Multilinear monogamy relations for multiqubit states

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(Received 13 May 2021; accepted 23 June 2021; published 28 July 2021)

The monogamy of entanglement means that entanglement cannot be freely shared. In 2014, Oliveira *et al.* [T. R. de Oliveira, M. F. Cornelio, and F. F. Fanchini, Phys. Rev. A **89**, 034303 (2014)] proposed a monogamy relation in the linear version and considered it in terms of entanglement of formation. Here we generalize the above version and consider a multilinear monogamy relation for a multiqubit system in terms of entanglement of formation and concurrence. Based on the above results, we present an entanglement criterion for genuine entangled states; also we consider the absolutely maximally entangled states and present what an absolutely maximally entangled state is for a three-qubit system. Last, we apply our results to a three-qubit pure state in terms of quantum discord.

DOI: 10.1103/PhysRevA.104.012426

I. INTRODUCTION

Quantum entanglement is an essential feature of quantum mechanics. It plays an important role in quantum information and quantum computation theory [1], such as superdense coding [2], teleportation [3], and the speedup of quantum algorithms [4].

As a property of multipartite entanglement, monogamy of entanglement presents that entanglement cannot be shared arbitrarily among many parties, which is different from classical correlations [5]. This property has been applied in many areas in quantum information. It can be applied to prove the security of quantum cryptography [6–8] and the bound of the regularization of its Holevo information for arbitrary channels [9]. It can also be applied to distinguish inequivalent classes of pure states in a tripartite system [10,11]. Recently, the authors showed there exist restrictions of indistinguishability for entangled systems due to monogamy relations [12].

Mathematically, for a tripartite system with parties A, B, and C, the general monogamy in terms of an entanglement measure $\mathcal{E}$ implies that the entanglement between A and BC satisfies

$$\mathcal{E}_{A|BC} \geqslant \mathcal{E}_{AB} + \mathcal{E}_{AC}. \quad (1)$$

Here $\mathcal{E}_{AB}$ and $\mathcal{E}_{AC}$ means the entanglement between the parties A, B and A, C. This relation was first proved for qubit systems in terms of the 2-tangle [10,13]. Bai *et al.* showed that the inequality Eq. (1) is valid in terms of the squared entanglement of formation (EoF) for n-qubit systems [14]. Zhu and Fei investigated the monogamy relations related to the concurrence and the entanglement of formation [15]. Recently, the authors of Refs. [16,17] presented generalized monogamy relations, and Jin *et al.* proposed tighter monogamy relations for n-qubit systems [18]. Yu *et al.* utilized the conversion relation between the coherence and the entanglement to establish the monogamy inequalities for high-dimensional coherence-induced entanglement in terms of the relative entropy of entanglement and the negativity [19]. Zhang *et al.* studied the monogamy relations for multiqubit quantum systems in product norm [20].

However, it is well known that the EoF (E) does not satisfy the inequality Eq. (1). In 2014, Oliveira *et al.* proposed a linear monogamy relation in terms of EoF and numerically obtained the bound for a three-qubit system. This result indicates that entanglement cannot be freely shared in terms of EoF [21]. In 2015, Liu *et al.* proved this bound analytically [22]. There they also computed the bound of the linear monogamy relation in terms of concurrence for a three-qubit system [22]. Moreover, Cornelio proposed another interesting monogamy relation in terms of the squared concurrence for three-qubit systems [23]. They called the relations multipartite monogamy relations.

One of the motivations of this paper is to better understand the monogamy relations within the theory of multipartite entanglement [24–27]. Although in Ref. [28] the authors mentioned a similar function of a three-qubit pure state in terms of some entanglement measure, there they aimed to investigate the robustness of a three-qubit pure state against loss of a qubit. Here we characterize the distribution of the entanglement for an n-qubit system in terms of EoF and concurrence. In Ref. [28], the authors only showed the function numerically in terms of EoF and the bound of the function in terms of the squared concurrence among three-qubit pure states. Crucially, we present a multilinear monogamy relation in terms of entanglement of formation for a three-qubit pure state analytically. We generalize this bound to a three-qubit mixed state in terms of EoF and concurrence. Also, we present that only the local-unitary-equivalent class of the W state can reach the upper

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bound among three-qubit mixed states. That is, this can be seen to detect whether a three-qubit pure state is the W state. Due to the importance of the W state in quantum computation and communication [29–32], this result is meaningful.

In this work, we consider a multilinear monogamy relation in terms of EoF and concurrence for a multiqubit system. We present that the W state is the unique state that can reach the upper bound of multilinear monogamy relations in terms of concurrence and EoF up to the local unitary (LU) transformations. We also present the condition when the states reach the minimum of the multilinear monogamy relation in terms of concurrence. Last, we present some applications of our results to build an entanglement criterion and consider the absolutely maximally entangled states for a three-qubit system mainly. We also get a similar bound for the discord of three-qubit pure states.

This article is organized as follows. First we review the preliminary knowledge needed. Then we prove our main results. We present multilinear monogamy relations in terms of EoF and concurrence. We also present some applications of our results on the entanglement witness. Last, based on the relation between the EoF and the discord, we present a similar result for the sum of all bipartite quantum discord for a three-qubit pure state.

II. PRELIMINARIES

An n-partite pure state $|\psi\rangle_{A_1A_2\cdots A_n}$ is full product if it can be written as

$$|\psi\rangle_{A_1A_2\cdots A_n} = |\phi_1\rangle_{A_1}|\phi_2\rangle_{A_2}\cdots|\phi_n\rangle_{A_n}; \tag{2}$$

otherwise, it is entangled. A multipartite pure state is called genuinely entangled if

$$|\psi\rangle_{A_1A_2\cdots A_n} \neq |\phi\rangle_S|\varphi\rangle_{\overline{S}}, \tag{3}$$

for any bipartition $S|\overline{S}$; here S is a subset of $\boldsymbol{A} = \{A_1, A_2, \dots, A_n\}$, and $\overline{S} = \boldsymbol{A} - S$.

Assume $|\psi\rangle_{AB}$ is a bipartite pure state. Due to the Schmidt decomposition, $|\psi\rangle_{AB}$ can always be written as

$$|\psi\rangle_{AB} = \sum_i \sqrt{\lambda_i}|i\rangle_A|i\rangle_B,$$

where $\lambda_i \geqslant 0$, $\sum_i \lambda_i = 1$, and $\{|i\rangle_{A(B)}\}$ is an orthonormal basis of the Hilbert space $A(B)$. First we recall the EoF. The EoF of $|\psi\rangle_{AB}$ is given by

$$E(|\psi\rangle_{AB}) = S(\rho_A) = -\sum \lambda_i \log_2 \lambda_i, \tag{4}$$

where λ_i are the eigenvalues of $\rho_A = \mathrm{Tr}_B\, |\psi\rangle_{AB}\langle\psi|$. For a mixed state ρ_{AB}, the EoF is defined by the convex roof extension method,

$$E(\rho_{AB}) = \min_{\{p_i,|\phi_i\rangle_{AB}\}} \sum_i p_i E(|\phi_i\rangle_{AB}), \tag{5}$$

where the minimum is taken over all the decompositions of $\rho_{AB} = \sum_i p_i|\phi_i\rangle_{AB}\langle\phi_i|$, with $p_i \geqslant 0$ and $\sum p_i = 1$.

The other important entanglement measure is the concurrence (C). The concurrence of a pure state $|\psi\rangle_{AB}$ is defined as

$$C(|\psi\rangle_{AB}) = \sqrt{2\left(1 - \mathrm{Tr}\,\rho_A^2\right)} = \sqrt{2\left(1 - \sum_i \lambda_i^2\right)}. \tag{6}$$

For a mixed state ρ_{AB}, it is defined as

$$C(\rho_{AB}) = \min_{\{p_i,|\phi_i\rangle_{AB}\}} \sum_i p_i C(|\phi_i\rangle_{AB}), \tag{7}$$

where the minimum takes over all the decompositions of $\rho_{AB} = \sum_i p_i|\phi_i\rangle_{AB}\langle\phi_i|$, with $p_i \geqslant 0$ and $\sum p_i = 1$.

