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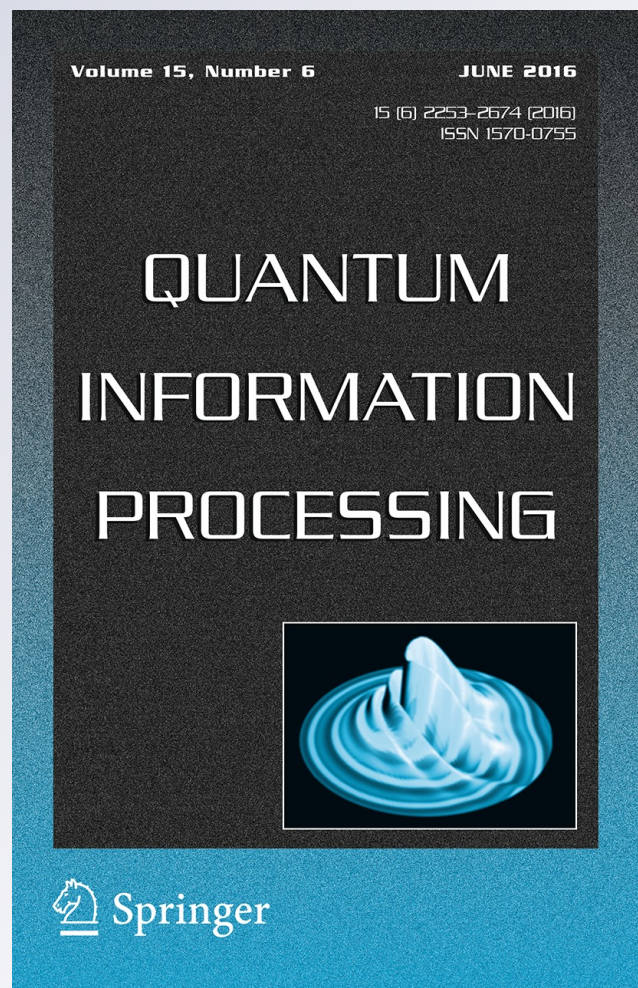
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Study of a monogamous entanglement measure for three-qubit quantum systems

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Abstract The entanglement quantification and classification of multipartite quantum states is an important research area in quantum information. In this paper, in terms of the reduced density matrices corresponding to all possible partitions of the entire system, a bounded entanglement measure is constructed for arbitrary-dimensional multipartite quantum states. In particular, for three-qubit quantum systems, we prove that our entanglement measure satisfies the relation of monogamy. Furthermore, we present a necessary condition for characterizing maximally entangled states using our entanglement measure.

Keywords Entanglement quantification · Arbitrary-dimensional multipartite
systems · Monogamy · Maximally entangled state

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1 Introduction

Entanglement, as a significant feature of quantum mechanics, plays a vital role in quantum information, such as quantum key distribution, quantum teleportation, quantum dense coding, quantum secret sharing, quantum secure direct communication, quantum simulation and quantum computation [1–14]. Mathematically, a pure state in a quantum system is called entangled if it cannot be factorized into the direct product of states on the subsystems; a mixed state is entangled if it cannot be written as a convex mixture of direct products of local states.

Quantifying entanglement has attracted much attention in recent years. For bipartite system, quantum entanglement measures have been given, such as the von Neumann entropy of entanglement [15], the entanglement of formation [16], concurrence [17] and the negativity [18]. In the case of multipartite states, given that there does not exist a single measure that can successfully account for all possible entanglement characteristics and applications, each measure usually performs better for a specific purpose and is always needed to choose the one that better fits our needs [19–26].

One of the most important properties of entanglement is monogamy [27–37], which quantifies the relation of entanglement between different parties in multipartite setting. Monogamy is also a fascinating characterization related to many areas of physics, such as quantum key distribution [38,39], the foundations of quantum mechanics [40,41], statistical mechanics [40], condensed matter physics [42–44] and even black-hole physics [45]. Let E be an entanglement measure for a tripartite system $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$. If the entanglement of the particles A and BC satisfies the inequality

$$E_{A|BC} \geqslant E_{AB} + E_{AC},$$

we call the entanglement measure E satisfies the monogamous relation. In this paper, we will propose an entanglement measure which itself has the monogamous relation. Moreover, as an application, we use our measure to establish the relation between maximally entangled states and single-qubit reduced states. We give a necessary condition for characterizing maximally entangled states.

We consider throughout this paper an n-partite system $\mathcal{H} = \mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2} \otimes \cdots \otimes \mathcal{H}^{d_n}$, where the dimension of a local space $\mathcal{H}^{d_i}$ is d_i with $i = 1, 2, \cdots, n$. A partition $\mathscr{A}$ of the system $\mathcal{H} = \mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2} \otimes \cdots \otimes \mathcal{H}^{d_n}$ is called a k-partition $(2 \leqslant k \leqslant n)$ if it contains k disjoint nonempty subsets $A_1, A_2, \ldots, A_k$ such that $\{\mathcal{H}^{d_1}, \mathcal{H}^{d_2}, \ldots, \mathcal{H}^{d_n}\} = A_1 \bigcup A_2 \bigcup \cdots \bigcup A_k$. Denote by $\mathscr{A}_k = A_1|A_2|\cdots|A_k$ the k-partition of $\mathcal{H}$. Every partition $\mathscr{A}_k = A_1|A_2|\cdots|A_k$ corresponds to a family of subsystems $A_1, A_2, \ldots, A_k$.

Let $|\psi\rangle \in \mathcal{H}$ be a pure state. It is called k-separable if there is a k-partition $\mathscr{A}_k = A_1|A_2|\cdots|A_k$ of $\mathcal{H}$ such that

$$|\psi\rangle = |\psi_1\rangle_{A_1} \otimes |\psi_2\rangle_{A_2} \otimes \cdots \otimes |\psi_k\rangle_{A_k},$$

where $|\psi_l\rangle_{A_l}$ is a pure state in the subsystem A_l $(l = 1, 2, \ldots, k)$. An n-partite mixed state ρ is called k-separable if there exist k-separable pure states $|\psi_j\rangle$ with respect to different subsets of parties and $p_j > 0$ with $\sum_j p_j = 1$, such that

$$\rho = \sum_j p_j \, |\psi_j\rangle \langle \psi_j| \, .$$

An n-partite state is called genuinely entangled if it is not 2-separable. It is called fully separable if and only if it is n-separable.

The coefficient matrices, which are constructed through arrangement of the coefficients of pure states in lexicographical order, have been used as important tools in the research into entanglement. The mathematical connection between entanglement classification and the coefficient matrices was established in [46,47]. In this work, the coefficient matrices of the pure state $|\psi\rangle$ are written as $M_{s_1 \ldots s_l}(|\psi\rangle)$ (see Sect. 6), where $1 \leqslant l \leqslant n$ and $\{s_1, s_2, \ldots, s_l\} \in \{1, 2, \ldots, n\}$.

The following theorem was proved in [48].

