Multipartite entanglement measure and complete monogamy relation

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Although many different entanglement measures have been proposed so far, much less is known in the multipartite case, which leads to the previous monogamy relations in the literature being not complete. We establish here a strict framework for defining the multipartite entanglement measure (MEM): apart from the postulates of the bipartite measure, i.e., vanishing on separable measures and nonincreasing under local operations and classical communication, a complete MEM should additionally satisfy the *unification condition* and the *hierarchy condition*. We then come up with a *complete monogamy* formula for the unified MEM (an MEM is called a *unified MEM* if it satisfies the unification condition) and a *tightly complete monogamy* relation for the complete MEM (an MEM is called a *complete MEM* if it satisfies both the unification condition and the hierarchy condition). Consequently, we propose MEMs which are multipartite extensions of entanglement of formation (EoF), concurrence, tangle, Tsallis q entropy of entanglement, Rényi α entropy of entanglement, the convex-roof extension of negativity, and negativity. We show that (i) the extensions of EoF, concurrence, tangle, and Tsallis q entropy of entanglement are complete MEMs; (ii) multipartite extensions of Rényi α entropy of entanglement, negativity, and the convex-roof extension of negativity are unified MEMs but not complete MEMs; and (iii) all these multipartite extensions are completely monogamous, and the ones which are defined by the convex-roof structure (except for the Rényi α entropy of entanglement and the convex-roof extension of negativity) are not only completely monogamous but also tightly completely monogamous. In addition, as a byproduct, we find a class of states that satisfy the additivity of EoF. We also find a class of tripartite states one part of which can be maximally entangled with the other two parts simultaneously according to the definition of mixed maximally entangled state (MMES) in Li *et al.* [Z. Li, M. Zhao, S. Fei, H. Fan, and W. Liu, Quantum Inf. Comput. 12, 0063 (2012)]. Consequently, we improve the definition of maximally entangled state (MES) and prove that the only MES is the pure MES.

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I. INTRODUCTION

Entanglement is recognized as the most important resource in quantum information processing tasks [1]. A fundamental problem in this field is to quantify entanglement. Many entanglement measures have been proposed for this purpose, such as the distillable entanglement [2], entanglement cost [2,3], entanglement of formation (EoF) [3,4], concurrence [5–7], tangle [8], relative entropy of entanglement [9,10], negativity [11,12], geometric measure [13–15], squashed entanglement [16,17], conditional entanglement of mutual information [18], three-tangle [19], generalizations of concurrence [20–22], sensation level (SL) invariant multipartite measure of entanglement [23–28], and α-entanglement entropy [29]. However, apart from the SL invariant measures and the α-entanglement entropy, all other measures are either only defined in the bipartite case or discussed with only the axioms of the bipartite case.

One of the most important issues closely related to the entanglement measure is the monogamy relation of entanglement [30], which states that, unlike classical correlations, if two parties A and B are maximally entangled, then neither of them can share entanglement with a third party C. Entanglement monogamy has many applications not only in quantum physics [31–33] but also in other area of physics, such as no-signaling theories [34,35], condensed-matter physics [36–38], statistical mechanics [31], and even black-hole physics [39]. Particularly, it is the crucial property that guarantees secure quantum key distribution [30,40]. An important basic issue in this field is to determine whether a given entanglement measure is monogamous. Considerable efforts have been devoted to this task in the last two decades [19,34,41–68] ever since Coffman, Kundu, and Wootters (CKW) presented the first quantitative monogamy relation in Ref. [19] for three-qubit states. So far, we have known that the one-way distillable entanglement (see Theorem 6 in Ref. [41]) and squashed entanglement (see Theorem 8 in Ref. [41]) and all the other measures that are defined by the convex-roof extension are monogamous [60] according to the original spirit of the CKW inequality for the monogamy relation in which a measure of entanglement E is said to be monogamous if it satisfies

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$E(A|BC) \geqslant E(AB) + E(AC)$ for all states. Notice that most of the monogamy relations in the literature are discussed via the bipartite measures of entanglement and, in general, only the relation between $A|BC$, AB, and AC is revealed; the global correlation in ABC and the correlation contained in part BC are missed [see Eqs. (5) and (6) below], where the vertical bar indicates the bipartite split across which we will measure the (bipartite) entanglement. From this point of view, the monogamy relation in the sense of the original CKW inequality is not "complete." We thus need to explore a complete monogamy relation which can exhibit the entanglement between ABC, AB, AC, and BC in extenso. [We remark here that, apart from the research on the original CKW relation, other routes of extending monogamy relations that could exhibit "completeness" were also studied extensively, such as the multipartite qubits extensions of CKW inequalities [62–65,67] and the monogamy relations by means of the linear entropy [66,68]. These monogamy relations are based on the two basic axioms of entanglement measures (see conditions E-1 and E-2 below). In this paper, we investigate a complete monogamy relation based on the unified multipartite entanglement measure (MEM).]

The phenomenon becomes much more complex when moving from the bipartite case to the multipartite case [29,69–71]. For an m-partite system, we have to encounter entanglement for both m-partite and k-partite cases, $k \leqslant m$. Particularly, a "complete monogamy relation" involves both the MEM and bipartite measures, which requires a "unified" way, i.e., the unification condition, to define entanglement measures. In Ref. [29], Szalay developed two kinds of indicator functions for characterizing multipartite entanglement based on the complex lattice-theoretic structure of partial separability classification for multipartite states. But the second kind in fact cannot quantify entanglement effectively and the unification condition was not considered as a necessary requirement of the MEM. The purpose of this paper is to give, concisely, "richer" postulates in defining a complete MEM from which we can quantify and compare the amount of entanglement for both bipartite and multipartite systems in a unified way. We then explore the complete monogamy relation under these postulates and illustrate with several MEMs which are multipartite extensions of EoF, concurrence, tangle, Tsallis q entropy of entanglement, Rényi α entropy of entanglement, negativity, and the convex-roof extension of negativity. Hereafter, we let $\mathcal{H}^{ABC}$ be a tripartite Hilbert space with finite dimension and let $\mathcal{S}^X$ be the set of density operators acting on $\mathcal{H}^X$.

The rest of this paper is organized as follows. We review the postulates of the bipartite entanglement measure and the associated monogamy relation in Sec. II, and explore the additional postulates for multipartite entanglement measures in Sec. III. Section IV proposes the complete monogamy relation and the tight complete monogamy relation for multipartite measures with the additional postulates. We then extend some well-known bipartite entanglement measures to the tripartite case, and discuss their complete monogamy properties. Particularly, we find a class of states that are additive under the tripartite entanglement of formation. Section VI mainly discusses what is the maximally entangled state (MES). We give a definition of the maximally entangled state by means of its extension. Finally, in Sec. VII, we summarize our main findings and conclusions.