For a two-qubit mixed state ρ_{AB}, Wootters derived an analytical formula [33]:

$$E(\rho_{AB}) = h\left(\frac{1 + \sqrt{1 - C_{AB}^2}}{2}\right), \tag{8}$$

$$h(x) = -x\log_2 x - (1-x)\log_2(1-x), \tag{9}$$

$$C_{AB} = \max\{\sqrt{\mu_1} - \sqrt{\mu_2} - \sqrt{\mu_3} - \sqrt{\mu_4}, 0\}, \tag{10}$$

where μ_1, μ_2, μ_3, and μ_4, are the eigenvalues of the matrix $\rho_{AB}(\sigma_y \otimes \sigma_y)\rho_{AB}^*(\sigma_y \otimes \sigma_y)$ with nonincreasing order.

III. MAIN RESULTS

For a three-qubit pure state $|\psi\rangle_{ABC}$, the pairwise correlations are described by the reduced density operators ρ_{AB}, ρ_{BC}, and ρ_{CA}. In 2014, de Oliveira *et al.* [21] numerically presented that the following inequality is valid for a three-qubit pure state in terms of EoF and concurrence,

$$E_{A|B} + E_{A|C} \leqslant \lambda, \tag{11}$$

where λ is a constant. When E is the EoF, they conjectured $\lambda = 1.2018$. In 2015, Liu *et al.* [22] proved the above inequality for a three-qubit pure state in terms of EoF analytically; there they denoted the above inequality as the linear monogamy relation.

From Eq. (11), we find that although the EoF does not satisfy Eq. (1) for three-qubit generic states, the entanglement cannot be freely shared in terms of EoF. Here we mainly consider a linear monogamy relation which we call the multilinear monogamy relation. The main difference between ours and the linear monogamy relations is that the left-hand side takes over all bipartitions within the multipartite entanglement. For the three-qubit states, this means in terms of some entanglement measure $\mathcal{E}$ that the following inequality is valid:

$$M\mathcal{E} = \mathcal{E}_{A|B} + \mathcal{E}_{A|C} + \mathcal{E}_{B|C} \leqslant \nu. \tag{12}$$

Here ν is a constant. We can also generalize the relations to n-qubit states $\rho_{A_1A_2\cdots A_n}$, we denote the following inequality in terms of some entanglement measure $\mathcal{E}$ as the multilinear monogamy relation:

$$\sum_{i<j} \mathcal{E}_{i|j} \leqslant \eta. \tag{13}$$

Here η is a constant.

A. Multipartite linear monogamy relations in terms of EoF

In this subsection, we first present a theorem on the multilinear monogamy relation in terms of EoF for a three-qubit pure state.

Theorem 1. For a three-qubit pure state, the W state reaches the upper bound $c_{\max} = 3h(\frac{1}{2} + \frac{\sqrt{5}}{6})$ of multilinear monogamy relation in terms of EoF.

The proof of Theorem 1 is given in Appendix A.

We can extend this result to the mixed state ρ_{ABC}. Assume that $\{s_h, |\phi_h\rangle_{ABC}\}$ is a decomposition of ρ_{ABC}, then we have.

$$\begin{aligned} &E(\rho_{AB}) + E(\rho_{AC}) + E(\rho_{BC}) \\ &= \sum_i p_i E(|\phi_i\rangle_{AB}) + \sum_j q_j E(|\theta_j\rangle_{AC}) + \sum_k r_k E(|\zeta_k\rangle_{BC}) \\ &\leqslant \sum_h s_h\big[E(\rho^h_{AB}) + E(\rho^h_{AC}) + E(\rho^h_{BC})\big] \\ &\leqslant \sum_h s_h \times c_{\max} = c_{\max}. \end{aligned} \tag{14}$$

Here we assume that in the first equality, $\{p_i, |\phi_i\rangle\}$, $\{q_j, |\theta_j\rangle\}$, and $\{r_k, |\zeta_k\rangle\}$ are the optimal decompositions of ρ_{AB}, ρ_{AC}, and ρ_{BC} in terms of the EoF correspondingly. The first equality is due to the definition of the EoF for the mixed states, and the second inequality is due to the equality (A15). In the first inequality, we denote $\mathrm{Tr}_C\, |\phi^h\rangle\langle\phi^h| = \rho^h_{AB}$, $\mathrm{Tr}_B\, |\phi^h\rangle\langle\phi^h| = \rho^h_{AC}$, and $\mathrm{Tr}_A\, |\phi^h\rangle\langle\phi^h| = \rho^h_{BC}$.

For a three-qubit pure state, Dür *et al.* [28] showed that there are two inequivalent kinds of genuinely entangled states, i.e., the W-class states and the Greenberger-Horne-Zeilinger (GHZ)-class states. The W-class states $|\psi\rangle$ are all LU equivalent to the following states:

$$|\phi\rangle = r_0|000\rangle + r_1|001\rangle + r_2|010\rangle + r_3|100\rangle, \tag{15}$$

where $r_1, r_2, r_3 > 0$ and $\sum_{i=0}^3 |r_i|^2 = 1$. From simple computation, we have $C^2(\rho_{AB}) = 4|r_2r_3|^2$, $C^2(\rho_{AC}) = 4|r_1r_3|^2$, and $C^2(\rho_{BC}) = 4|r_1r_2|^2$. We see that the function $E(\rho_{AB}) + E(\rho_{AC}) + E(\rho_{BC})$ ranges over $(0, c_{\max}]$ for the W class states. When $|\psi\rangle = \frac{|000\rangle+|111\rangle}{\sqrt{2}}$, $E(\rho_{AB}) + E(\rho_{AC}) + E(\rho_{BC}) = 0$, and as the GHZ class states is dense [34], the function $E(\rho_{AB}) + E(\rho_{AC}) + E(\rho_{BC})$ ranges over $[0, c_{\max})$.

B. Multipartite linear monogamy relations in terms of concurrence

In this subsection, we present a theorem on the multilinear monogamy relation in terms of the concurrence for a three-qubit pure state $|\psi\rangle_{ABC}$.

Lemma 1. Up to the local unitary transformations, the W state is the unique state that can reach the upper bound in terms of the function. $C^M(\psi) = C_{AB} + C_{BC} + C_{AC}$ for a three-qubit pure state.

We give the proof of Lemma 1 in Appendix B.

By a method similar to that we present under Theorem 1, we can also extend the above results on the mixed states.

Next we present an example on the multilinear monogamy relation in terms of concurrence for a three-qubit mixed state.

Example 1. Example 1 is as follows:

$$\rho = p_1|W\rangle\langle W| + p_2|\overline{W}\rangle\langle\overline{W}|.$$

Here we denote that $|\overline{W}\rangle = \frac{1}{3}(|110\rangle + |101\rangle + |011\rangle)$.

Through simple computation,

$$\rho_{AB} = \rho_{AC} = \rho_{BC},$$

$$\rho_{AB} = \frac{p_1}{3}|00\langle 00|\rangle + \frac{1}{3}(|01\rangle + |10\rangle)(\langle 10| + \langle 01|) + \frac{p_2}{3}|11\rangle\langle 11|,$$

we have

$$C(\rho_{AB}) = C(\rho_{AC}) = C(\rho_{BC}) = \frac{2 - 2\sqrt{p_1p_2}}{3};$$

if $p_i > 0$, $i = 1$ and 2, we have $C^M(\rho_{ABC}) < 2$.

The Lemma 1 can be generalized to the three-qubit mixed states.

Theorem 2. Up to the local unitary transformations, the W state is the unique state that can reach the upper bound in terms of the function $C^M(\cdot)$ for a three-qubit mixed state.

The proof of Theorem 2 is given in Appendix C.

Next we present a necessary and sufficient condition when the function $C^M(\cdot)$ attains the minimum 0.