Theorem *Let $|\psi\rangle$, $|\phi\rangle$ be any two pure states in the n-partite system $\mathcal{H} = \mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2} \otimes \cdots \otimes \mathcal{H}^{d_n}$. If there exist complex square matrices A_i ($1 \leqslant i \leqslant n$) such that*

$$|\psi\rangle = A_1 \otimes A_2 \otimes \cdots \otimes A_n |\phi\rangle,$$

then, for any $1 \leqslant l < n$,

$$M_{1 \ldots l}(|\psi\rangle) = A_1 \otimes \cdots \otimes A_l M_{1 \ldots l}(|\phi\rangle)(A_{l+1} \otimes \cdots \otimes A_n)^T,$$

where $(A_{l+1} \otimes \cdots \otimes A_n)^T$ is the transpose matrix of the matrix $A_{l+1} \otimes \cdots \otimes A_n$.

A simple and effective application of the coefficient matrices is to concretely represent the reduced density matrix that provides a way to associate a density matrix with each component system. For $i \in \{1, \ldots, k\}$. Denote by ρ_{A_i} the reduced density matrix of $|\psi\rangle\langle\psi|$ on subsystem A_i. Then ρ_{A_i} ($1 \leqslant i \leqslant k$) has a factorization in terms of the corresponding coefficient matrix and its conjugate transpose [49],

$$\rho_{A_i} = M_{A_i} M_{A_i}^\dagger.$$

Naturally, for the reduced density matrices of two pure states, the following corollary can be reached.

Corollary *Let $|\psi\rangle$, $|\phi\rangle$ be any two pure states in the n-partite system $\mathcal{H} = \mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2} \otimes \cdots \otimes \mathcal{H}^{d_n}$. If there exist unitary matrices U_i ($1 \leqslant i \leqslant n$) such that*

$$|\psi\rangle = U_1 \otimes U_2 \otimes \cdots \otimes U_n |\phi\rangle,$$

then their corresponding reduced density matrices $\rho_{1 \ldots l}(|\psi\rangle)$ and $\rho_{1 \ldots l}(|\phi\rangle)$ ($1 \leqslant l < n$) satisfy the relation that

$$\rho_{1 \ldots l}(|\psi\rangle) = U_1 \otimes \cdots \otimes U_l \rho_{1 \ldots l}(|\phi\rangle) (U_1 \otimes \cdots \otimes U_l)^\dagger.$$

This paper is organized as follows. In Sect. 2, an entanglement monotone (denoted by $\mathcal{E}_k$) for n-qudit states is constructed. Furthermore, we transform our entanglement

monotone to a three-qubit monogamous entanglement measure in Sect. 3. By our entanglement measure, we give in Sect. 4 a necessary condition for characterizing maximally entangled states. Section 5 contains a brief summary.

2 An entanglement monotone

Let $|\psi\rangle$ be an n-qudit pure state in the n-partite quantum system $\mathcal{H} = \mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2} \otimes \cdots \otimes \mathcal{H}^{d_n}$. For arbitrary but fixed $k (2 \leqslant k \leqslant n)$, we define a map $\mathcal{E}_k$ as

$$
\mathcal{E}_k (|\psi\rangle) = \min_{\mathscr{A}_k} \left[\frac{\sum_{i=1}^{k} \left(tr \sqrt{\rho_{A_i}} \right)^2}{k} \right], \tag{1}
$$

where the minimum $\min_{\mathscr{A}_k}$ is taken over all possible k-partitions $\mathscr{A}_k = A_1 | \cdots | A_k$ of the system $\mathcal{H}$.

Theorem 1 *The $\mathcal{E}_k (|\psi\rangle)$ defined in Eq. (1) is an entanglement monotone for any pure state $|\psi\rangle$.*

Proof We will prove that $\mathcal{E}_k$ does not increase, on average, under local operations and classical communication (LOCC).

Because any protocol consists of a series of local positive operator valued measures (POVMs) such that only one subsystem be operated and $\mathcal{E}_k$ keeps invariant under permutations of the particles, it suffices to consider a general local POVM in only one part of a partition. Without loss of generality, we may assume that the local POVM is performed on the part A_1.

We note that any local POVM can be written as a sequence of two-outcome POVMs in analogy to the method in Ref. [50]. Let F_1 and F_2 be two POVM elements operated in the part A_1 such that $F_1 + F_2 = \mathbf{1}_{A_1}$. Then there exist matrices P_j such that $F_j = P_j^{\dagger} P_j$ $(j = 1, 2)$. Choose a proper unitary matrix V and decompose $P_j = U_j D_j V$ $(j = 1, 2)$. Here U_j $(j = 1, 2)$ are unitary matrices; D_1 and D_2 are both diagonal matrices with nonnegative real numbers $\mu_1, \mu_2, \ldots, \mu_{n_{A_1}}$ and $\sqrt{1 - \mu_1^2}, \sqrt{1 - \mu_2^2}, \ldots, \sqrt{1 - \mu_{n_{A_1}}^2}$ on their respective diagonals, where n_{A_1} stands for the dimension of the part A_1.

Let $M_{A_1} (|\psi\rangle)$ be the coefficient matrix of $|\psi\rangle$ corresponding to the part A_1, then by the singular value decomposition $M_{A_1} (|\psi\rangle) = S \Omega T^{\dagger}$, where S, T are unitary matrices and Ω is a matrix with the diagonal entries $\{ \omega_1, \omega_2, \ldots, \omega_{n_{A_1}} \}$.

Because any local unitary operations do not cause a change of the entanglement, some local unitary operation H preceding the POVM can be implemented in the initial state $|\psi\rangle$. We select $H = V^{\dagger} S^{\dagger}$ only for simplicity of proof.

Hence, after local actions H and POVM, the initial state $|\psi\rangle$ is transformed into new states

$$
\begin{aligned}
|\eta_j\rangle &= \frac{\left(P_j H \otimes \mathbf{1}_{\overline{A_1}}\right)|\psi\rangle}{\sqrt{p_j}} \\
&= \frac{\left(U_j D_j V V^\dagger S^\dagger \otimes \mathbf{1}_{\overline{A_1}}\right)|\psi\rangle}{\sqrt{p_j}},
\end{aligned}
\tag{2}
$$

where $j = 1, 2$; $\overline{A_1} = A_2 \otimes \cdots \otimes A_k$ is the complement of A_1; $p_j = \langle\theta_j|\theta_j\rangle$ with $|\theta_j\rangle = \left(U_j D_j S^\dagger \otimes \mathbf{1}_{\overline{A_1}}\right)|\psi\rangle$; $p_1 + p_2 = 1$.