II. REVIEW OF THE BIPARTITE ENTANGLEMENT MEASURE

We begin by reviewing the bipartite entanglement measure. A function $E : \mathcal{S}^{AB} \to \mathbb{R}_+$ is called an *entanglement measure* if it satisfies [10] the following conditions.

(E-1) $E(\rho) = 0$ if ρ is separable.

(E-2) E cannot increase under local operations and classical communication (LOCC), i.e., $E(\Phi(\rho)) \leqslant E(\rho)$ for any LOCC Φ [condition E-2 implies that E is invariant under local unitary operations, i.e., $E(\rho) = E(U^A \otimes U^B \rho U^{A,\dagger} \otimes U^{B,\dagger})$ for any local unitaries U^A and U^B]. The map Φ is completely positive and trace preserving (CPTP).

In general, LOCC can be stochastic, in the sense that ρ can be converted to σ_j with some probability p_j. [It is possible that $E(\sigma_{j_0}) > E(\rho)$ for some j_0.] In this case, the map from ρ to σ_j cannot be described in general by a CPTP map. However, by introducing a "flag" system A', we can view the ensemble $\{\sigma_j, p_j\}$ as a classical quantum state $\sigma' := \sum_j p_j |j\rangle\langle j|^{A'} \otimes \sigma_j$. Hence, if ρ can be converted by LOCC to σ_j with probability p_j, then there exists a CPTP LOCC map Φ such that $\Phi(\rho) = \sigma'$. Therefore, the definition above of a measure of entanglement captures also probabilistic transformations. Particularly, E must satisfy $E(\sigma') \leqslant E(\rho)$.

Almost all measures of entanglement studied in the literature (although not all [73]) satisfy

$$E(\sigma') = \sum_j p_j E(\sigma_j), \tag{1}$$

which is very intuitive since A' is just a classical system encoding the value of j. In this case the condition $E(\sigma') \leqslant E(\rho)$ becomes

$$\sum_j p_j E(\sigma_j) \leqslant E(\rho).$$

That is, LOCC cannot increase entanglement on average. An entanglement measure E is said to be an entanglement monotone [72] if it satisfies Eq. (1) and is convex additionally.

Let E be a bipartite measure of entanglement. The entanglement of formation associated with E, denoted by E_F, is defined as the average pure-state measure minimized over all pure-state decompositions:

$$E_F(\rho) := \min \sum_{j=1}^{n} p_j E(|\psi_j\rangle\langle\psi_j|), \tag{2}$$

which is also called the convex-roof extension of E. In general, for pure state $|\psi\rangle \in \mathcal{H}^{AB}$, $\rho^A = \mathrm{Tr}_B|\psi\rangle\langle\psi|$,

$$E(|\psi\rangle\langle\psi|) = h(\rho^A) \tag{3}$$

for some positive function h. Vidal (see Theorem 2 in Ref. [72]) showed that E_F, defined as Eqs. (2) and (3), is an entanglement monotone if and only if h is also *concave*, i.e.,

$$h[\lambda\rho_1 + (1-\lambda)\rho_2] \geqslant \lambda h(\rho_1) + (1-\lambda)h(\rho_2) \tag{4}$$

for any states ρ_1 and ρ_2, and any $\lambda \in [0, 1]$. Very recently, Guo and Gour [60] showed that, if h is strictly concave, then

E_F is monogamous; i.e., for any $\rho^{ABC} \in \mathcal{S}^{ABC}$ that satisfies the disentangling condition

$$E_F(\rho^{AB}) = E_F(\rho^{A|BC}) \quad (5)$$

we have that $E_F(\rho^{AC}) = 0$ or, equivalently (for continuous measures [59]), there exists some $\alpha > 0$ such that

$$E_F^\alpha(\rho^{A|BC}) \geqslant E_F^\alpha(\rho^{AB}) + E_F^\alpha(\rho^{AC}) \quad (6)$$

holds for all $\rho^{ABC} \in \mathcal{S}^{ABC}$.

For convenience, we list some bipartite entanglement measures. The first convex-roof extended measure is EoF [2,4], E_f, which is defined by

$$E_f(|\psi\rangle) = E(|\psi\rangle) := S(\rho^A), \quad \rho^A = \mathrm{Tr}_B|\psi\rangle\langle\psi|, \quad (7)$$

for pure state $|\psi\rangle \in \mathcal{H}^{AB}$, where $S(\rho) := -\mathrm{Tr}(\rho \ln \rho)$ is the von Neumann entropy, and

$$E_f(\rho) := \min_{\{p_i,|\psi_i\rangle\}} \sum_i p_i E(|\psi_i\rangle) \quad (8)$$

for the mixed state, where the minimum is taken over all pure-state decompositions $\{p_i, |\psi_i\rangle\}$ of $\rho \in \mathcal{S}^{AB}$ (throughout this paper, we identify the original bipartite entanglement of formation with E_f; the notation E_F with capital F in the subscript denotes other general convex-roof extended measures). For bipartite pure state $|\psi\rangle \in \mathcal{H}^{AB}$, concurrence [5–7] and tangle [8] are defined by

$$C(|\psi\rangle) = \sqrt{2[1 - \mathrm{Tr}(\rho^A)^2]}$$

and

$$\tau(|\psi\rangle) = C^2(|\psi\rangle),$$

respectively. For the mixed state, they are defined by the convex-roof extension as Eq. (2). The negativity [11,12] is defined by

$$N(\rho) = \tfrac{1}{2}(\|\rho^{T_a}\|_{\mathrm{Tr}} - 1), \quad \rho \in \mathcal{S}^{AB},$$

where T_x denotes the transpose with respect to the subsystem X, and $\|\cdot\|_{\mathrm{Tr}}$ denotes the trace norm. The convex-roof extension of N, N_F, is defined as Eq. (2) (i.e., taking $E = N$). Any function that can be expressed as

$$H_g(\rho) = \mathrm{Tr}[g(\rho)] = \sum_j g(p_j), \quad (9)$$

where p_j denotes the eigenvalues of ρ, is strictly concave if $g''(p) < 0$ for all $0 < p < 1$ [60]. This includes the quantum Tsallis q entropy [74–76] T_q with $q > 0$ and the Rényi α entropy [77–79] R_α with $\alpha \in [0, 1]$. Consequently, according to Eq. (5), it is proved that all bipartite entanglement monotones are monogamous for pure states and all E_F in the literature so far—such as E_f, C, τ, N_F, Tsallis q entropy of entanglement ($q > 0$), and Rényi α entropy of entanglement ($0 < \alpha < 1$)—are monogamous [60].