Theorem 3. Assume $|\psi\rangle$ is a three-qubit pure state, then $C^M(|\psi\rangle) = 0$ if and only if $|\psi\rangle$ can be represented as $|\psi\rangle = r_0|000\rangle + r_1|111\rangle$ up to local unitary operations when $0 \leqslant r_0$ and $r_1 \leqslant 1$.

The proof of Theorem 3 is given in Appendix D.

Theorem 4. Up to the local unitary transformations, the W state is the unique state that can reach the upper bound in terms of the function $E(\rho_{AB}) + E(\rho_{AC}) + E(\rho_{BC})$ for a three-qubit mixed state.

Theorem 4 can be proved in a process similar to that used in the proof of Theorem 2.

Next we consider the multilinear monogamy relations for the n-qubit W-class states. These states were proposed by San Kim *et al.* [35] in order to study the monogamy relations in terms of convex roof extended negativity for higher-dimensional systems.

Example 2. Example 2 is as follows:

$$|\phi\rangle_{A_1A_2\cdots A_n} = \sqrt{p}|GW\rangle_n + \sqrt{1-p}|0\rangle_n.$$

Here we assume $|GW\rangle = a_1|10\cdots 0\rangle + a_2|010\cdots\rangle + \cdots + a_n|00\cdots 1\rangle$, $\sum_i |a_i|^2 = 1$.

Through simple computation, we have $C(\rho_{A_1A_i}) = 2p|a_1a_i|$, and

$$\begin{aligned} C^M(|\phi\rangle) &= 2p\sum_{i<j}|a_ia_j| \\ &= p\left[\left(\sum_i |a_i|\right)^2 - \sum_i |a_i|^2\right] \\ &= p\left[\left(\sum_i |a_i|\right)^2 - 1\right]. \end{aligned} \tag{16}$$

By the method of the Lagrange multiplier, we see when $a_i = \frac{1}{\sqrt{n}}$ and $p = 1$, that is, when $|\phi\rangle = |W\rangle$, the value in Eq. (16) attains the maximum.

In Ref. [36], the authors presented that, for an n-qubit symmetric pure state $|\phi\rangle$, the maximal value between any pair of qubits in terms of concurrence is $\frac{2}{n}$, and when $|\phi\rangle = |W\rangle$, it attains the maximum. Then we may propose a conjecture.

Conjecture 1. For an n-qubit genuinely entangled pure state $|\phi\rangle$, the maximum $C^M(\phi)$ is attained when $|\phi\rangle = |W\rangle$.

Remark 1. Under Conjecture 1, we can generalize the above results to n-qubit mixed states.

First, we prove that when $|\phi\rangle_{A_1A_2\cdots A_n}$ is an n-qubit pure state, the maximum of $C^M(\phi)$ is attained when $|\phi\rangle = |W\rangle$, that is, $\max_\phi C^M(|\phi\rangle) = n - 1$.

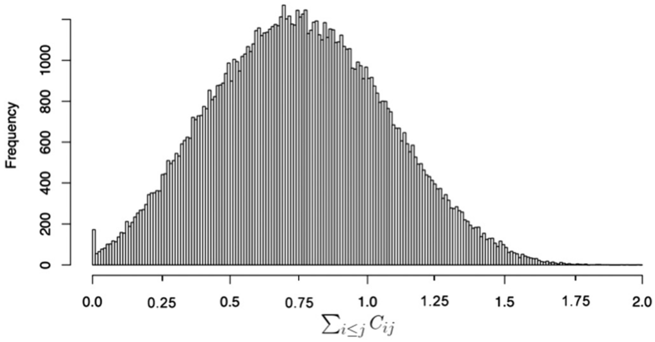

FIG. 1. In this figure, we present the frequency of the function $\sum_{i\leqslant j} C_{ij}$ for random pure states of four-qubit states. The unit of the Y axis is the number of times that the value of the function $\sum_{i\leqslant j} C_{ij}$ occurs.

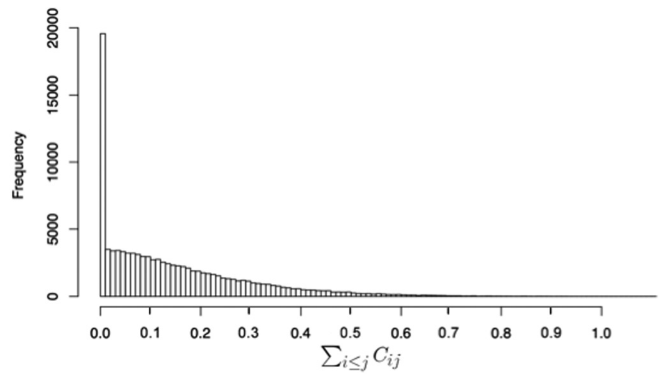

FIG. 2. In this figure, we present the frequency of the function $\sum_{i\leqslant j} C_{ij}$ for random pure states of five-qubit states. The unit of the Y axis is the number of times that the value of the function $\sum_{i\leqslant j} C_{ij}$ occurs.

If $|\phi\rangle$ is not genuinely entangled, we can always assume that $|\phi\rangle_{A_1A_2\cdots A_n}$ is biseparable, i.e., $|\phi\rangle_{A_1A_2\cdots A_n} = |\theta_1\rangle_{A_1A_2\cdots A_m}|\theta_2\rangle_{A_{m+1}A_{m+2}\cdots A_n}$, here $|\theta_i\rangle$, $i=1$ and 2, are genuinely entangled. As $|\phi\rangle$ is biseparable,

$$\begin{aligned} C^M(|\phi\rangle) &= C^M(|\theta_1\rangle) + C^M(|\theta_2\rangle) \\ &\leqslant m-1+n-m-1 \\ &= n-2 \\ &< n-1. \end{aligned} \tag{17}$$

Then by a proof similar to that of Theorem 2 and the statement above, we can get the results on mixed states: when $\rho_{A_1A_2\cdots A_n}$ is an n-qubit mixed state, up to the local unitary transformations, the W state is the unique state that can reach the upper bound in terms of the function $\sum_{i<j} C_{ij}$.

Then we pick 10^5 four- and five-qubit pure states randomly and compute their $C^M(\cdot)$; these results may verify Conjecture 1 numerically. In Fig. 1, we present a histogram of the value of $\sum_{i\leqslant j} C_{ij}$ for random pure states of four qubits sampled uniformly. Here we find the function $C^M(\cdot)$ mainly distributes in the section [0,1.8], and in the section [1.8,2], there are few states. Figure 1 supports Conjecture 1 for $n=4$.

In Fig. 2 , we present a histogram of the value of $\sum_{i\leqslant j} C_{ij}$ for random pure states of five qubits sampled uniformly. From the figure, we have that the sum of $C^M(\cdot)$ mainly distributes in the section [0,0.6]. In Ref. [37], the authors considered the multipartite correlations in four-qubit pure states. Here, through Fig. 2, we have that the quantity of the bipartite correlations of most five-qubit pure states is few; then it seems that comparing with the separable states, the set of the entangled states for five-qubit pure states is bigger.