By the theorem in the introduction, the coefficient matrices of new states $|\eta_j\rangle$ ($j = 1, 2$) are

$$
M_{A_1}\left(|\eta_j\rangle\right) = \frac{1}{\sqrt{p_j}} U_j D_j S^\dagger M_{A_1}\left(|\psi\rangle\right) = \frac{1}{\sqrt{p_j}} U_j D_j \Omega T^\dagger.
\tag{3}
$$

It follows that

$$
\begin{aligned}
tr\sqrt{\rho_{A_1}\left(|\eta_1\rangle\right)} &= tr\sqrt{M_{A_1}\left(|\eta_1\rangle\right) M_{A_1}\left(|\eta_1\rangle\right)^\dagger} \\
&= tr\sqrt{\frac{1}{p_1}\left(U_1 D_1 \Omega T^\dagger\right)\left(U_1 D_1 \Omega T^\dagger\right)^\dagger} \\
&= tr\sqrt{\frac{1}{p_1}\left(D_1 \Omega\right)\left(D_1 \Omega\right)^\dagger} \\
&= \sum_{m=1}^{n_{A_1}} \frac{\omega_m \mu_m}{\sqrt{p_1}},
\end{aligned}
\tag{4}
$$

and similarly that

$$
tr\sqrt{\rho_{A_1}\left(|\eta_2\rangle\right)} = \sum_{m=1}^{n_{A_1}} \frac{\omega_m\sqrt{1 - \mu_m^2}}{\sqrt{p_2}}.
\tag{5}
$$

We denote by $\langle\mathcal{E}_k(|\psi\rangle)\rangle$ the average entanglement after LOCC , then $\langle\mathcal{E}_k(|\psi\rangle)\rangle = p_1\mathcal{E}_k\left(|\eta_1\rangle\right) + p_2\mathcal{E}_k\left(|\eta_2\rangle\right)$.

Note that $p_1 + p_2 = 1$ and $\rho_{A_i}\left(|\psi\rangle\right) = \rho_{A_i}\left(|\eta_1\rangle\right) = \rho_{A_i}\left(|\eta_2\rangle\right)$, $i = 2, 3, \ldots, k$, it follows that

$$
\begin{aligned}
&p_1\mathcal{E}_k\left(|\eta_1\rangle\right) + p_2\mathcal{E}_k\left(|\eta_2\rangle\right) \\
&= p_1\left\{\min_{\mathscr{A}_k}\left[\frac{\left(\sum_{i=1}^{k}\left(tr\sqrt{\rho_{A_i}\left(|\eta_1\rangle\right)}\right)\right)^2}{k}\right]\right\}
\end{aligned}
$$

$$+ p_2 \left\{ \min_{\mathscr{A}_k} \left[\frac{\sum_{i=1}^{k} \left(tr \sqrt{\rho_{A_i} (|\eta_2\rangle)} \right)^2}{k} \right] \right\}$$

$$\leqslant \min_{\mathscr{A}_k} \left[\frac{p_1 \sum_{i=1}^{k} \left(tr \sqrt{\rho_{A_i} (|\eta_1\rangle)} \right)^2}{k} + \frac{p_2 \sum_{i=1}^{k} \left(tr \sqrt{\rho_{A_i} (|\eta_2\rangle)} \right)^2}{k} \right]$$

$$= \min_{\mathscr{A}_k} \left[\frac{\left(\sum_{m=1}^{n_{A_1}} \omega_m \mu_m \right)^2 + \left(\sum_{m=1}^{n_{A_1}} \omega_m \sqrt{1 - \mu_m^2} \right)^2}{k} \right.$$

$$\left. + \frac{\sum_{i=2}^{k} \left(tr \sqrt{\rho_{A_i} (|\psi\rangle)} \right)^2}{k} \right]. \tag{6}$$

Because

$$\left(\sum_{m=1}^{n_{A_1}} \omega_m \mu_m \right)^2 + \left(\sum_{m=1}^{n_{A_1}} \omega_m \sqrt{1 - \mu_m^2} \right)^2$$

$$= \sum_{m=1}^{n_{A_1}} \omega_m^2 \mu_m^2 + \sum_{\substack{1 \leqslant k,l \leqslant n_{A_1} \\ k \neq l}} \omega_k \mu_k \omega_l \mu_l + \sum_{m=1}^{n_{A_1}} \omega_m^2 \left(1 - \mu_m^2 \right)$$

$$+ \sum_{\substack{1 \leqslant k,l \leqslant n_{A_1} \\ k \neq l}} \omega_k \sqrt{1 - \mu_k^2} \omega_l \sqrt{1 - \mu_l^2}$$

$$= \sum_{m=1}^{n_{A_1}} \omega_m^{\;2} + \sum_{\substack{1 \leqslant k,l \leqslant n_{A_1} \\ k \neq l}} \omega_k \omega_l \left(\mu_k \mu_l + \sqrt{1 - \mu_k^2} \cdot \sqrt{1 - \mu_l^2} \right)$$

$$\leqslant \sum_{m=1}^{n_{A_1}} \omega_m^{\;2} + \sum_{\substack{1 \leqslant k,l \leqslant n_{A_1} \\ k \neq l}} \omega_k \omega_l \sqrt{\mu_k^{\;2} + \left(\sqrt{1 - \mu_k^2} \right)^2} \cdot \sqrt{\mu_l^{\;2} + \left(\sqrt{1 - \mu_l^2} \right)^2}$$

$$= \sum_{m=1}^{n_{A_1}} \omega_m^{\;2} + \sum_{\substack{1 \leqslant k,l \leqslant n_{A_1} \\ k \neq l}} \omega_k \omega_l = \left(\sum_{m=1}^{n_{A_1}} \omega_m \right)^2 = \left(tr \sqrt{\rho_{A_1} (|\psi\rangle)} \right)^2, \tag{7}$$

it is obtained that

$$\langle \mathcal{E}_k(|\psi\rangle)\rangle \leqslant \min_{\mathscr{A}_k} \left[\frac{\sum_{i=1}^{k} \left(tr\sqrt{\rho_{\mathrm{A}_i}(|\psi\rangle)} \right)^2}{k} \right] = \mathcal{E}_k(|\psi\rangle). \tag{8}$$

So the average entanglement $\langle \mathcal{E}_k(|\psi\rangle)\rangle$ does not increase after LOCC, and then $\mathcal{E}_k(|\psi\rangle)$ is an entanglement monotone.

This completes the proof of Theorem 1. □

We now turn to consider the mixed states. For an n-qudit mixed state ρ in the n-partite quantum system $\mathcal{H}$, we define

$$\mathcal{E}_k(\rho) = \inf_{\{p_i,|\psi_i\rangle\}} \sum_i p_i \mathcal{E}_k(|\psi_i\rangle), \tag{9}$$

where the infimum is taken over all possible pure state decomposition $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. On the basis of Theorem 1, it can be straightforwardly verified that $\mathcal{E}(\rho)$ defined in Eq. (9) is an entanglement monotone for any n-qudit mixed state ρ.