III. POSTULATES FOR THE MULTIPARTITE ENTANGLEMENT MEASURE

A. Multipartite entanglement monotone

We now turn to the discussion of multipartite measures of entanglement. A function $E^{(m)} : \mathcal{S}^{A_1A_2\cdots A_m} \to \mathbb{R}_+$ is called a m-partite entanglement measure in the literature [20,21,69] if it satisfies the following conditions.

(E1) $E^{(m)}(\rho) = 0$ if ρ is fully separable.

(E2) $E^{(m)}$ cannot increase under m-partite LOCC.

In addition, $E^{(m)}$ is said to be an m-partite entanglement monotone if it is convex and does not increase on average under m-partite stochastic LOCC. For simplicity, throughout this paper, we call $E_F^{(m)}$ defined as

$$E_F^{(m)}(\rho) := \min \sum_i p_i E^{(m)}(|\psi_i\rangle) \quad (10)$$

an m-partite entanglement of formation associated with $E^{(m)}$ provided that $E^{(m)}$ is an m-partite entanglement measure on pure states. From now on, we only consider the tripartite system $\mathcal{H}^{ABC}$ unless otherwise stated, and the case for $m \geqslant 3$ could be argued analogously. As a generalization of Vidal's scenario for the bipartite entanglement monotone proposed in Ref. [72], we give at first a necessary-sufficient criterion of the tripartite entanglement monotone (TEM).

Proposition 1. Let $E^{(3)} : \mathcal{H}^{ABC} \to \mathbb{R}_+$ be a function defined by

$$E^{(3)}(|\psi\rangle) = h^{(3)}(\rho^A \otimes \rho^B \otimes \rho^C), \quad |\psi\rangle \in \mathcal{H}^{ABC} \quad (11)$$

and let $E_F^{(3)}$ be a function defined as Eq. (10). Then $E_F^{(3)}$ is a TEM if and only if (1) $h^{(3)}$ is invariant under local unitary operations and (2) $h^{(3)}$ is LOCC concave, i.e.,

$$h^{(3)}(\rho^A \otimes \rho^B \otimes \rho^C) \geqslant \sum_k p_k h^{(3)}\big(\sigma_k^A \otimes \sigma_k^B \otimes \sigma_k^C\big) \quad (12)$$

holds for any stochastic LOCC $\{\Phi_k\}$ acting on $|\psi\rangle\langle\psi|$, where $\sigma_k^x = \mathrm{Tr}_{\bar{x}}\sigma_k$, $p_k\sigma_k = \Phi_k(|\psi\rangle\langle\psi|)$.

Proof. According to the scenario in Ref. [11], we only need to consider a family $\{\Phi_k\}$ consisting of completely positive linear maps such that $\Phi_k(\rho) = p_k\sigma_k$, where

$$\Phi_k(\rho) = M_k\rho M_k^\dagger = M_k^A \otimes I^{BC}\rho M_k^{A,\dagger} \otimes I^{BC}$$

transforms pure states to some scalar multiple of pure states, $\sum_k M_k^{A,\dagger}M_k^A = I^A$. We assume at first that the initial state $\rho \in \mathcal{S}^{ABC}$ is pure. Then it yields that $E^{(3)}(\rho) \geqslant \sum_k p_k E^{(3)}(\sigma_k)$ holds if and only if $h^{(3)}$ is LOCC concave. Apparently, $E^{(3)}(\rho) = h^{(3)}(\rho^A \otimes \rho^B \otimes \rho^C)$ and $E^{(3)}(\sigma_k) = h^{(3)}(\sigma_k^A \otimes \sigma_k^B \otimes \sigma_k^C)$ since σ_k still is a pure state for each k. Therefore, the inequality $E^{(3)}(\rho) \geqslant \sum_k p_k E^{(3)}(\sigma_k)$ can be rewritten as

$$h^{(3)}(\rho^A \otimes \rho^B \otimes \rho^C) \geqslant \sum_k p_k h^{(3)}\big(\sigma_k^A \otimes \sigma_k^B \otimes \sigma_k^C\big).$$

That is, if $h^{(3)}$ is LOCC concave, then $E^{(3)}$ does not increase on average under LOCC for pure states and vice versa. So it remains to be shown that $E_F^{(3)}$ does not increase on average under LOCC for mixed states with the assumption that $h^{(3)}$ is LOCC concave. For any mixed state $\rho \in \mathcal{S}^{ABC}$, there exists an ensemble $\{t_j, |\eta_j\rangle\}$ such that

$$E_F^{(3)}(\rho) = \sum_j t_j E^{(3)}(|\eta_j\rangle).$$

For each j, let

$$t_{jk}\sigma_{jk} = \Phi_k(|\eta_j\rangle\langle\eta_j|), \quad t_{jk} = \mathrm{Tr}[\Phi_k(|\eta_j\rangle\langle\eta_j|)].$$

Then we obtain that

$$E_F^{(3)}(\rho) = \sum_j t_j E^{(3)}(|\eta_j\rangle) \geqslant \sum_{j,k} t_j t_{jk} E^{(3)}(\sigma_{jk}) \geqslant \sum_k p_k E_F^{(3)}(\sigma_k),$$

where $p_k = \sum_j t_j t_{jk}$. In addition, it is well known that entanglement is invariant under local unitary operation, which is equivalent to the fact that h is invariant under local unitary operation. The proof is completed. ■

Remark 1. The inequality (12) in condition 2 above reduces to Eq. (4) for the bipartite case. That is, for the bipartite case, concavity is equivalent to LOCC concavity, but it is unknown whether it also true for the tripartite case.

B. Unification condition for the multipartite entanglement measure

As mentioned before, for MEM, a natural question that arisen from the monogamy relation is whether it obeys:

(E3): *the unification condition*, i.e., $E^{(3)}$ is consistent with $E^{(2)}$.