In the last part of this section, we consider the $C^M(\cdot)$ for a class of pure states in a system with more qubits studied in Ref. [34]. They are useful kinds of entanglement states for quantum teleportation and error correction:

$$|\psi\rangle = a|\mathrm{GHZ}\rangle_m|W\rangle_n + b|W\rangle_m|\mathrm{GHZ}\rangle_n.$$

Here $|a|^2+|b|^2=1$, and $m,n\geqslant 2$. Due to the shape of $|\psi\rangle$, we have that the set of the bipartite reduced density matrices for the pure state $|\psi\rangle$ consists of three kinds:

$$\begin{aligned} \rho^1 &= \frac{|a|^2}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|) + \frac{|b|^2}{m}[(m-2)|00\rangle\langle 00| + (|01\rangle+|10\rangle)(\langle 01|+\langle 10|)], \\ \rho^2 &= \frac{|b|^2}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|) + \frac{|a|^2}{n}[(n-2)|00\rangle\langle 00| + (|01\rangle+|10\rangle)(\langle 01|+\langle 10|)], \\ \rho^3 &= \left(\frac{a}{\sqrt{2n}}|01\rangle + \frac{b}{\sqrt{2m}}|10\rangle\right)\left(\frac{\bar{a}}{\sqrt{2n}}\langle 01| + \frac{\bar{b}}{\sqrt{2m}}\langle 10|\right) + \left[\frac{(n-1)|a|^2}{2n} + \frac{(m-1)|b|^2}{2m}\right]|00\rangle\langle 00| + \frac{(n-1)|a|^2}{2n}|10\rangle\langle 10| \\ &\quad + \frac{|a|^2}{2n}|11\rangle\langle 11| + \frac{(m-1)|b|^2}{2m}|01\rangle\langle 01| + \frac{|b|^2}{2m}|11\rangle\langle 11|, \end{aligned} \tag{18}$$

and then we have

$$\begin{aligned} C(\rho^1) &= \max\left\{0, \frac{2|b|^2}{m} - 2\sqrt{\frac{|a|^2}{2}\left(\frac{|a|^2}{2} + \frac{m-2}{m}|b|^2\right)}\right\} \\ &= \begin{cases} 0, & |a|^2 \in (g(m), 1], \\ \frac{2|b|^2}{m} - 2\sqrt{\frac{|a|^2}{2}\left(\frac{|a|^2}{2} + \frac{m-2}{m}|b|^2\right)}, & |a|^2 \in [0, g(m)], \end{cases} \end{aligned} \tag{19}$$

$$C(\rho^2) = \max\left\{0, \frac{2|a|^2}{n} - 2\sqrt{\frac{|b|^2}{2}\left(\frac{|b|^2}{2} + \frac{n-2}{n}|a|^2\right)}\right\}$$

$$= \begin{cases} 0, & |a|^2 \in [0, h(n)], \\ \frac{2|a|^2}{n} - 2\sqrt{\frac{|b|^2}{2}\left(\frac{|b|^2}{2} + \frac{n-2}{n}|a|^2\right)}, & |a|^2 \in [h(n), 1], \end{cases} \quad (20)$$

$$C(\rho^3) = 0. \quad (21)$$

Here $g(m) = \frac{m^2-2m+4-m\sqrt{m^2-4m+8}}{(m-2)^2}$, and $h(n) = \frac{n\sqrt{n^2-4n+8}-2n}{(n-2)^2}$.

Let $x = |a|^2$, and $f(x) = C^M(|\psi\rangle)$. First we compute the maximum when $(m, n) \in \{(2, 2), (2, 3), (3, 2), (3, 3), (2, 4), (4, 2)\}$.

When $m = n = 2$, we have

$$f(x) = \begin{cases} 1 - 2x, & x \in [0, 1/2], \\ 2x - 1, & x \in [1/2, 1], \end{cases} \quad (22)$$

and then the maximum is 1, when $x = 0$ or 1.

When $m = 2$ and $n = 3$, we have

$$f(x) = \begin{cases} 1 - 2x, & x \in (0, 1/2), \\ 0, & x \in [1/2, 3\sqrt{5} - 6], \\ 2x - \sqrt{3x^2 - 12x + 9}, & x \in (3\sqrt{5} - 6, 1], \end{cases} \quad (23)$$

and then when $x = 1$, we have $f(x)$ gets the maximum 2.

When $m = 3$ and $n = 2$, we have

$$f(x) = \begin{cases} 2(1 - x) - \sqrt{3x(x + 2)}, & x \in [0, 7 - 3\sqrt{5}], \\ 0, & x \in \left[7 - 3\sqrt{5}, \frac{1}{2}\right], \\ 2x - 1, & x \in [1/2, 1], \end{cases} \quad (24)$$

and when $x = 0$, $f(x)$ gets the maximum 2.

When $m = n = 3$, we have

$$f(x)= \begin{cases} 3(1-x)-\sqrt{3x(x + 2)}, & x \in [0, 7 - 3\sqrt{5}], \\ 0, & x \in (7 - 3\sqrt{5}, 3\sqrt{5} - 6), \\ 2x - \sqrt{3x^2 - 12x + 9}, & x \in (3\sqrt{5} - 6, 1], \end{cases} \quad (25)$$

and when $x = 0$ or $x = 1$, $f(x)$ gets the maximum, 2.

When $m = 4$ and $n = 2$, we have

$$f(x) = \begin{cases} 3 - 3x - 6\sqrt{x}, & x \in [0, 3 - 2\sqrt{2}], \\ 0, & x \in [3 - 2\sqrt{2}, 1/2], \\ 2x - 1, & x \in [1/2, 1], \end{cases} \quad (26)$$

and when $x = 0$, $f(x)$ gets the maximum 3.

When $m = 2$ and $n = 4$, we have

$$f(x) = \begin{cases} 1 - 2x, & x \in [0, 1.2], \\ 0, & x \in (1/2, 2\sqrt{2} - 2), \\ 3x - 12\sqrt{\frac{1}{4} - \frac{x}{4}}, & x \in [2\sqrt{2} - 2, 1], \end{cases} \quad (27)$$

and then $\max_{x\in[0,1]} f(x) = 3$.

Next from simple computation, we have $\forall m, n \geqslant 3, h(n) \geqslant g(m)$, then

$$f(x) = \begin{cases} (m - 1)(1 - x) - 2\sqrt{\frac{4-m}{4m}x^2 + \frac{m-2}{2m}x}, & x \in [0, g(m)], \\ 0, & x \in [g(m), h(n)], \\ (n - 1)x - n(n - 1)\sqrt{\frac{1}{4} - \frac{x}{n} + \frac{4-n}{4n}x^2}, & x \in [g(n), 1], \end{cases} \quad (28)$$

when $x \in [0, g(m)]$ and $m \geqslant 4$, $f(x)$ is monotone decreasing; then when $x = 0$, $f(x) = m - 1$; when $x \in [g(n), 1]$, $f(x)$ is monotone increasing and then $\max_{x\in[g(n,1)]} f(x) = n - 1$, that is, when $m \geqslant 4$, $f(x) = \max(m - 1, n - 1)$.

In the next section, we present some applications of our results.

IV. APPLICATION

The structure of a multipartite entanglement system is complex. In this section, we apply our results above on the genuine entanglement detection. We also make some comments on the absolutely maximally entangled states (AMES), and we apply Theorem 3 to present when a pure state is an AMES in a three-qubit system.

A. An entanglement criterion for genuine entangled states

On the other hand, an important problem in entanglement theory is to determine whether a multipartite state is genuinely entangled, biseparable, or fully separable. A widely accepted method for attacking the problem is to construct entanglement witnesses (EWs) [1]. The EW W is a Hermitian operator when $\mathrm{Tr}(W\sigma) \geqslant 0$ for every biseparable state σ and $\mathrm{Tr}(W\rho) < 0$ for some entangled state ρ. The EW is a theoretical and experimental method compared with mathematical criteria, such as positive partial transpose [38] and computable cross norm [39]. For a review we refer readers to Refs. [1,24]. EWs have been constructed to detect the entanglement of many physically realizable states, such as the GHZ diagonal states [40,41], GHZ-like states [42], and noisy Dicke states [43]. In the following we connect EWs to $C^M(\phi)$.