The entanglement monotone $\mathcal{E}_k$ has an physical interpretation in terms of the fidelity, which is defined by $F(\rho, \sigma) \equiv tr\sqrt{\rho^{1/2}\sigma\rho^{1/2}}$. When ρ and σ are both pure states, the square of fidelity is the transition probability from σ to ρ [51]. In the general case of mixed states, a simple operational interpretation of the fidelity is also provided in Ref. [52]. If we re-write $\mathcal{E}_k$ as

$$\mathcal{E}_k(|\psi\rangle) = \min_{\mathscr{A}_k} \left[\frac{\sum_{i=1}^{k} n_{\mathrm{A}_i} \left(tr\sqrt{\left(\frac{1}{n_{\mathrm{A}_i}} I_{n_{\mathrm{A}_i}}\right)^{1/2} \rho_{\mathrm{A}_i} \left(\frac{1}{n_{\mathrm{A}_i}} I_{n_{\mathrm{A}_i}}\right)^{1/2}} \right)^2}{k} \right]$$

$$= \min_{\mathscr{A}_k} \left[\frac{\sum_{i=1}^{k} n_{\mathrm{A}_i} F\left(\frac{1}{n_{\mathrm{A}_i}} I_{n_{\mathrm{A}_i}}, \rho_{\mathrm{A}_i}\right)^2}{k} \right],$$

where $F\left(\frac{1}{n_{\mathrm{A}_i}} I_{n_{\mathrm{A}_i} \times n_{\mathrm{A}_i}}, \rho_{\mathrm{A}_i}\right)^2$ is the square of fidelity for the reduced state ρ_{A_i} and its system's totally mixed state $\frac{1}{n_{\mathrm{A}_i}} I_{n_{\mathrm{A}_i}}$, and $I_{n_{\mathrm{A}_i}}$ denotes an identity matrix on subsystem $\mathcal{H}_{\mathrm{A}_i}$. Then the $\mathcal{E}_k$ can be explained as the minimum of all weighed averages of the square of fidelity, corresponding to all possible k-partitions ($2 \leqslant k \leqslant n$) of the system $\mathcal{H}$.

3 A monogamous entanglement measure

Monogamous relation is an important criteria for the judgment of good measures of multipartite entanglement, because the entanglement measures that satisfy this relation can show us that quantum entanglement, differing from classical correlation, is not shareable at liberty when distributed among three or more parties. For an n-qudit pure state $|\psi\rangle$ in the n-partite quantum system $\mathcal{H} = \mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2} \otimes \cdots \otimes \mathcal{H}^{d_n}$, let

$$\mathcal{E}^M\left(|\psi\rangle\right) = \min_{2 \leqslant k \leqslant n} \min_{\mathscr{A}_k} \sqrt{\widetilde{d}^n} \left[\frac{\sum_{i=1}^k \left(tr\sqrt{\rho_{A_i}}\right)^2}{k} - 1 \right], \qquad (10)$$

where the minimum $\min_{\mathscr{A}_k}$ is taken over all possible k-partitions $\mathscr{A}_k = A_1|\cdots|A_k$ of the system $\mathcal{H}$ and $\widetilde{d} = \frac{\sum_{i=1}^n d_i}{n}$. It is clear to see that $\mathcal{E}^M\left(|\psi\rangle\right) \geqslant 0$ for any pure state $|\psi\rangle$ and $\mathcal{E}^M\left(|\psi\rangle\right) = 0$ if and only if $|\psi\rangle$ is separable. By corollary in the introduction, $\mathcal{E}^M\left(|\psi\rangle\right)$ keeps invariant under local unitary transformations. Then, by the proof of Theorem 1, we know that $\mathcal{E}^M$ is an entanglement monotone. Therefore $\mathcal{E}^M$ becomes an entanglement measure.

For an n-qudit mixed state ρ in the n-partite quantum system $\mathcal{H}$, we define

$$\mathcal{E}^M\left(\rho\right) = \inf_{\{p_i, |\psi_i\rangle\}} \sum_i p_i \mathcal{E}^M\left(|\psi_i\rangle\right), \qquad (11)$$

where the infimum is taken over all possible pure state decomposition $\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$. According to the analysis of the preceding context, we can draw a conclusion that $\mathcal{E}^M(\rho)$ defined in Eq. (11) is an entanglement measure for any n-qudit mixed state ρ. Obviously, $\mathcal{E}^M$ satisfies the subadditivity [53]. In addition, we can verify that $\mathcal{E}^M$ satisfies the convexity by its definition :

$$\mathcal{E}^M\left(\sum_i p_i \rho_i\right) \leqslant \sum_i p_i \mathcal{E}^M\left(\rho_i\right).$$

Next we prove that $\mathcal{E}^M$ is monogamous for three-qubit systems.

Theorem 2 *For a three-qubit system $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, $\mathcal{E}^M$ satisfies a monogamy inequality*

$$\mathcal{E}^M_{AB} + \mathcal{E}^M_{AC} \leqslant \mathcal{E}^M_{A|BC},$$

where $\mathcal{E}^M_{AB}$, $\mathcal{E}^M_{AC}$, and $\mathcal{E}^M_{A|BC}$ mean the entanglement of the respective parts of the system.

Proof First, analogously to Eq. (7) in [54], we use the Schmidt decomposition for a general pure state $|\psi\rangle_{ABC}$ in the system $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$,

$$|\psi\rangle_{ABC} = \sqrt{p}\,|\phi_0\rangle_{AB}\,|0\rangle_C + \sqrt{1-p}\,|\phi_1\rangle_{AB}\,|1\rangle_C,$$

with $0 \leqslant p \leqslant 1$, $|\phi_0\rangle_{AB}$ and $|\phi_1\rangle_{AB}$ being the orthonormal states of biqubit system $\mathcal{H}_A \otimes \mathcal{H}_B$ and $|0\rangle_C$ and $|1\rangle_C$ being the orthonormal basis of qubit system $\mathcal{H}_C$. When $p = 0$ or $p = 1$, $|\psi\rangle_{ABC}$ is separable, the inequality holds clearly. Now we assume that $0 < p < 1$. According to the Schmidt number of $|\phi_0\rangle_{AB}$ and $|\phi_1\rangle_{AB}$, they can be categorized into three classes:

1. there is no Schmidt rank-2 state,
2. there is only one Schmidt rank-2 state,
3. there are two Schmidt rank-2 states.

Case 1 There is no Schmidt rank-2 state in $|\phi_0\rangle_{AB}$ and $|\phi_1\rangle_{AB}$.

With a proper basis $\{|\widetilde{0}\rangle_A, |\widetilde{1}\rangle_A\}$, $\{|\widetilde{0}\rangle_B, |\widetilde{1}\rangle_B\}$ and $\{|0\rangle_C, |1\rangle_C\}$ of $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H}_C$, respectively; $|\psi\rangle_{ABC}$ can be expressed as

$$\begin{aligned}|\psi\rangle_{ABC} &= \sqrt{p}|\widetilde{0}\rangle_A|\widetilde{0}\rangle_B|0\rangle_C \\ &\quad + \sqrt{1-p}|\widetilde{1}\rangle_A(\sqrt{a}|\widetilde{0}\rangle_B + \sqrt{1-a}|\widetilde{1}\rangle_B)|1\rangle_C,\end{aligned}$$

where $0 < p < 1$ and $0 \leqslant a \leqslant 1$. A direct calculation implies that

$$\begin{aligned}\mathcal{E}^M_{A|BC} &= \mathcal{E}^M\left[\rho_A\left(|\psi\rangle_{ABC}\right)\right] = 4\sqrt{2p(1-p)}, \\ \mathcal{E}^M_{AB} &= \mathcal{E}^M\left[\rho_{AB}\left(|\psi\rangle_{ABC}\right)\right] = 0.\end{aligned}$$

It remains to calculate $\mathcal{E}^M_{AC}$.