That is, when we analyze the entanglement contained in a given tripartite state $\rho^{ABC} \in \mathcal{S}^{ABC}$, we have to cope with not only the total entanglement in ρ^{ABC} measured by $E^{(3)}$ but also the entanglement in ρ^{AB}, ρ^{AC}, ρ^{BC}, $\rho^{A|BC}$, $\rho^{B|AC}$, and $\rho^{AB|C}$ measured by $E^{(2)}$, and thus $E^{(3)}$ and $E^{(2)}$ must be defined in the same way. Then, how can we define them in the same way? We begin with a simple observation. Let $|\psi\rangle^{ABC}$ be a biseparable pure state in $\mathcal{H}^{ABC}$, e.g., $|\psi\rangle^{ABC} = |\psi\rangle^{AB}|\psi\rangle^{C}$. It is clear that the only entanglement of such a state is contained in $|\psi\rangle^{AB}$, namely, we must have

$$E^{(3)}(|\psi\rangle^{AB}|\psi\rangle^{C}) = E^{(2)}(|\psi\rangle^{AB}). \tag{13}$$

In this way, we can find the link between $E^{(2)}$ and $E^{(3)}$ (or $h^{(2)}$ and $h^{(3)}$). For instance, if $E^{(3)}(|\psi\rangle^{ABC}) = h^{(3)}(\rho^A \otimes \rho^B \otimes \rho^C)$, we have $E^{(2)}(|\psi\rangle^{AB}) = h^{(2)}(\rho^A \otimes \rho^B)$ with the same "action" of function h [e.g., EoF and the tripartite EoF (also see Sec. V): $E^{(2)}(|\psi\rangle^{AB}) = h^{(2)}(\rho^A \otimes \rho^B) = \frac{1}{2}S(\rho^A \otimes \rho^B)$ while $E^{(3)}(|\psi\rangle^{ABC}) = h^{(3)}(\rho^A \otimes \rho^B \otimes \rho^C) = \frac{1}{2}S(\rho^A \otimes \rho^B \otimes \rho^C)$]. In general, $E^{(2)}$ is uniquely determined by $E^{(3)}$ but not vice versa. It is worth mentioning that $h^{(2)}(\rho^A \otimes \rho^B)$ can exist instead by $h(\rho^A)$ since any bipartite pure state has Schmidt decomposition, which guarantees that the eigenvalues of ρ^A coincide with those of ρ^B. That is, $h(\rho^A)$ is in fact $h^{(2)}(\rho^A \otimes \rho^B)$, and part A and part B are symmetric, or, equivalently,

$$h^{(2)}(\rho^A \otimes \rho^B) = h^{(2)}(\rho^B \otimes \rho^A).$$

So, as one may expect, for the multipartite case, the unification condition requires that the measure of multipartite entanglement must be *invariant under the permutations of the subsystems*. Namely, the amount of entanglement contained in a state is fixed:

$$E^{(3)}(\rho^{ABC}) = E^{(3)}(\rho^{\pi(ABC)}), \tag{14}$$

where π is a permutation of the subsystems [note that $E(\rho^{A|BC}) \neq E(\rho^{X|YZ})$ in general whenever $X \neq A$, $X, Y, Z \in \{A, B, C\}$]. For instance, the three-tangle of three qubits is invariant under permutations of the qubits [19]. In addition, we always have

$$E^{(3)}(ABC) \geqslant E^{(2)}(XY), \quad X, Y, \in \{A, B, C\} \tag{15}$$

since the partial trace is a special LOCC. $E^{(3)}$ is called a *unified* multipartite entanglement measure if it satisfies condition E3. Hereafter, we always assume that $E^{(3)}$ is a unified measure unless otherwise specified.

We note here that, although the analytic formulas for $E^{(2)}$ and $E^{(3)}$ cannot be uniquely determined, namely, the "same action" of h has a little ambiguity since they are defined on different systems, $E^{(2)}$ can be uniquely determined for any given $E^{(3)}$ by the requirements in Eqs. (13) and (14) generally.

C. Hierarchy condition for the multipartite entanglement measure

There are different kinds of separability in the tripartite case: the fully separable state, two-partite separable state, and genuinely entangled state. We denote by $E^{(3-2)}$ the two-partite entanglement measure associated with $E^{(3)}$, which is defined by

$$E^{(3-2)}(|\psi\rangle) := \min\{E^{(2)}(|\psi\rangle^{A|BC}), E^{(2)}(|\psi\rangle^{AB|C}), E^{(2)}(|\psi\rangle^{B|AC})\}. \tag{16}$$

For any given $\rho^{ABC} \in \mathcal{S}^{ABC}$, $E^{(3)}(\rho^{ABC})$ extracts the "total entanglement" contained in the state while $E^{(2)}(\rho^{X|YZ})$ only quantifies the "bipartite entanglement" up to some bipartite cutting $X|YZ$, $X, Y, Z \in \{A, B, C\}$. For instance, for any entanglement monotone E, the pure state $|\psi\rangle^{ABC}$ satisfying the disentangling condition $E(|\psi\rangle^{A|BC}) = E(\rho^{AB})$ has the form of $|\psi\rangle^{AB_1}|\psi\rangle^{B_2C}$ for some subspace $\mathcal{H}^{B_1B_2}$ in $\mathcal{H}^B$ [58–60]. In such a case, $E(A|BC)$ only reflects the entanglement between A and BC; the entanglement between B and C is missed whenever $|\psi\rangle^{B_2C}$ is entangled (in fact, $|\psi\rangle^{B_2C}$ can be a maximally entangled sate; also see Sec. VI). We thus need additionally the *hierarchy condition*:

(E4): $E^{(3)}(\rho^{ABC}) \geqslant E^{(2)}(\rho^{X|YZ}) \geqslant E^{(3-2)}(\rho^{ABC})$ holds for all ρ^{ABC}, $X, Y, Z \in \{A, B, C\}$.

That is, a non-negative function $E^{(3)}$, as a "complete" tripartite entanglement measure, not only must obey conditions E1 and E2 but also must satisfy conditions E3 and E4. One can easily check that the tripartite squashed entanglement and the tripartite conditional entanglement of mutual information are complete entanglement monotones, i.e., they also satisfy conditions E3 and E4, but the k-ME concurrence [20] violates condition E4, and the three-tangle is even not a unified measure. Note that the three-tangle, denoted by τ_{ABC}, is defined by

$$\tau_{ABC} := C^2_{A|BC} - C^2_{AB} - C^2_{AC},$$

which is not symmetric up to the three parts A, B, and C in general (except for the three-qubit case [19]), and there are no uniform formulas for $h^{(2)}$ and $h^{(3)}$. In addition, it is worth mentioning that τ_{ABC} is different from $E^{(3)}$ here since the former only quantifies the genuine entanglement shared by the three parts simultaneously while the latter one reflects all the entanglement contained in the state.

Remark 2. Condition E4 is consistent with the multipartite monotonic indicator functions of the first kind [see Eq. (87) in

Ref. [29]]. From the arguments in this paper, the multipartite monotonic indicator function of the second kind in Ref. [29] is meaningless for defining the MEM.