In practice, we need to analyze the change of $C^M(\phi)$ of n-qubit pure states $|\varphi\rangle$ under white noise. Let $\rho(p) = p|\varphi\rangle\langle\varphi| + (1 - p)\frac{1}{2^n}I_{2^n}$, with $p \in (0, 1)$. By definition and simple computation, one can show that $C^M(\rho)$ monotonically increases with p. As an example, we assume that $|\varphi\rangle$ is the n-qubit W

state. Hence

$$\rho(p) = p|W_n\rangle\langle W_n| + (1-p)\frac{I}{2^n}. \tag{29}$$

Here we can find that the state (29) is symmetric. From computation, we have

$$C(\rho_{i\neq j}) = \max\left(0, \frac{2p}{n} - 2\sqrt{\frac{(1-p)(n+3np-8p)}{16n}}\right), \tag{30}$$

that is, when

$$16p^2 - n^2(1-p)^2 + 4np(n-2)(p-1) > 0, \tag{31}$$

$$C^M(\rho) = (n-1)p - (n-1)\sqrt{n(1-p)(n+3np-8p)}.$$

When $n=3$, from the analysis above, we have that when $p \geqslant \frac{\sqrt{155}-5}{8}$ the state $\rho(p)$ is a genuinely entangled state. In Ref. [43], the authors showed when $p \leqslant \frac{\sqrt{3}}{8+\sqrt{3}}$ the state $\rho(p)$ is fully separable; there the authors presented an optimal entanglement witness $\widehat{W}$ for the state $\rho(p)$ when $n=3$, and the witness $\widehat{W}$ was written as

$$\begin{aligned}\widehat{W} = &\frac{1}{d}|000\rangle\langle 000| - [|001\rangle(\langle 001| \\ &+ \langle 100|) + |010\rangle(\langle 001| + \langle 100|) \\ &+ |100\rangle(\langle 001| + \langle 010|)] \\ &+ d(|011\rangle + |101\rangle + |110\rangle)(\langle 011| \\ &+ \langle 101| + \langle 110|).\end{aligned}$$

Chen *et al.* [44] have shown that the state $\rho(p)$ is fully separable when $p \leqslant \frac{\sqrt{3}}{8+\sqrt{3}}$; they also showed when $p \in (\frac{\sqrt{3}}{8+\sqrt{3}}, 0.2095]$ the state $\rho(p)$ is biseparable but not fully separable. Here, if Conjecture 1 is true, then $C^M(\rho) > n-2$ implies that $\rho(p)$ is a genuinely entangled state. In particular, this is true when $n=3$ by Theorem 4. Thus proving Conjecture 1 is meaningful to the investigation of entanglement detection.

B. Absolutely maximally entangled state

Next we investigate AMES in n-qubit systems. A pure multipartite entangled state is called AMES if all reduced density operators obtained by tracing out at least half of the particles are maximally mixed [45]. So the function $C^M(\cdot)$ of every AMES is zero, though the converse fails because the n-qubit non-AMES may have separable reduced density operators. An example is the GHZ state. Hence, we have constructed a necessary condition by which a multipartite state is an AMES. Next we consider the AMES in a three-qubit system.

Corollary 1. The sole class of AMES $|\psi\rangle$ in a three-qubit system are the states that are LU equivalent to $|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$.

We give the proof of the corollary in Appendix E.

C. An upper bound of the sum of all bipartite quantum discord

Here we present an upper bound of the sum of all bipartite quantum discord for a three-qubit pure state. The quantum discord was presented by Henderson and Vedral [46] and Ollivier and Zurek [47] independently. Quantum discord is a measure of nonclassical correlation. It is defined as

$$\delta_{AB}^{\leftarrow} = I_{AB} - J_{AB}^{\leftarrow} = I_{AB} - \max_{\{\Pi_x^B\}}\left(S(\rho_A) - \sum_x p_x S(\rho_A^x)\right),$$

where the maximum takes over all the positive-operator-valued measurements $\{\Pi_x^B\}$ performed on the subsystem B, $p_x = \mathrm{Tr}\,\Pi_x^B\rho_{AB}\Pi_x^B$, and $\rho_A^x = \mathrm{Tr}_B(\Pi_x^B\rho_{AB}\Pi_x^B)/p_x$. From its definition, it quantifies at least how much a bipartite state of one system is changed on average by the measurement of the other system. In the last decade, there are some results suggesting that quantum discord plays an important role in quantum information and computation tasks [48–52]. Recently, Guo *et al.* considered the complete monogamy relation for multiparty quantum discord [53].

Next we recall a conservation law for distributed EoF and quantum discord of a three-qubit pure state [54],

$$E_{AB} + E_{AC} = \delta_{AB}^{\leftarrow} + \delta_{AC}^{\leftarrow}. \tag{32}$$

The law depends on the Koashi-Winter relation $E_{AB} + J_{AC}^{\leftarrow} = S_A$ [55].

Here we present an upper bound of the sum of all the bipartite discord for a three-qubit pure state; from Eq. (32), we have

$$\begin{aligned}&\delta_{AB}^{\leftarrow} + \delta_{BC}^{\leftarrow} + \delta_{CA}^{\leftarrow} + \delta_{BA}^{\leftarrow} + \delta_{AC}^{\leftarrow} + \delta_{CB}^{\leftarrow} \\ &= E_{AB} + E_{AC} + E_{BC} + E_{BA} + E_{CA} + E_{CB} \\ &\leqslant 2 \times c_{\max} = 2c_{\max}.\end{aligned} \tag{33}$$

Thus, we have that quantum discord owns a multilinear monogamy relation for a three-qubit pure state.

V. CONCLUSIONS

Here we have mainly considered the shareablility of the entanglement for a multiqubit state in terms of EoF. We have presented that, up to the local unitary transformations, the W state is the unique one that can reach the upper bound of $C^M(\cdot)$ for a three-qubit state; these results may tell us that the entanglement cannot be shared freely for a three-qubit system. We have also picked 10^5 four- and five-qubit pure states randomly and computed their $C^M(\cdot)$ values, which have verified Conjecture 1 numerically. Finally, we also have presented some applications of our results. We think the methods we used here can be generalized to consider the upper bound of the multilinear monogamy relation in terms of other bipartite entanglement measures such as Rényi entanglement for an n-qubit pure state. We believe that our results are helpful in the study of monogamy relations for multipartite entanglement systems.

ACKNOWLEDGMENTS

The authors were supported by the NNSF of China (Grant No. 11871089) and the Fundamental Research Funds for the Central Universities (Grant No. ZG216S2005).

APPENDIX A: THE PROOF OF THEOREM 1

For a three-qubit pure state, the W state reaches the upper bound of the multilinear monogamy relation in terms of EoF.

Proof. Here we denote that

$$f(x) = h\left(\frac{1+\sqrt{1-x}}{2}\right), \quad x = C_{AB}^2,$$

$$y = C_{AC}^2 + C_{AB}^2, \quad c = C_{AC}^2 + C_{AB}^2 + C_{BC}^2,$$

$$g(x,y) = f(x) + f(y-x) + f(c-y), \tag{A1}$$

$$\frac{\partial g}{\partial x} = f'(x) - f'(y-x) = 0,$$

$$\frac{\partial g}{\partial y} = f'(y-x) - f'(c-y) = 0. \tag{A2}$$

As $f''(x) < 0$, $f'(x)$ is monotonously decreasing [56], $-f'(y-x)$ is also monotonously decreasing in terms of x, and by the equality (A2), we have that

$$C_{AB}^2 = C_{AC}^2 = C_{BC}^2 \tag{A3}$$

is the only case when Eq. (A2) is valid. Furthermore, as $f(x)$ is a monotonic function [56], we have that, when (A3) is valid, $E(\rho_{AB}) + E(\rho_{AC}) + E(\rho_{BC})$ achieves the upper bound for a three-qubit pure state.