For the sake of simplicity, we write

$$\begin{aligned}|\widetilde{0}\rangle_A|0\rangle_C &= |e_{00}\rangle, \\ |\widetilde{0}\rangle_A|1\rangle_C &= |e_{01}\rangle, \\ |\widetilde{1}\rangle_A|0\rangle_C &= |e_{10}\rangle, \\ |\widetilde{1}\rangle_A|1\rangle_C &= |e_{11}\rangle.\end{aligned}$$

Then the reduced density matrix of the subsystem $\mathcal{H}_A \otimes \mathcal{H}_C$ can be represented as

$$\begin{aligned}\rho_{AC}\left(|\psi\rangle_{ABC}\right) &= p|e_{00}\rangle\langle e_{00}| + \sqrt{ap(1-p)}|e_{00}\rangle\langle e_{11}| \\ &\quad + \sqrt{ap(1-p)}|e_{11}\rangle\langle e_{00}| + (1-p)|e_{11}\rangle\langle e_{11}|.\end{aligned}$$

Consider a pure state decomposition of ρ_{AC}

$$\rho_{AC}\left(|\psi\rangle_{ABC}\right) = r_1|\varphi_1\rangle\langle\varphi_1| + r_2|\varphi_2\rangle\langle\varphi_2|,$$

where

$$r_1 = p + a(1 - p),$$
$$r_2 = (1 - a)(1 - p),$$
$$|\varphi_1\rangle = \frac{1}{\sqrt{p + a(1 - p)}} \left(\sqrt{p}|e_{00}\rangle + \sqrt{a(1 - p)}|e_{11}\rangle \right),$$
$$|\varphi_2\rangle = |e_{11}\rangle.$$

Then we have

$$
\begin{aligned}
\mathcal{E}_{AC}^M &= \mathcal{E}^M [\rho_{AC} (|\psi\rangle_{ABC})] \\
&\leqslant r_1 \mathcal{E}^M (|\varphi_1\rangle) + r_2 \mathcal{E}^M (|\varphi_2\rangle) \\
&= r_1 \left\{ 2 \left[\left(tr \sqrt{\rho_A (|\varphi_1\rangle)} \right)^2 - 1 \right] \right\} \\
&= [p + a(1 - p)] \left\{ 2 \left[\left(\frac{\sqrt{p} + \sqrt{a(1 - p)}}{\sqrt{p + a(1 - p)}} \right)^2 - 1 \right] \right\} \\
&= 4\sqrt{ap(1 - p)} \\
&< 4\sqrt{2p(1 - p)} = \mathcal{E}_{A|BC}^M.
\end{aligned}
$$

This leads us to the conclusion that $\mathcal{E}_{AB}^M + \mathcal{E}_{AC}^M < \mathcal{E}_{A|BC}^M$.

Case 2 There is only one Schmidt rank-2 state in $|\phi_0\rangle_{AB}$ and $|\phi_1\rangle_{AB}$. Without lose of generality, we might as well assume that $|\phi_0\rangle_{AB}$ is a Schmidt rank-2 state.

With the proper choice of basis sets, $|\psi\rangle_{ABC}$ can be expressed as

$$
\begin{aligned}
|\psi\rangle_{ABC} &= \sqrt{p}(\sqrt{b}|\tilde{0}\rangle_A|\tilde{0}\rangle_B + \sqrt{1 - b}|\tilde{1}\rangle_A|\tilde{1}\rangle_B)|0\rangle_C \\
&\quad + \sqrt{1 - p}(\alpha_1|\tilde{0}\rangle_A + \alpha_2|\tilde{1}\rangle_A)(\beta_1|\tilde{0}\rangle_B + \beta_2|\tilde{1}\rangle_B)|1\rangle_C,
\end{aligned}
$$

where $0 < b < 1$ and the complex numbers $\alpha_i (i = 1, 2)$ and $\beta_i (i = 1, 2)$ satisfy $\sum_{i=1}^{2} |\alpha_i|^2 = 1$ and $\sum_{i=1}^{2} |\beta_i|^2 = 1$, respectively. Similarly to the discussion in Case 1, we get

$$
\begin{aligned}
\mathcal{E}_{A|BC}^M &= \mathcal{E}^M [\rho_A (|\psi\rangle_{ABC})] \\
&= 4\sqrt{2 \left[b(1 - b)p^2 + p(1 - b)(1 - p) |\alpha_1|^2 + bp(1 - p) |\alpha_2|^2 \right]}, \\
\mathcal{E}_{AB}^M &= \mathcal{E}^M [\rho_{AB} (|\psi\rangle_{ABC})] \leqslant 4p\sqrt{b(1 - b)}, \\
\mathcal{E}_{AC}^M &= \mathcal{E}^M [\rho_{AC} (|\psi\rangle_{ABC})] \\
&\leqslant 4 |\alpha_2 \beta_1| \sqrt{pb(1 - p)} + 4 |\alpha_1 \beta_2| \sqrt{p(1 - p)(1 - b)}.
\end{aligned}
$$

It can be directly checked that $\mathcal{E}_{AB}^M + \mathcal{E}_{AC}^M \leqslant \mathcal{E}_{A|BC}^M$.

Case 3 Both $|\phi_0\rangle_{AB}$ and $|\phi_1\rangle_{AB}$ are Schmidt rank-2 states.

By choosing a proper basis, we can get the expression of $|\psi\rangle_{ABC}$

$$
\begin{aligned}
|\psi\rangle_{ABC} = {} & \sqrt{p}(\sqrt{c}|\tilde{0}\rangle_A|\tilde{0}\rangle_B + \sqrt{1-c}|\tilde{1}\rangle_A|\tilde{1}\rangle_B)|0\rangle_C \\
& + \sqrt{1-p}(a_1|\tilde{0}\rangle_A|\tilde{0}\rangle_B + a_2|\tilde{0}\rangle_A|\tilde{1}\rangle_B \\
& + a_3|\tilde{1}\rangle_A|\tilde{0}\rangle_B + a_4|\tilde{1}\rangle_A|\tilde{1}\rangle_B)|1\rangle_C,
\end{aligned}
$$

where $0 < c < 1$ and $\sum_{i=1}^{4}|a_i|^2 = 1$. A similar discussion just as in Case 1 implies that

$$
\begin{aligned}
\mathcal{E}_{A|BC}^M &= \mathcal{E}^M\left[\rho_A\left(|\psi\rangle_{ABC}\right)\right] \\
&= 4\sqrt{2}\left\{c(1-c)p^2 + p(1-p)\left[(1-c)(|a_1|^2 + |a_2|^2) + c(|a_3|^2 + |a_4|^2)\right]\right. \\
&\quad \left. + (1-p)^2(|a_1|^2|a_3|^2 + |a_1|^2|a_4|^2 + |a_2|^2|a_3|^2 + |a_2|^2|a_4|^2)\right\}^{1/2}, \\
\mathcal{E}_{AB}^M &= \mathcal{E}^M\left[\rho_{AB}\left(|\psi\rangle_{ABC}\right)\right] \\
&\leqslant 4\left[(1-p)\left|a_1a_4 - a_2a_3\right| + p\sqrt{c(1-c)}\right], \\
\mathcal{E}_{AC}^M &= \mathcal{E}^M\left[\rho_{AC}\left(|\psi\rangle_{ABC}\right)\right] \\
&\leqslant 4|a_2|\sqrt{p(1-p)(1-c)} + 4|a_3|\sqrt{p(1-p)c};
\end{aligned}
$$

which entails that $\mathcal{E}_{AB}^M + \mathcal{E}_{AC}^M \leqslant \mathcal{E}_{A|BC}^M$. The proof of Theorem 2 is complete. □