Remark 3. Hereafter, the tripartite squashed entanglement, a little bit different from the one in Ref. [17], is defined by

$$E_{\rm sq}^{(3)}(\rho^{ABC}) := \tfrac{1}{2}\inf I(A:B:C|E), \tag{17}$$

where

$$I(A:B:C|E) = I(A:B|E) + I(C:AB|E),$$

with $I(A:B|E)$ the conditional mutual information, i.e.,

$$I(A:B|E) = S(AE) + S(BE) - S(ABE) - S(E),$$

and where the infimum is taken over all extensions ρ^{ABCE} of ρ^{ABC}, i.e., over all states satisfying $\mathrm{Tr}_E(\rho^{ABCE}) = \rho^{ABC}$. In Ref. [17], the tripartite squashed entanglement, denoted by $E_{\rm sq}^q$, is defined by $E_{\rm sq}^q(\rho^{ABC}) := \inf I(A:B:C|E)$. Observe that

$$E_{\rm sq}^{(3)}(\rho^{ABC}) = \tfrac{1}{2}\inf[S(\rho^{AE}) + S(\rho^{BE}) + S(\rho^{CE}) - S(\rho^{ABCE}) - 2S(\rho^E)]$$

and, by definition Eq. (17), it is immediate that this formula is symmetric with respect to the subsystems A, B, and C though parties A, B, and C in the definition are asymmetric. Therefore we conclude that $E_{\rm sq}^{(3)}$ is a unified tripartite monotone.

IV. COMPLETE MONOGAMY RELATION FOR THE MULTIPARTITE MEASURE

A. Complete monogamy relation for the unified MEM

Since there is no bipartite cut among the subsystems when we consider the complete MEM, we thus, following the spirit of the bipartite case proposed in Ref. [59], give the following definition of monogamy for the unified tripartite measure of entanglement.

Definition 1. Let $E^{(3)}$ be a unified tripartite entanglement measure. $E^{(3)}$ is said to be completely monogamous if for any $\rho^{ABC} \in \mathcal{S}^{ABC}$ that satisfies

$$E^{(3)}(\rho^{ABC}) = E^{(2)}(\rho^{AB}) \tag{18}$$

we have that $E^{(2)}(\rho^{AC}) = E^{(2)}(\rho^{BC}) = 0$.

We remark here that, for tripartite measures, the subsystems A and B are symmetric in the *tripartite disentangling condition* (18), which is different from that of the bipartite disentangling condition (5). The tripartite disentangling condition (18) means that, for a given tripartite state shared by Alice, Bob, and Charlie, if the entanglement between A and B reached the "maximal amount" which is limited by the "total amount" of the entanglement contained in the state, i.e., $E^{(3)}(ABC)$, then both part A and part B cannot be entangled with part C additionally. While the monogamy relation up to bipartite measures is not complete (we can call it the *partial monogamy relation*), Definition 1 (or Proposition 2 below) captures the nature of the monogamy law of entanglement since it reflects the distribution of entanglement thoroughly and we thus call it *completely monogamous*. The difference between these two kinds of monogamy relations, i.e., Eqs. (6) and (19) (see below) [or equivalently, Eqs. (5) and (18)], is illustrated in Fig. 1. By the proof of Theorem 1 in Ref. [59], the following theorem is obvious.

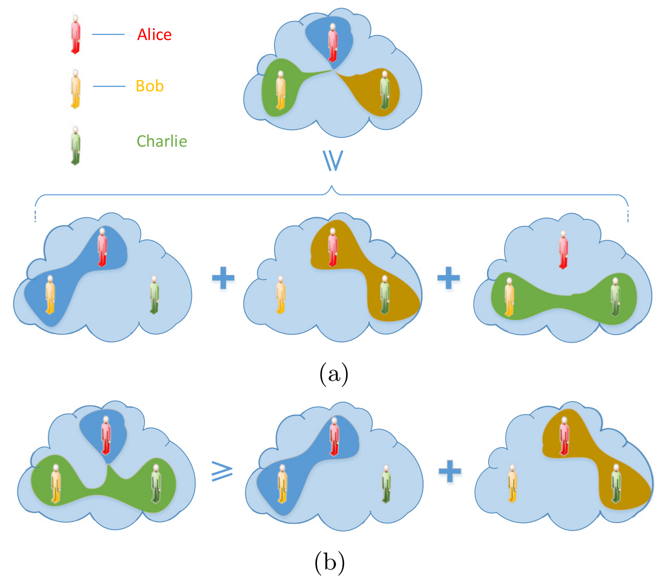

FIG. 1. Schematic picture of the monogamy relation under (a) the unified tripartite entanglement measure and (b) the bipartite entanglement measure.

Proposition 2. Let $E^{(3)}$ be a continuous unified tripartite entanglement measure. Then $E^{(3)}$ is completely monogamous if and only if there exists $0 < \alpha < \infty$ such that

$$E^{\alpha}(\rho^{ABC}) \geqslant E^{\alpha}(\rho^{AB}) + E^{\alpha}(\rho^{AC}) + E^{\alpha}(\rho^{BC}), \tag{19}$$

for all $\rho^{ABC} \in \mathcal{S}^{ABC}$ with fixed $\dim \mathcal{H}^{ABC} = d < \infty$, where we omit the superscript $^{(3)}$ of $E^{(3)}$ for brevity.

As with the monogamy exponent α in Eq. (6) for the bipartite measure, we call the smallest possible value for α satisfying Eq. (19) in a given dimension $d = \dim \mathcal{H}^{ABC}$ the *monogamy exponent* associated with a unified measure $E^{(3)}$, and we identify it with $\alpha(E^{(3)})$. That is, the completely monogamous measure $E^{(3)}$ together with its monogamy exponent $\alpha(E^{(3)})$ exhibit the monogamy relation more clearly. In general, the monogamy exponent is hard to calculate. It is worth mentioning that almost all entanglement measures by now are continuous [59]. Hence, it is clear that, to decide whether $E^{(3)}$ is completely monogamous, the approach in Definition 1 is much easier than the one from Proposition 2 since we only need to check the states that satisfy the tripartite disentangling condition in (18) while all states should be verified in Eq. (19).

Let $E_F^{(3)}$ be a unified TEM defined as in Eq. (10). By replacing $E_f(A|BC)$ and $E_f(A|B)$ with $E_F^{(3)}$ and $E_F^{(2)}$ in Theorem 3 in Ref. [59], respectively, we can conclude that, if $E_F^{(3)}$ is completely monogamous in pure tripartite states in $\mathcal{H}^{ABC}$, then it is also completely monogamous in tripartite mixed states acting on $\mathcal{H}^{ABC}$.