From Ref. [57], we have that a three-qubit pure state $|\psi\rangle_{ABC}$ can be written in the generalized Schmidt decomposition:

$$|\psi\rangle = l_0|000\rangle + l_1 e^{i\theta}|100\rangle + l_2|101\rangle + l_3|110\rangle + l_4|111\rangle, \tag{A4}$$

where $\theta \in [0, \pi)$, $l_i \geqslant 0$ $(i = 0, 1, 2, 3, 4)$, and $\sum_{i=0}^4 l_i^2 = 1$. From simple computation, we have

$$C_{AB}^2 = 4l_0^2 l_2^2, \quad C_{AC}^2 = 4l_0^2 l_3^2, \tag{A5}$$

$$C_{BC}^2 = 4l_2^2 l_3^2 + 4l_1^2 l_4^2 - 8l_1 l_2 l_3 l_4 \cos\theta. \tag{A6}$$

As $f(x)$ is monotone [56], then we only need to obtain the maximum of $4l_0^2 l_2^2$ by using the Lagrange multiplier:

$$m(l_0, l_1, l_2, l_4, \lambda, \mu) = 4l_0^2 l_2^2 + \lambda\left(l_0^2 + l_1^2 + 2l_2^2 + l_4^2 - 1\right) + \mu\left(l_0^2 l_2^2 - l_2^4 - l_1^2 l_4^2 + 2l_1 l_2^2 l_4 \cos\theta\right), \tag{A7}$$

$$\frac{\partial m}{\partial l_0} = 8l_0 l_2^2 + 2\lambda l_0 + 2\mu l_0 l_2^2, \tag{A8}$$

$$\frac{\partial m}{\partial l_1} = 2\lambda l_1 + 2\mu l_2^2 l_4 \cos\theta - 2\mu l_1 l_4^2, \tag{A9}$$

$$\frac{\partial m}{\partial l_2} = 8l_0^2 l_2 + 4\lambda l_2 + 2\mu l_0^2 l_2 - 4\mu l_2^3 + 4\mu l_1 l_2 l_4 \cos\theta, \tag{A10}$$

$$\frac{\partial m}{\partial l_4} = 2\lambda l_4 - 2\mu l_1^2 l_4 + 2\mu l_1 l_2^2 \cos\theta, \tag{A11}$$

$$\frac{\partial m}{\partial \theta} = -2\mu l_1 l_2^2 l_4 \sin\theta, \tag{A12}$$

$$\frac{\partial m}{\partial \lambda} = l_0^2 + l_1^2 + 2l_2^2 + l_4^2 - 1, \tag{A13}$$

$$\frac{\partial m}{\partial \mu} = l_0^2 l_2^2 - l_2^4 - l_1^2 l_4^2 + 2l_1 l_2^2 l_4 \cos\theta. \tag{A14}$$

When formulas (A8)–(A14) equal to 0, we have $l_0 = l_2 = l_3 = \frac{1}{\sqrt{3}}$, and $l_1 = l_4 = 0$ is the only case when $C^2(\rho_{AB})$ attains the maximum, that is,

$$\max_{|\psi\rangle_{ABC}} [E(\rho_{AB}) + E(\rho_{AC}) + E(\rho_{BC})] := c_{\max} = 3h\left(\frac{1}{2} + \frac{\sqrt{5}}{6}\right). \tag{A15}$$

When computing Eqs. (A8)–(A14) equal to 0, according to Eq. (A12), we have that at least one of the equalities in the set $\{\mu = 0,\ l_1 = 0,\ l_2 = 0,\ l_4 = 0,\ \sin\theta = 0\}$ is valid. Then by using the method of exclusion, we could get the result. By the way, in the method of exclusion, we mainly use that when $|\psi\rangle$ is separable the function $E^M(\cdot)$ cannot get the maximum.

When we take the operation σ_x on the first system, we get the W state $\frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$. ■

APPENDIX B: THE PROOF OF LEMMA 1

Up to the local unitary transformations, the W state is the unique state that can reach the upper bound in terms of the function $C^M(\psi) = C_{AB} + C_{BC} + C_{AC}$ for a three-qubit pure state.

Proof. We will compute the maximum of the six classes of a three-qubit state respectively according to Ref. [58].

Case i. When $|\psi\rangle_{ABC}$ is $A - B - C$, $C^M(\psi) = 0$.

Case ii. When $|\psi\rangle_{ABC}$ is biseparable, if $|\psi\rangle_{ABC} = |\phi_1\rangle_A \otimes |\phi_2\rangle_{BC}$, $C_{AB} = C_{AC} = 0$, and $C^M(\psi) = C_{BC} \leqslant 1$, the other cases are similar.

Case iii. When $|\psi\rangle_{ABC}$ belongs to the W class, according to the formula (15), $C^M(\psi) = 2r_2r_3 + 2r_1r_3 + 2r_1r_2$. Trivially, when $r_1 = r_2 = r_3$, that is, $|\psi\rangle_{ABC} = |W\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |110\rangle)$, $C^M(\psi)$ gets the maximum.

Case iv. When $|\psi\rangle_{ABC}$ belongs to the GHZ class, according to Ref. [58], assume $|\psi\rangle = M_1 \otimes M_2 \otimes M_3|\text{GHZ}\rangle$, $M_i = (\vec{u}_i, \vec{v}_i)$, $\vec{u}_i = (u_i\cos\theta_i, u_i\sin\theta_i)^T$, $\vec{v}_i = [v_i\cos(\phi_i + \theta_i), v_i\sin(\phi_i + \theta_i)]^T$, and

$$C^M(\psi) = \frac{|c_1s_2s_3| + |c_2s_1s_3| + |c_3s_1s_2|}{r + c_1c_2c_3}. \tag{B1}$$

Here we denote $c_i = \cos\phi_i$, $s_i = \sin\phi_i$, $i = 1, 2, 3$, $2r = \frac{u_1u_2u_3}{v_1v_2v_3} + \frac{v_1v_2v_3}{u_1u_2u_3}$, and $r \geqslant 1$. In order to let C^M be the maximum, assume $r = 1$. When $c_i < 0$, C^M will get the maximum. Then let $\phi_i \in [0, \frac{\pi}{2}]$, and $C^M(\psi) = \frac{c_1s_2s_3 + c_2s_1s_3 + c_3s_1s_2}{1 - c_1c_2c_3}$. Next we prove $C^M(\psi) \leqslant 2$. First we define $l(c_1, c_2, c_3)$ as follows:

$$l(c_1, c_2, c_3) = c_1\cos(\phi_2 - \phi_3) + c_2\cos(\phi_1 - \phi_3) + c_3\cos(\phi_1 - \phi_2) - c_1c_2c_3.$$

Assume $c_1 > c_2 \geqslant c_3$, then we obtain

$$l(c_1, c_2, c_3) \leqslant l(c_1, c_1, c_1).$$

When $c_1 = c_2 = c_3$, the function $l(c_1, c_1, c_1)$ is a monotonic function of c_1. When $c_1 \to 1$, the function $l(c_1, c_1, c_1)$ gets the maximum, that is, $C^M(\psi) \to 2$. Then we prove that, if $|\psi\rangle_{ABC}$ is a GHZ class state, then $C^M(|\psi\rangle_{ABC}) \leqslant 2$. However, from the above analysis, when $C^M(|\psi\rangle_{ABC}) = 2$, we have $c_1 = c_2 = c_3 \to 1$; that is, the matrix M_i is singular; this is impossible. ■

APPENDIX C: THE PROOF OF THEOREM 2

Up to the local unitary transformations, the W state is the unique state that can reach the upper bound in terms of the function $C^M(\cdot)$ for a three-qubit state.

Proof. Combining with Lemma 1, we only need to present that the mixed states cannot reach the upper bound of the multilinear monogamy relations in terms of concurrence.