4 Application

In Ref. [55], the authors conjecture that for an n-qubit state maximally entangled with respect to their entanglement measure, all single-qubit reduced states are totally mixed. In this section, by our entanglement measure, we prove that all single-qubit reduced states of a maximally entangled state are totally mixed. In order to do this, we first gives the boundedness of the entanglement measure $\mathcal{E}^M$.

Theorem 3 *Let $|\psi\rangle$ be an n-partite pure state in the system $\mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2} \otimes \cdots \otimes \mathcal{H}^{d_n}$, then*

$$
0 \leqslant \mathcal{E}^M(|\psi\rangle) \leqslant (\tilde{d} - 1)\sqrt{\tilde{d}^n},
$$

with $\tilde{d} = \frac{\sum_{i=1}^{n} d_i}{n}$.

For a rigorous proof of this theorem the reader can refer to Sect. 7.

It can be seen from the theorem above that $\mathcal{E}^M$ is a bounded entanglement measure for any given system. For a pure state $|\psi\rangle$, it is separable if and only if $\mathcal{E}^M(|\psi\rangle) = 0$; if it is a genuine entangled state, then $\mathcal{E}^M(|\psi\rangle) > 0$; if its entanglement degree reaches the upper bound of $\mathcal{E}^M$, i.e., $\mathcal{E}^M(|\psi\rangle) = (\tilde{d} - 1)\sqrt{\tilde{d}^n}$, then we say that it is maximally entangled. Recall that a state is totally mixed if its density matrix is the scalar multiplication of an identity matrix.

Theorem 4 *If an n-qubit pure state* $|\psi\rangle$ *is maximally entangled with respect to* $\mathcal{E}^M$, *then all single-qubit reduced states of* $|\psi\rangle$ *are totally mixed.*

Proof We assert that

$$\min_{2\leqslant k\leqslant n}\min_{\mathscr{A}_k}\left[\frac{\sum_{i=1}^{k}\left(tr\sqrt{\rho_{A_i}}\right)^2}{k}-1\right]=\min_{\mathscr{A}_2}\left[\left(tr\sqrt{\rho_{A_1}}\right)^2-1\right], \qquad (12)$$

Otherwise, it can be assumed that the minimum on the right side of Eq. (12) is obtained at a certain k'-partition with $2<k'\leqslant n$, i.e.,

$$\min_{2\leqslant k\leqslant n}\min_{\mathscr{A}_k}\left[\frac{\sum_{i=1}^{k}\left(tr\sqrt{\rho_{A_i}}\right)^2}{k}-1\right]=\frac{\sum_{i=1}^{k'}\left(tr\sqrt{\rho_{A_i}}\right)^2}{k'}-1.$$

Without loss of generality, we may as well assume that

$$tr\sqrt{\rho_{A_1}}=\min\left\{tr\sqrt{\rho_{A_i}}|i=1,2,\ldots,k'\right\}.$$

Then we have

$$\min_{2\leqslant k\leqslant n}\min_{\mathscr{A}_k}\left[\frac{\sum_{i=1}^{k}\left(tr\sqrt{\rho_{A_i}}\right)^2}{k}-1\right]\geqslant\left[\left(tr\sqrt{\rho_{A_1}}\right)^2-1\right]$$

$$\geqslant\min_{\mathscr{A}_2}\left[\left(tr\sqrt{\rho_{A_1}}\right)^2-1\right]$$

$$>\left[\frac{\sum_{i=1}^{k'}\left(tr\sqrt{\rho_{A_i}}\right)^2}{k'}-1\right]$$

$$=\min_{2\leqslant k\leqslant n}\min_{\mathscr{A}_k}\left[\frac{\sum_{i=1}^{k}\left(tr\sqrt{\rho_{A_i}}\right)^2}{k}-1\right].$$

This leads to a contradiction.

So $\mathcal{E}^M(|\psi\rangle)=\min_{\mathscr{A}_2}\sqrt{\widetilde{d^n}}\left[\left(tr\sqrt{\rho_{A_1}}\right)^2-1\right]$. For an n-qubit pure state $|\psi\rangle$, assume that it is maximally entangled. Then

$$\mathcal{E}^M(|\psi\rangle)=\sqrt{2^n}$$

and

$$\min_{\mathscr{A}_2}\left[\left(tr\sqrt{\rho_{A_1}}\right)^2-1\right]=1.$$

Assume that there is a single-qubit reduced state ρ_A, satisfying that $(tr\sqrt{\rho_A})^2 - 1 > 1$. We might as well assume that ρ_A has eigenvalues λ_1 and λ_2; then,

$$(\sqrt{\lambda_1} + \sqrt{\lambda_2})^2 - 1 > 1$$

and

$$\lambda_1 + \lambda_2 = 1.$$

This implies that

$$\left(\lambda_1 - \frac{1}{2}\right)^2 < 0.$$

But it is impossible. So for all single-qubit reduced state ρ_A, we have $(tr\sqrt{\rho_A})^2 - 1 = 1$ and hence $\rho_A = \frac{1}{2}I$, namely, ρ_A is totally mixed. The proof is finished. $\square$

It should be pointed out that Theorem 4 is not sufficient for maximal entanglement. In fact, there exists a separable state whose single-qubit reduced states are all totally mixed. For example, the state

$$|\alpha\rangle = \left(\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle\right) \otimes \left(\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle\right)$$

is separable. However, all single-qubit reduced states of $|\alpha\rangle$ are

$$\frac{1}{2}|00\rangle\langle00| + \frac{1}{2}|11\rangle\langle11|,$$

which is a totally mixed state.