The first disentangling theorem was investigated in Ref. [58] with respect to bipartite negativity. Very recently, Guo and Gour showed in Ref. [60] that the disentangling theorem is valid for any bipartite entanglement monotone in pure states and also valid for any bipartite convex-roof extended measures so far. We present here the analogous one up to tripartite measures. One can check, following the argument of Theorem 4 and Corollary 5 in Ref. [59], that Lemma 1 below is valid.

Lemma 1. Let $E^{(3)}$ be a unified tripartite entanglement monotone, and let ρ^{ABC} be a pure tripartite state satisfying the disentangling condition (18). Then,

$$E^{(2)}(\rho^{AB}) = E_F^{(2)}(\rho^{AB}) = E_a^{(2)}(\rho^{AB}), \tag{20}$$

where $E_F^{(2)}$ is defined as in (10), and $E_a^{(2)}$ is also defined as in (10) but with a maximum replacing the minimum.

By Lemma 1 we have the following result that characterizes the form of the states satisfying the tripartite disentangling condition in detail.

Theorem 1. Let $E^{(3)}$ be a complete TEM for which h, induced from $h^{(3)}$ as defined in (3), i.e., $h(\rho^A) = E^{(2)}(|\psi\rangle^{A|BC})$ whenever $h^{(3)}(\rho^A\otimes\rho^B\otimes\rho^C) = E^{(3)}(|\psi\rangle^{ABC})$, is strictly concave. Then, if ρ^{ABC} is a tripartite state and $E_F^{(3)}(\rho^{ABC}) = E_F^{(2)}(\rho^{AB})$, then

$$\rho^{ABC} = \sum_x p_x|\psi_x\rangle\langle\psi_x|^{ABC}, \tag{21}$$

where $\{p_x\}$ is some probability distribution, and each pure state $|\psi_x\rangle^{ABC}$ admits the form

$$|\psi\rangle^{ABC} = |\phi\rangle^{AB}|\eta\rangle^{C}\,. \tag{22}$$

Proof. By Lemma 1, we can derive that if ρ^{ABC} is a pure tripartite state satisfying the disentangling condition (18) then

$$E^{(2)}(\rho^{AB}) = E_F^{(2)}(\rho^{AB}) = E_a^{(2)}(\rho^{AB}),$$

where $E_F^{(2)}$ is defined as in (10), and $E_a^{(2)}$ is also defined as in (10) but with a maximum replacing the minimum. Let $\rho^{AB} = \sum_{j=1}^n p_j|\psi_j\rangle\langle\psi_j|^{AB}$ be an arbitrary pure state decomposition of ρ^{AB} with $n = \mathrm{rank}(\rho^{AB})$. Then,

$$E^{(2)}(\rho^{AB}) \leqslant E_F^{(2)}(\rho^{AB}) = \sum_{j=1}^n p_jE^{(2)}(|\psi_j\rangle\langle\psi_j|^{AB}).$$

On the other hand,

$$E_F^{(2)}(\rho^{AB}) \leqslant E^{(3)}(|\psi\rangle\langle\psi|^{ABC}) = h^{(3)}(\rho^A\otimes\rho^B\otimes\rho^C).$$

Therefore, denoting by $\rho_j^{A,B} := \mathrm{Tr}_{B,A}|\psi_j\rangle\langle\psi_j|^{AB}$ and writing

$$h\big(\rho_j^A\big) = h\big(\rho_j^B\big) = h^{(2)}\big(\rho_j^A\otimes\rho_j^B\big) \tag{23}$$

we conclude that if Eq. (18) holds then we must have

$$\sum_{j=1}^n p_jh\big(\rho_j^A\big) = \sum_{j=1}^n p_jh\big(\rho_j^B\big) = h(\rho^A) = h(\rho^B)$$

since

$$\begin{aligned} h(\rho^A) &= E^{(2)}(|\psi\rangle^{A|BC}) \leqslant E^{(3)}(|\psi\rangle^{ABC})\\ &= h^{(3)}(\rho^A\otimes\rho^B\otimes\rho^C),\\ h(\rho^B) &= E^{(2)}(|\psi\rangle^{B|AC}) \leqslant h^{(3)}(\rho^A\otimes\rho^B\otimes\rho^C). \end{aligned}$$

Given that $\rho^A = \sum_{j=1}^n p_j\rho_j^A$, $\rho^B = \sum_{j=1}^n p_j\rho_j^B$, and $h^{(2)}$ is strictly concave we must have

$$\rho_j^A = \rho^A,\ \rho_j^B = \rho^B, \quad j = 1,\dots,n. \tag{24}$$

This leads to $|\psi\rangle^{ABC} = |\psi\rangle^{AB}|\psi\rangle^{C}$. The case of the mixed state can be easily followed. ■

Comparing with the theorem in Ref. [60], we can see that the strict concavity of $h^{(2)}$ for the tripartite case is stronger than that of the bipartite case, which leads to the fact that the state satisfying the tripartite disentangling condition is a special case of the one satisfying the bipartite disentangling condition. This also indicates that the complete monogamy formula is really different from the previous monogamy relations up to the bipartite measures.

For the case of the m-partite case, $m\geqslant 4$, we can easily derive the following disentangling conditions with the same spirit as that of the tripartite disentangling condition in mind (we take $m = 4$ for example): Let $E^{(4)}$ be a unified tripartite entanglement measure. $E^{(4)}$ is said to be *monogamous* if (i) either for any $\rho^{ABCD}\in\mathcal{S}^{ABCD}$ that satisfies

$$E^{(4)}(\rho^{ABCD}) = E^{(2)}(\rho^{AB}) \tag{25}$$

we have that $E^{(2)}(\rho^{AB|CD}) = E^{(2)}(\rho^{CD}) = 0$ or (ii) for any $\rho^{ABCD}\in\mathcal{S}^{ABCD}$ that satisfies

$$E^{(4)}(\rho^{ABCD}) = E^{(3)}(\rho^{ABC}) \tag{26}$$

we have that $E^{(2)}(\rho^{ABC|D}) = 0$.

The difference between the two kinds of disentangling conditions can also be revealed by the following theorem, which is the complement of the theorem in Ref. [60].