Due to Lemma 1, for a three-qubit pure state $|\psi\rangle$, $C^M(|\psi\rangle)$ gets the maximum, only when $|\psi\rangle$ is LU equivalent to $|W\rangle$. Assume ρ is a three-qubit mixed system, and $\{(p_i, |\phi_i\rangle)|i = 1, 2, \dots, k\}$ is a decomposition of ρ, we can always assume $k = 2$. For the cases when $k > 2$, we can prove similarly. As $|\phi_i\rangle$ is LU equivalent to $|W\rangle$, we can always assume $\{(p_1, |W\rangle), (p_2, U_1 \otimes U_2 \otimes U_3|W\rangle)\}$ is a decomposition of ρ, and then

$$\begin{aligned} C^M(\rho) &= C(\rho_{AB}) + C(\rho_{AC}) + C(\rho_{BC}) \\ &= C(\sigma_1) + C(\sigma_2) + C(\sigma_3). \end{aligned} \tag{C1}$$

Here we assume

$$\begin{aligned} \sigma_1 &= \frac{p_1}{3}(|00\rangle\langle 00| + 2|\phi^+\rangle\langle\phi^+|) + \frac{p_2}{3}\tau_1, \\ \sigma_2 &= \frac{p_1}{3}[|00\rangle\langle 00| + 2|\phi^+\rangle\langle\phi^+|] + \frac{p_2}{3}\tau_2, \\ \sigma_3 &= \frac{p_1}{3}[|00\rangle\langle 00| + 2|\phi^+\rangle\langle\phi^+|] + \frac{p_2}{3}\tau_3, \\ |\phi^+\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \end{aligned}$$

where we denote $\tau_1 = [(U_1 \otimes U_2)|00\rangle\langle 00|(U_1 \otimes U_2)^\dagger + 2(U_1 \otimes U_2)|\phi^+\rangle\langle\phi^+|(U_1 \otimes U_2)^\dagger]$, $\tau_2 = [(U_1 \otimes U_3)|00\rangle\langle 00|(U_1 \otimes U_3)^\dagger + 2(U_1 \otimes U_3)|\phi^+\rangle\langle\phi^+|(U_1 \otimes U_3)^\dagger]$, and $\tau_3 = [(U_2 \otimes U_3)|00\rangle\langle 00|(U_2 \otimes U_3)^\dagger + 2(U_2 \otimes U_3)|\phi^+\rangle\langle\phi^+|(U_2 \otimes U_3)^\dagger]$, then we have

$$\begin{aligned} C(\sigma_1) \leqslant{} & \tfrac{2}{3}C[p_1|\phi^+\rangle\langle\phi^+| + p_2(U_1 \otimes U_2)|\phi^+\rangle \\ & \times \langle\phi^+|(U_1 \otimes U_2)^\dagger]. \end{aligned} \tag{C2}$$

By Lemmas 2, 3, and 4, we have $(U_1 \otimes U_2)|\phi^+\rangle = e^{ix}|\phi^+\rangle$ is a sufficient and necessary condition of $C[p_1|\phi^+\rangle\langle\phi^+| + p_2(U_1 \otimes U_2)|\phi^+\rangle\langle\phi^+|(U_1 \otimes U_2)^\dagger] = 1$; here e^{ix} is a global phase factor. Then we can get the similar result for σ_2 and σ_3. As $\text{Sr}(|01\rangle) = \text{Sr}(|10\rangle) = 1$, here we denote that $\text{Sr}(\cdot)$ is the Schmidt rank; then we have $U_i = \begin{pmatrix} e^{i\theta_i} & 0 \\ 0 & 1 \end{pmatrix}$, $i = 1, 2,$ and 3, that is, $\rho = |W\rangle\langle W|$. Then we finish the proof. ■

Here we prove that $(U_1 \otimes U_2)|\phi^+\rangle = e^{ix}|\phi^+\rangle$ is a sufficient and necessary condition of $C[p_1|\phi^+\rangle\langle\phi^+| + p_2(U_1 \otimes U_2)|\phi^+\rangle\langle\phi^+|(U_1 \otimes U_2)^\dagger] = 1$. As $\Longrightarrow$ is trivial, $\Longleftarrow$: first we present a lemma.

Lemma 2. Assume $A, B \in \text{Pos}(\mathbb{H})$, here we denote that $\text{Pos}(\mathbb{H})$ is a linear space consisting of all the semidefinite positive operators of a bounded Hilbert space $\mathbb{H}$. Here we denote that $\text{Eig}(A)$ and $\text{Eig}(B)$ are two sets consisting of all the eigenvalues of the matrix A and B, respectively. If the biggest elements in the set $\text{Eig}(A)$ and $\text{Eig}(B)$ are 1 or less, then the biggest element in the set $\text{Eig}(AB)$ is 1 or less.

Proof. Assume that the eigenvalues of A are λ_i with their eigenvectors $|\alpha_i\rangle$, the eigenvalues of B are μ_j with their eigenvectors $|\beta_j\rangle$, and the eigenvalues of AB are χ_k with their eigenvectors $|\gamma_k\rangle$. Here we always assume that the range of A and B are nonsingular; then we have

$$\begin{aligned} AB|\gamma_k\rangle &= AB\sum_j x_{jk}|\beta_j\rangle \\ &= A\sum_j \mu_j x_{jk}|\beta_j\rangle \\ &= \sum_{ij} \lambda_i\mu_j x_{jk}y_{ij}|\alpha_i\rangle, \end{aligned} \tag{C3}$$

$$AB|\gamma_k\rangle = \chi_k|\gamma_k\rangle = \chi_k\sum_{ij} x_{jk}y_{ij}|\alpha_i\rangle. \tag{C4}$$

In the formula (C3), we denote that $|\gamma_k\rangle = \sum_j x_{jk}|\beta_j\rangle$ and $|\beta_j\rangle = \sum_i y_{ij}|\alpha_i\rangle$. From the equalities (C3) and (C4), we have

$$\chi_k = \frac{\sum_{ij}\lambda_i\mu_j x_{jk}y_{ij}}{\sum_{ij} x_{jk}y_{ij}} \leqslant 1. \tag{C5}$$

Here, Eq. (C5) is due to $\lambda_i \leqslant 1$ and $\mu_j \leqslant 1$. Then we finish the proof. ■

As ρ is semidefinite positive, then $(\sigma_y \otimes \sigma_y)\overline{\rho}(\sigma_y \otimes \sigma_y)$ is semidefinite positive. Then due to Lemma 2, we have that all the eigenvalues of $\rho(\sigma_y \otimes \sigma_y)\overline{\rho}(\sigma_y \otimes \sigma_y)$ are 1 or less. Then due to Eq. (10), we have that only when $\text{Rank}[\rho(\sigma_y \otimes \sigma_y)\overline{\rho}(\sigma_y \otimes \sigma_y)] = 1$ and λ_1 in Eq. (10) equals to 1 can $C(\rho) = 1$. As $\sigma_y \otimes \sigma_y$ is nonsingular, we only need $\text{Rank}(\rho) = 1$.

Lemma 3. $\text{Rank}[p_1|\phi^+\rangle\langle\phi^+| + p_2(U_1 \otimes U_2)|\phi^+\rangle\langle\phi^+|(U_1 \otimes U_2)^\dagger] = 1$ if and only if $(U_1 \otimes U_2)|\phi^+\rangle = e^{ix}|\phi^+\rangle$, where e^{ix} is a global phase factor.

Proof. Here we denote $\sigma = p_1|\phi^+\rangle\langle\phi^+| + p_2(U_1 \otimes U_2)|\phi^+\rangle\langle\phi^+|(U_1 \otimes U_2)^\dagger$. If $(U_1 \otimes U_2)|\phi^+\rangle \neq e^{ix}|\phi^+\rangle$, then $(U_1 \otimes U_2)|\phi^+\rangle$ and $|\phi^+\rangle$ are linear independent, $\dim[\text{span}\{|\phi^+\rangle, (U_1 \otimes U_2)|\phi^+\rangle\}] = 2$, $\dim[\text{span}\{|\phi^+\rangle, (U_1 \otimes U_2)|\phi^+\rangle\}]^\perp = n - 2$. As $\forall|\alpha\rangle \in \dim(\text{span}\{|\phi^+\rangle, (U_1 \otimes U_2)|\phi^+\rangle\}^\perp$, $\sigma|\alpha\rangle = 0$, that is, $\text{Rank}(\sigma) \leqslant 2$. As we cannot find a nontrivial vector $|\beta\rangle$ in the subspace $\text{span}\{|\phi^+\rangle, (U_1 \otimes U_2)|\phi^+\rangle\}$ such that $\sigma|\beta\rangle = 0$, then we finish the proof. ■

Lemma 4. Assume $\theta = p_1|\phi^+\rangle\langle\phi^+| + p_2U_1 \otimes U_2)|\phi^+\rangle\langle\phi^+|(U_1 \otimes U_2)^\dagger$ with $\text{Rank}(\theta) = 2$, then $\text{Rank}[(\sigma_y \otimes \sigma_y)\tilde{\theta}(\sigma_y \otimes \sigma_y)\theta] = 2$.