In Ref. [56], the authors conjecture that the following state in four-qubit system $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \otimes \mathcal{H}_D$

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

is maximally entangled, where $\omega = e^{\frac{2\pi i}{3}}$. Under our entanglement measure $\mathcal{E}^M$, this conjecture is true. A straightforward calculation shows that

$$\rho_A(|\beta\rangle) = \rho_B(|\beta\rangle) = \rho_C(|\beta\rangle) = \rho_D(|\beta\rangle) = \frac{1}{2}|00\rangle\langle00| + \frac{1}{2}|11\rangle\langle11|,$$

$$\rho_{AB}(|\beta\rangle) = \frac{1}{6}|00\rangle\langle00| + \frac{1}{3}|01\rangle\langle01| + \frac{1}{6}|01\rangle\langle10| + \frac{1}{6}|10\rangle\langle01|$$
$$+ \frac{1}{3}|10\rangle\langle10| + \frac{1}{6}|11\rangle\langle11|$$

and

$$\rho_{AC}(|\beta\rangle) = \rho_{AD}(|\beta\rangle) = \frac{1}{6}|00\rangle\langle 00| + \frac{1}{3}|01\rangle\langle 01| - \frac{1}{6}|01\rangle\langle 10| - \frac{1}{6}|10\rangle\langle 01|$$
$$+ \frac{1}{3}|10\rangle\langle 10| + \frac{1}{6}|11\rangle\langle 11|.$$

Then,

$$\left(tr\sqrt{\rho_A(|\beta\rangle)}\right)^2 = \left(tr\sqrt{\rho_B(|\beta\rangle)}\right)^2 = \left(tr\sqrt{\rho_C(|\beta\rangle)}\right)^2 = 2$$

and

$$\left(tr\sqrt{\rho_{AB}(|\beta\rangle)}\right)^2 = \left(tr\sqrt{\rho_{AC}(|\beta\rangle)}\right)^2 = \left(tr\sqrt{\rho_{AD}(|\beta\rangle)}\right)^2 = 2 + \sqrt{3}.$$

Hence,

$$\mathcal{E}^M(|\beta\rangle) = \min_{\mathscr{A}_2} 4\left[\left(tr\sqrt{\rho_{A_1}(|\beta\rangle)}\right)^2 - 1\right] = 4.$$

This means that the entanglement degree of $|\beta\rangle$ reaches the upper bound of $\mathcal{E}^M$ in four-qubit system; namely, $|\beta\rangle$ is maximally entangled with respect to $\mathcal{E}^M$.

5 Conclusion

In this paper, we propose an entanglement measure $\mathcal{E}^M$ for arbitrary-dimensional multipartite quantum states, starting with the entanglement monotone $\mathcal{E}_k$. Our entanglement measure is equipped with useful properties for any states, including boundedness, convexity and subadditivity. It vanishes for and only for the separable states. Furthermore, it satisfies the monogamous relation for three-qubit quantum systems. We hope that this result can be generalized to entanglement monogamy of n-qubit quantum states. We also establish a connection between a maximally entangled state and its single-qubit reduced states. A necessary condition to characterize maximally entangled states is obtained as an application of measure $\mathcal{E}^M$.

6 Appendix 1

Here we introduce the concept of the coefficient matrix. Every pure state $|\psi\rangle$ in system $\mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2} \otimes \cdots \otimes \mathcal{H}^{d_n}$ can be represented as

$$|\psi\rangle = \sum_{j=0}^{\prod_{k=1}^{n} d_k - 1} \lambda_j |t_j\rangle,$$

where, for $j = 0, 1, \ldots, \prod_{k=1}^{n} d_k - 1$, coefficients λ_j are complex numbers satisfying

$$\sum_{j=0}^{\prod_{k=1}^{n} d_k - 1} |\lambda_j|^2 = 1$$

and $|t_j\rangle$ are the basis states in $\mathcal{H}$.

We denote the n systems by numbers $1, 2, \ldots, n$, respectively. Let q_i ($i = 1, 2, \ldots n$) be positive integers such that $0 \leqslant q_i \leqslant d_i - 1$, then the state $|\psi\rangle$ can be rewritten as

$$|\psi\rangle = \sum_{q_1=0}^{d_1-1} \sum_{q_2=0}^{d_2-1} \cdots \sum_{q_n=0}^{d_n-1} a_{q_1,q_2,\ldots,q_n} |q_1 q_2 \ldots q_n\rangle,$$

which induces the following $\left(\prod_{i=1}^{l} d_i\right) \times \left(\prod_{i=l+1}^{n} d_i\right)$ coefficient matrices whose entries $a_{q_1 q_2 \ldots q_n}$ are arranged according to the subscript $q_1 q_2 \ldots q_n$ in lexicographical ascending order

$$M_{1\cdots l,l+1\cdots n}(|\psi\rangle)$$

$$= \begin{pmatrix} a_{\underbrace{0\cdots0}_{l}\underbrace{0\cdots0}_{n-l}} & \cdots & a_{\underbrace{0\cdots0}_{l}\underbrace{d_{l+1}-1\cdots d_n-1}_{n-l}} \\ a_{\underbrace{0\cdots1}_{l}\underbrace{0\cdots0}_{n-l}} & \cdots & a_{\underbrace{0\cdots1}_{l}\underbrace{d_{l+1}-1\cdots d_n-1}_{n-l}} \\ \vdots & \ddots & \vdots \\ a_{\underbrace{d_1-1\cdots d_l-1}_{l}\underbrace{0\cdots0}_{n-l}} & \cdots & a_{\underbrace{d_1-1\cdots d_l-1}_{l}\underbrace{d_{l+1}-1\cdots d_n-1}_{n-l}} \end{pmatrix}$$

We abbreviate the coefficient matrix $M_{1\cdots l,l+1\cdots n}(|\psi\rangle)$ as $M_{1\cdots l}(|\psi\rangle)$ by omitting the column subscripts $l+1\cdots n$. Each realignment of the n particles, described simply as $s_1 s_2 \cdots s_l s_{l+1} \cdots s_n$, a permutation of the set $\{1, 2, \ldots, n\}$, generates correspondingly a $\left(\prod_{i=1}^{l} d_{s_i}\right) \times \left(\prod_{i=l+1}^{n} d_{s_i}\right)$ coefficient matrix where l is an arbitrary but fixed positive integer satisfying $1 \leqslant l \leqslant n$,

$$M_{s_1\cdots s_l}(|\psi\rangle)$$

$$= \begin{pmatrix} a_{\underbrace{0\cdots0}_{l}\underbrace{0\cdots0}_{n-l}} & \cdots & a_{\underbrace{0\cdots0}_{l}\underbrace{d_{s_{l+1}}-1\cdots d_{s_n}-1}_{n-l}} \\ a_{\underbrace{0\cdots1}_{l}\underbrace{0\cdots0}_{n-l}} & \cdots & a_{\underbrace{0\cdots1}_{l}\underbrace{d_{s_{l+1}}-1\cdots d_{s_n}-1}_{n-l}} \\ \vdots & \ddots & \vdots \\ a_{\underbrace{d_{s_1}-1\cdots d_{s_l}-1}_{l}\underbrace{0\cdots0}_{n-l}} & \cdots & a_{\underbrace{d_{s_1}-1\cdots d_{s_l}-1}_{l}\underbrace{d_{s_{l+1}}-1\cdots d_{s_n}-1}_{n-l}} \end{pmatrix}$$

7 Appendix 2

This appendix is devoted to prove Theorem 3. In order to prove this theorem, we need the following lemma.