Theorem 2. Let $E^{(2)}$ be an entanglement monotone for which $h^{(2)}$, as defined in Eq. (3), is strictly concave, and let $|\psi\rangle^{ABC}$ be a pure state in $\mathcal{H}^{ABC}$. Then,

$$E^{(2)}(\rho^{AB}) = E^{(2)}(|\psi\rangle^{A|BC}) \text{ iff } \rho^{AC} = \rho^A\otimes\rho^C,$$

and in turn, if and only if

$$|\psi\rangle^{ABC} = |\psi\rangle^{AB_1}|\psi\rangle^{B_2C}$$

for some subspaces $\mathcal{H}^{B_1}$ and $\mathcal{H}^{B_2}$ in $\mathcal{H}^B$ up to some local unitary on part B, where $|\psi\rangle^{AB_1}\in\mathcal{H}^{AB_1}$ and $|\psi\rangle^{B_1C}\in\mathcal{H}^{B_1C}$, if ρ^{AC} is separable but $\rho^{AC}\neq\rho^A\otimes\rho^C$, then $E^{(2)}(\rho^{AB}) < E^{(2)}(|\psi\rangle^{A|BC})$.

Proof. Let $|\psi\rangle^{ABC}$ be a pure state. If $\rho^{AC} = \rho^A\otimes\rho^C$, we assume that $\mathrm{rank}(\rho^A) = m$ with spectrum decomposition $\rho^A = \sum_i(\lambda_i^A)^2|\psi_i\rangle\langle\psi_i|^A$ and $\mathrm{rank}(\rho^C) = n$ with spectrum decomposition $\rho^C = \sum_j(\lambda_j^C)^2|\psi_j\rangle\langle\psi_j|^C$. It follows that $|\psi\rangle^{ABC}$ admits the form

$$|\psi\rangle^{ABC} = \sum_{i,j}\lambda_i^A\lambda_j^C|\psi_i\rangle^A|\psi_{ij}\rangle^B|\psi_j\rangle^C$$

with $\langle\psi_{ij}|\psi_{kl}\rangle^B = \delta_{ik}\delta_{jl}$. Let $\mathcal{K} := \mathrm{span}\{|\psi_{ij}\rangle^B\}\subseteq\mathcal{H}^B$; then $\mathcal{K}\cong\mathcal{H}^{B_1}\otimes\mathcal{H}^{B_2}$ for some subspaces $\mathcal{H}^{B_1}$ and $\mathcal{H}^{B_2}$. We thus conclude that there exists a unitary operator U^B acting on $\mathcal{H}^B$ such that

$$U^B|\psi_{ij}\rangle^B = |x_i\rangle^{B_1}|y_j\rangle^{B_2}, \quad \forall i, j.$$

This implies that

$$|\psi\rangle^{ABC} = |\psi\rangle^{AB_1}|\psi\rangle^{B_2C}$$

with $|\psi\rangle^{AB_1} = \sum_i\lambda_i^A|\psi_i\rangle^A|x_i\rangle^{B_1}$ and $|\psi\rangle^{B_2C} = \sum_j\lambda_j^C|y_j\rangle^{B_2}|\psi_j\rangle^C$ up to local unitary operator U^B. It is now clear that $E(\rho^{AB}) = E(|\psi\rangle^{A|BC})$.

Together with the theorem in Ref. [60], we get

$$\rho^{AC} = \rho^A\otimes\rho^C \Leftrightarrow E^{(2)}(\rho^{AB}) = E^{(2)}(|\psi\rangle^{A|BC}).$$

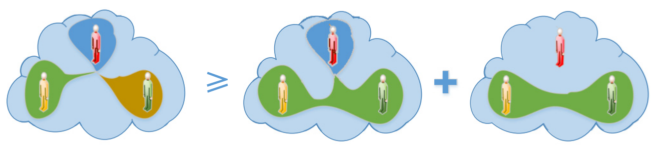

FIG. 2. Schematic picture of the tight monogamy relation.

That is, if ρ^{AC} is separable but $\rho^{AC}\neq\rho^A\otimes\rho^C$, then $E^{(2)}(\rho^{AB})<E^{(2)}(\rho^{A|BC})$. For example, we let

$$|\psi\rangle^{ABC}=\sum_k\lambda_k|k\rangle^A|k\rangle^B|k\rangle^C$$

be a generalized Greenberger-Horne-Zeilinger state; then ρ^{AC} is separable but $\rho^{AC}\neq\rho^A\otimes\rho^C$ and $E^{(2)}(\rho^{AB})=0<E^{(2)}(|\psi\rangle^{A|BC})$. ■

The bipartite squashed entanglement is shown to be monogamous [16] with the monogamy exponent being at most 1. We prove here that $E_{sq}^{(3)}$ is complete monogamous.

Proposition 3. $E_{sq}^{(3)}$ is completely monogamous; i.e.,

$$E_{sq}^{(3)}(\rho^{ABC})\geqslant E_{sq}(\rho^{AB})+E_{sq}(\rho^{AC})+E_{sq}(\rho^{BC}) \quad (27)$$

holds for any $\rho^{ABC}\in\mathcal{S}^{ABC}$.

Proof. By the chain rule for the conditional mutual information with any state extension ρ^{ABCE}, it is obvious that

$$\begin{aligned}&\tfrac{1}{2}I(A:B:C|E)\\&=\tfrac{1}{2}I(A:B|E)+\tfrac{1}{2}I(C:A|E)+\tfrac{1}{2}I(C:B|AE)\\&\geqslant E_{sq}(\rho^{AB})+E_{sq}(\rho^{AC})+E_{sq}(\rho^{BC}).\end{aligned}$$

The proof is completed. ■

Moreover, if there exists an optimal extension ρ^{ABCE} such that $E_{sq}^{(3)}(\rho^{ABC})=\frac{1}{2}I(A:B:C|E)$, then ρ^{ABC} is the tripartite disentangling condition (18) with respect to $E_{sq}^{(3)}$ if and only if ρ^{ABEC} is a Markov state [80], which implies that

$$\rho^{ABC}=\sum_j q_j\rho_j^{AB}\otimes\rho_j^C,$$

where $\{q_j\}$ is a probability distribution.

B. Tight complete monogamy relation for the complete MEM

For the complete MEM, condition E4 exhibits the relation between $E^{(3)}(ABC)$, $E^{(2)}(A|BC)$, and $E^{(2)}(AB)$. This motivates us to discuss the following *tight complete monogamy relation* which connects the two different kinds of monogamy relations, i.e., the monogamy relation up to the bipartite measure and the complete one, together (see Fig. 2).

Definition 2. Let $E^{(3)}$ be a unified MEM. We say $E^{(3)}$ is tightly complete monogamous if for any state $\rho^{ABC}\in\mathcal{S}^{ABC}$ satisfying

$$E^{(3)}(\rho^{ABC})=E^{(2)}(\rho^{A|BC}) \quad (28)$$

we have $E^{(2)}(\rho^{BC})=0$.