Proof. As $\sigma_y \otimes \sigma_y$ is invertible, we only need to prove $\text{Rank}[\tilde{\theta}(\sigma_y \otimes \sigma_y)\theta] = 2$. As $\text{Rank}[\tilde{\theta}(\sigma_y \otimes \sigma_y)\theta] = \text{Rank}[\theta\tilde{\theta}(\sigma_y \otimes \sigma_y)]$, then if we can prove $\text{Rank}[\theta\tilde{\theta}] = 2$, we finish the proof. As $\theta = \theta^\dagger$, then $\text{Rank}[\theta\tilde{\theta}] = \text{Rank}[\theta\theta^T] = \text{Rank}(\theta) = 2$. ■

APPENDIX D: THE PROOF OF THEOREM 3

Assume $|\psi\rangle$ is a three-qubit pure state, then $C^M(|\psi\rangle) = 0$ if and only if $|\psi\rangle$ can be represented as $|\psi\rangle = r_0|000\rangle + r_1|111\rangle$ up to local unitary operations when $0 \leqslant r_0$ and $r_1 \leqslant 1$.

Proof. First we recall $C^M(|\psi\rangle_{ABC}) = C_{AB}^2 + C_{AC}^2 + C_{BC}^2$.

$\Leftarrow$: When $|\psi\rangle = r_0|000\rangle + r_1|111\rangle$, then $\rho_{AB} = \rho_{AC} = \rho_{BC} = r_0^2|00\rangle\langle 00| + r_1^2|11\rangle\langle 11|$, $C(\rho_{AB}) = C(\rho_{AC}) = C(\rho_{BC}) = 0$, that is, $C^M(|\psi\rangle) = 0$.

$\Rightarrow$: In the proof of Theorem 1, we present that for a three-qubit pure state $|\psi\rangle_{ABC} = l_0|000\rangle + l_1e^{i\theta}|100\rangle + l_2|101\rangle +$

$l_3|110\rangle + l_4|111\rangle$, where $l_i \geqslant 0$ $(i = 0, 1, 2, 3, 4)$, $\theta \in [0, \pi)$,

$$C_{AB}^2 = 4l_0^2l_2^2, \quad C_{AC}^2 = 4l_0^2l_3^2,$$
$$C_{BC}^2 = 4l_2^2l_3^2 + 4l_1^2l_4^2 - 8l_1l_2l_3l_4\cos\theta. \tag{D1}$$

When $C^M(|\psi\rangle) = 0$, we have that

$$l_0l_2 = l_0l_3 = 0, \quad l_2^2l_3^2 + l_1^2l_4^2 = 2l_1l_2l_3l_4\cos\theta. \tag{D2}$$

When $l_0 \neq 0$, we have $l_2 = l_3 = 0$, that is, $l_1l_4 = 0$, then $|\psi\rangle = l_0|000\rangle + l_4|111\rangle$ or $|\psi\rangle = (l_0|0\rangle + l_1e^{i\theta}|1\rangle)|00\rangle$. When $|\psi\rangle$ is the second state, let U_1 be a unitary on the first system such that $U_1(|l_0|0\rangle + l_1e^{i\theta}|1\rangle\rangle) = |0\rangle$, then the second state is LU equivalent to the state $|000\rangle$. Below we denote U_i to be a unitary on the ith system, $i = 1, 2$, and 3.

When $l_0 = 0$, then from the third formula in Eq. (D1),

$$(l_2l_3\cos\theta - l_1l_4)^2 + l_2^2l_3^2(\sin\theta)^2 = 0, \tag{D3}$$

that is, $l_2l_3\cos\theta = l_1l_4$ and $l_2l_3\sin\theta = 0$. When $\sin\theta = 0$ and $l_i \geqslant 0$ $(i = 1, 2, 3, 4)$, $\cos\theta = 1$. That is, $(l_1, l_2) = a(l_3, l_4)$, then $|\psi\rangle = |1\rangle(|0\rangle + a|1\rangle)(l_1|0\rangle + l_2|1\rangle)$. When $U_2(|0\rangle + a|1\rangle) = \sqrt{1 + a^2}|0\rangle$ and $U_3(l_1|0\rangle + l_2|1\rangle) = \sqrt{l_1^2 + l_2^2}|0\rangle$, then we obtain that the above state is LU equivalent to $|000\rangle$. When $l_2 = 0$, then $l_1l_4 = 0$. If $l_1 = 0$, then $|\psi\rangle$ can be represented as $|\phi_1\rangle = l_3|110\rangle + l_4|111\rangle$. Let $U_3(l_3|0\rangle + l_4|1\rangle) = |1\rangle$, then it is LU equivalent to the state $|111\rangle$. If $l_4 = 0$, then $|\psi\rangle$ can be represented as $|\phi_2\rangle = e^{i\theta}l_1|100\rangle + l_3|110\rangle$. Let $U_2(e^{i\theta}l_1|0\rangle + l_3|1\rangle) = |1\rangle$ and $U_3 = \sigma_X$, then it is LU equivalent to the state $|111\rangle$.

The case when $l_3 = 0$ is similar to the case when $l_2 = 0$. Then we finish the proof. ■

APPENDIX E: THE PROOF OF COROLLARY 1

The sole class of AMES $|\psi\rangle$ in a three-qubit system are the states that are LU equivalent to $|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$.

Proof. First we provide two methods to prove that ρ_{AB}, ρ_{AC}, and ρ_{BC} are separable. Assume $|\psi\rangle_{ABC}$ is an AMES in a three-qubit state, then

$$\rho_A = \rho_B = \rho_C = \frac{I}{2}.$$

Next as $\rho_A = \frac{I}{2}$, then any purification state $|\phi\rangle_{AB'}$ of ρ_A can be written as

$$|\phi\rangle_{ABC} = (I_A \otimes U_{BC})\frac{(|00\rangle + |11\rangle)|0\rangle}{\sqrt{2}},$$

where U_{BC} is a unitary operator; then we have

$$\rho_{BC} = |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|,$$
$$|\phi_1\rangle = U_{BC}|00\rangle, \quad |\phi_2\rangle = U_{BC}|10\rangle, \tag{E1}$$

that is, $r(\rho_{BC}) = 2$. Then due to Theorem 1 in Ref. [59], we have ρ_{BC} is separable. Similarly, we have ρ_{AB} and ρ_{AC} are separable.

Here we provide the other method to prove that ρ_{AB}, ρ_{AC}, and ρ_{BC} are separable. As $\rho_A = \rho_B = \frac{I}{2}$, then from Ref. [60], we have

$$\rho_{AB} = \lambda_1\Psi^+ + \lambda_2\Psi^- + \lambda_3\Phi^+ + \lambda_4\Phi^-, \tag{E2}$$
$$\Psi^+ = \tfrac{1}{2}(|00\rangle + |11\rangle)(\langle 11| + \langle 00|),$$
$$\Psi^- = \tfrac{1}{2}(|00\rangle - |11\rangle)(|00\rangle - \langle 11|),$$
$$\Phi^+ = \tfrac{1}{2}(|01\rangle + \langle 10|)(\langle 01| + \langle 10|),$$
$$\Phi^- = \tfrac{1}{2}(|01\rangle - |10\rangle)(\langle 01| - \langle 10|).$$

As ρ_C and ρ_{AB} are with the same spectrum, then we have only two of λ_i $(i = 1, 2, 3, 4)$ are $\frac{1}{2}$. Then ρ_{AB} is separable. Similarly, we have ρ_{AC} and ρ_{BC} are separable.

As all of ρ_{AB}, ρ_{AC}, and ρ_{BC} are separable, then we have

$$C^M(|\psi\rangle) = 0.$$

Then from Theorem 3, we have $|\psi\rangle = r_0|000\rangle + r_1|111\rangle$ up to unitary operations when $r_0, r_1 \in [0, 1]$. As $\rho_A = \rho_B = \rho_C = \frac{1}{2}$, then $|\psi\rangle = \frac{1}{2}(|000\rangle + |111\rangle)$ up to local unitary operations. ■

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