, because all coefficient matrices in (2.13) and (2.14) are of rank 2, we can ascertain that both the GHZ state and the W state are not separable with respect to any partition. The state $|\psi\rangle = \frac{1}{\sqrt{2}}|000\rangle + \frac{1}{\sqrt{2}}|011\rangle$ of a three-qubit system $\{A, B, C\}$ has coefficient matrices

$$C_A = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and

$$C_{AB} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

Since $\text{rank}(C_A) = 1$ and $\text{rank}(C_{AB}) = 2$, we can conclude that $|\psi\rangle$ is separable with respect to the bipartition $A(BC)$ but not separable with respect to the bipartition $(AB)C$. To show the use of criterion (VI), we again investigate the four coefficients $c_{0001} = 0$, $c_{0101} = \frac{1}{\sqrt{6}}\omega$, $c_{1001} = \frac{1}{\sqrt{6}}\omega^2$ and $c_{1101} = 0$ of the Higuchi–Sudbery state. Bipartition the four indices 0001, 1101, 0101 and 1001 into two partsAC and BD, respectively, and then we find that it holds that $\{00, 10\} = \{00, 10\}$ (corresponding to their respective AC parts) and $\{01, 11\} = \{11, 01\}$ (corresponding to their respective BD parts). On the other hand, $c_{0001}c_{1101} = 0 \neq c_{0101}c_{1001} = \omega^3/6 = 1/6$. Therefore, by criterion (VI), the Higuchi–Sudbery state is not separable with respect to the bipartition $(AC)(BD)$.

As we have mentioned at the end of section 2, the ranks of coefficient matrices appear to reflect some essential qualities of a multipartite pure state so that we can use them to characterize these qualities. Retrospectively, we can realize that in this section we have used the ranks of coefficient matrices to investigate the full and partial separability of a multipartite pure state.

4. Conclusions, discussions and open problems

In the former parts of this paper, we have introduced the concept, construction and some basic properties of coefficient matrices, and then given practical full and partial separability criteria for multipartite pure states based on coefficient matrices. In section 2, given a pure state of an n-partite quantum system, we have proposed step-by-step derivation for the equation $\rho = CC^*$, based on which coefficient matrices have been constructed. At first, by tracing out one subsystem, we have constructed the coefficient matrices of $n-1$ subsystems. Subsequently, by tracing out two subsystems, we have constructed coefficient matrices of $n-2$ subsystems. Along the same line, we have constructed the coefficient matrix of any partition. Finally, by the notion of purification, we have generalized the concept of coefficient matrices to any density matrix or any quantum system. Corollary 2.1 tells us that coefficient matrices are closely related to density matrices and their purifications. After the construction of coefficient matrices, we have given some of their basic properties. After the necessary groundwork is laid in section 2, we have obtained practical necessary and sufficient full and partial separability criteria for multipartite pure states in section 3 and we can see that coefficient matrices are very operational and convenient.

One simple but important thought throughout this paper is the idea of bipartition for a multipartite quantum system. For example, we note equation (2.20), which is the basis of theorems 3.1 and 3.2. Indeed, rank(ρ_P) is nothing but the Schmidt number of the Schmidt decomposition of a multipartite pure state $|\psi\rangle$ in any bipartition $\{P, \bar{P}\}$. Therefore, when we use the ranks of coefficient matrices to investigate the full and partial separability of a multipartite pure state, we actually use the Schmidt numbers in bipartitions for the entire multipartite quantum system to do so.

Some questions about the coefficient matrix method arise naturally. For example, are there more properties of coefficient matrices that will be helpful for investigating multipartite quantum systems? Can this method be extended to the case of mixed states? How can it be used to explore some quantitative entanglement problems like entanglement measure [17] and generalized concurrence [18]? Discussions about these questions are definitely beneficial and important.

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