Lemma 1 *Let $S = \{d_1, d_2, \ldots, d_n\}$ be a set of n positive numbers with $d_i \geqslant 1$ ($i = 1, 2, \ldots n$). Divide S into any k ($1 \leqslant k \leqslant n$) subsets $S_j = \left\{d_1^j, d_2^j, \ldots, d_{n_j}^j\right\}$, where $1 \leqslant j \leqslant k$ and $\sum_{j=1}^{k} n_j = n$. Then,*

$$\frac{\sum_{i=1}^{n} d_i}{n} \leqslant \frac{\sum_{j=1}^{k} \left(\prod_{m=1}^{n_j} d_m^j\right)}{k}.$$

Proof It is sufficient to verify that for any k ($1 \leqslant k \leqslant n - 1$) subsets $S_j = \left\{d_1^j, d_2^j, \ldots, d_{n_j}^j\right\}$ of the set S with $1 \leqslant j \leqslant k$ and $\sum_{j=1}^{k} n_j = n$, there exists $k + 1$ subsets $T_l = \left\{c_1^l, c_2^l, \ldots, c_{h_l}^l\right\}$ of the set S with $1 \leqslant l \leqslant k + 1$ and $\sum_{l=1}^{k+1} h_l = n$, such that

$$\frac{\sum_{l=1}^{k+1} \left(\prod_{m=1}^{h_l} c_m^l\right)}{k + 1} \leqslant \frac{\sum_{j=1}^{k} \left(\prod_{m=1}^{n_j} d_m^j\right)}{k}.$$

For k subsets $S_j = \left\{d_1^j, d_2^j, \ldots, d_{n_j}^j\right\}$ with $1 \leqslant j \leqslant k$ and $\sum_{j=1}^{k} n_j = n$, without loss of generality we assume $n_1 \geqslant 2$. Suppose that

$$
\begin{aligned}
T_1 &= \left\{c_1^1\right\} = \left\{d_1^1\right\}, \\
T_2 &= \left\{c_1^2, c_2^2 \ldots, c_{h_2}^2\right\} = \left\{d_2^1, d_3^1, \ldots, d_{n_1}^1\right\}, \\
T_l &= \left\{c_1^l, c_2^l, \ldots, c_{h_l}^l\right\} = S_{l-1} = \left\{d_1^{l-1}, d_2^{l-1}, \ldots, d_{n_{l-1}}^{l-1}\right\},
\end{aligned}
$$

with $3 \leqslant l \leqslant k + 1$.

It is apparent from the condition that

$$d_1^1 \geqslant 1,$$
$$\prod_{m=2}^{n_1} d_m^1 \geqslant 1,$$
$$\sum_{j=2}^{k} \left(\prod_{m=1}^{n_j} d_m^j\right) \geqslant k - 1.$$

A routine computation gives rise to

$$(k + 1) \sum_{j=1}^{k} \left(\prod_{m=1}^{n_j} d_m^j\right) - k \left[d_1^1 + \prod_{m=2}^{n_1} d_m^1 + \sum_{j=2}^{k} \left(\prod_{m=1}^{n_j} d_m^j\right)\right]$$

$$= \left(k d_1^1 + d_1^1\right) \left(\prod_{m=2}^{n_1} d_m^1 - 1\right) - k \prod_{m=2}^{n_1} d_m^1 + \sum_{j=2}^{k} \left(\prod_{m=1}^{n_j} d_m^j\right) + d_1^1$$

$$\geqslant \left(kd_1^1 + d_1^1\right)\left(\prod_{m=2}^{n_1} d_m^1 - 1\right) - k\prod_{m=2}^{n_1} d_m^1 + k - 1 + d_1^1$$

$$= \left(d_1^1 - 1\right) + \left[k\left(d_1^1 - 1\right) + d_1^1\right]\left(\prod_{m=2}^{n_1} d_m^1 - 1\right)$$

$$\geqslant 0.$$

Rearranging the preceding inequality leads to

$$\frac{d_1^1 + \prod_{m=2}^{n_1} d_m^1 + \sum_{j=2}^{k}\left(\prod_{m=1}^{n_j} d_m^j\right)}{k+1} \leqslant \frac{\sum_{j=1}^{k}\left(\prod_{m=1}^{n_j} d_m^j\right)}{k}.$$

Thus we arrive at the conclusion that

$$\frac{\sum_{l=1}^{k+1}\left(\prod_{m=1}^{h_l} c_m^l\right)}{k+1} \leqslant \frac{\sum_{j=1}^{k}\left(\prod_{m=1}^{n_j} d_m^j\right)}{k}.$$

This completes the proof of Lemma 1. □

Now we turn to prove Theorem 3.

Proof of Theorem 3 It can be immediately seen that $\mathcal{E}^M(|\psi\rangle) \geqslant 0$ for any pure state $|\psi\rangle$. It remains to show that the upper bound of $\mathcal{E}^M(|\psi\rangle)$ is $(\widetilde{d} - 1)\sqrt{\widetilde{d}^n}$. For any n_i-partite component system $A = \mathcal{H}^{d_1^i} \otimes \mathcal{H}^{d_2^i} \otimes \cdots \otimes \mathcal{H}^{d_{n_i}^i}$ $(d_1^i, d_2^i, \ldots, d_{n_i}^i \in \{d_1, d_2, \ldots, d_n\})$, let ρ_A has the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_{\prod_{m=1}^{n_i} d_m^i}$. Therefore,

$$\lambda_1 + \lambda_2 + \cdots + \lambda_{\prod_{m=1}^{n_i} d_m^i} = 1$$

and

$$tr\sqrt{\rho_A} = \sum_{j=1}^{\prod_{m=1}^{n_i} d_m^i} \sqrt{\lambda_j} \leqslant \sqrt{\left(\prod_{m=1}^{n_i} d_m^i\right)\sum_{j=1}^{\prod_{m=1}^{n_i} d_m^i} \lambda_j} = \sqrt{\prod_{m=1}^{n_i} d_m^i}.$$

Consequently, we infer that

$$\min_{\mathscr{A}_k}\left[\frac{\sum_{i=1}^{k}\left(tr\sqrt{\rho_{A_i}}\right)^2}{k} - 1\right] \leqslant \min_{\mathscr{A}_k}\left[\frac{\sum_{i=1}^{k}\left(\prod_{m=1}^{n_i} d_m^i\right)}{k} - 1\right].$$

Meanwhile, Lemma 1 tells us that

$$\min_{2 \leqslant k \leqslant n} \min_{\mathscr{A}_k} \left[\frac{\sum_{i=1}^{k} \left(\prod_{m=1}^{n_i} d_m^i \right)}{k} - 1 \right] = \frac{\sum_{i=1}^{n} d_i}{n} - 1 = \widetilde{d} - 1.$$

Hence,

$$\min_{2 \leqslant k \leqslant n} \min_{\mathscr{A}_k} \sqrt{\widetilde{d}^n} \left[\frac{\sum_{i=1}^{k} \left(tr \sqrt{\rho_{A_i}} \right)^2}{k} - 1 \right] \leqslant (\widetilde{d} - 1) \sqrt{\widetilde{d}^n},$$

which means that $\mathcal{E}^M (|\psi\rangle) \leqslant (\widetilde{d} - 1) \sqrt{\widetilde{d}^n}$. Thus Theorem 3 is completed. □

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