As one may expect, we show below that the tightly complete monogamy Eq. (28) is stronger than the complete monogamy relation Eq. (18) in general.

Theorem 3. Let $E^{(3)}$ be a complete multipartite entanglement monotone. If $E^{(3)}$ is tightly completely monogamous on pure states and $E_F^{(3)}$ is tightly completely monogamous, then $E^{(3)}$ is completely monogamous on pure states and $E_F^{(3)}$ is completely monogamous.

Proof. We assume that for any $|\psi\rangle^{ABC}$ that satisfies $E^{(3)}(|\psi\rangle^{ABC})=E^{(2)}(|\psi\rangle^{A|BC})$ we have $E^{(2)}(\rho^{BC})=0$. Therefore, if $E^{(2)}(\rho^{AB})=E^{(3)}(|\psi\rangle^{ABC})$, then

$$E^{(2)}(\rho^{AB})=E^{(2)}(|\psi\rangle^{A|BC})=E^{(3)}(|\psi\rangle^{ABC}) \quad (29)$$

since $E^{(2)}(\rho^{AB})\leqslant E^{(2)}(\rho^{A|BC})\leqslant E^{(3)}(\rho^{ABC})$ holds for any state ρ^{ABC}. This follows from the assumption that ρ^{BC} is separable. Together with Theorem 2, we can conclude that

$$|\psi\rangle^{ABC}=|\psi\rangle^{AB}|\psi\rangle^C. \quad (30)$$

That is, ρ^{AC} is a product state and thus $E(\rho^{AC})=0$. Namely, $E^{(3)}$ is completely monogamous for any pure state. We can easily check that $E_F^{(3)}$ is completely monogamous. ■

Notice in particular that, if $E_F^{(3)}$ is a TEM defined as in Eqs. (10) and (11), then condition E4 is equivalent to the following condition (E4′): $h(\rho^A\otimes\rho^B\otimes\rho^C)\geqslant h(\rho^A\otimes\rho^{BC})$, $\forall|\psi\rangle\in\mathcal{H}^{ABC}$. By Definition 2, the following can be easily checked.

Theorem 4. Let $E_F^{(3)}$, defined as in Eq. (10), be a unified TEM for which h, as defined in (11), satisfies condition E4′ where the equality holds if and only if $\rho^{BC}=\rho^B\otimes\rho^C$. Then $E_F^{(3)}$ is tightly completely monogamous.

V. EXTENDING BIPARTITE MEASURES TO COMPLETE MULTIPARTITE MEASURES

A. Tripartite extension of bipartite measures

Observing that, for pure state $|\psi\rangle\in\mathcal{H}^{AB}$,

$$\begin{aligned}E_f^{(2)}(|\psi\rangle)&=E_f(|\psi\rangle)=S(\rho^A)=S(\rho^B)\\&=\tfrac{1}{2}S(|\psi\rangle\langle\psi\|\rho^A\otimes\rho^B)=\tfrac{1}{2}S(\rho^A\otimes\rho^B)\\&=\tfrac{1}{2}[S(\rho^A)+S(\rho^B)],\end{aligned}$$

where $S(\rho\|\sigma):=\mathrm{Tr}[\rho(\ln\rho-\ln\sigma)]$ is the relative entropy, we thus define tripartite entanglement of formation as

$$\begin{aligned}E^{(3)}(|\psi\rangle)&:=\tfrac{1}{2}[S(|\psi\rangle\langle\psi\|\rho^A\otimes\rho^B\otimes\rho^C)]\\&=\tfrac{1}{2}[S(\rho^A)+S(\rho^B)+S(\rho^C)]\end{aligned} \quad (31)$$

for pure state $|\psi\rangle\in\mathcal{H}^{ABC}$, and then by the convex-roof extension, i.e.,

$$E_f^{(3)}(\rho^{ABC})=\min_{\{p_i,|\psi_i\rangle\}}\sum_i p_iE^{(3)}(|\psi_i\rangle) \quad (32)$$

for mixed state $\rho^{ABC}\in\mathcal{S}^{ABC}$, $E_f^{(3)}$ coincides with the α-entanglement entropy defined in Ref. [29].

Let $\mathcal{P}_3^2(|\psi\rangle)=\{\rho^A\otimes\rho^{BC},\rho^{AB}\otimes\rho^C,\rho^B\otimes\rho^{AC}\}$; then

$$E^{(3-2)}(|\psi\rangle):=\frac{1}{2}\min_{\sigma\in\mathcal{P}_3^2(|\psi\rangle)}S(|\psi\rangle\langle\psi\|\sigma). \quad (33)$$

For any mixed state $\rho\in\mathcal{S}^{ABC}$, the entanglements of formation associated with $E^{(3)}$ and $E^{(3-2)}$ are denoted by $E_f^{(3)}$ and $E_f^{(3-2)}$, respectively. (In order to remain consistent with the original bipartite entanglement of formation E_f, we call $E_f^{(3)}$ here the *tripartite EoF*, and denote it by $E_f^{(3)}$ throughout

TABLE I. Comparison of $E^{(3)}$ and $E^{(2)}$ (or $h^{(3)}$ and $h^{(2)}$ for entanglement of formation $E_F^{(3,2)}$) for $E_f^{(3)}$, tripartite concurrence $C^{(3)}$, tripartite tangle $\tau^{(3)}$, tripartite Tsallis q entropy of entanglement $T_q^{(3)}$, tripartite Rényi α entropy of entanglement $R_\alpha^{(3)}$, tripartite convex roof extended negativity $N_F^{(3)}$, tripartite negativity $N^{(3)}$, tripartite squashed entanglement $E_{\rm sq}^{(3)}$, tripartite conditional entanglement of mutual information $E_I^{(3)}$, tripartite relative entropy of entanglement $E_r^{(3)}$, and tripartite geometric measure of entanglement $E_G^{(3)}$. M denotes $E^{(2)}$ is monogamous, CM denotes $E^{(3)}$ is completely monogamous, and TCM denotes $E^{(3)}$ is tightly completely monogamous.

$E^{(3)}$	$E^{(3)}$ or $h^{(3)}(\rho^A\otimes\rho^B\otimes\rho^C)$	$E^{(2)}$ or $h^{(2)}(\rho^A\otimes\rho^B)$	E3	E4	M	CM	TCM
$E_f^{(3)}$	$\frac{1}{2}S(\rho^A\otimes\rho^B\otimes\rho^C)$	$\frac{1}{2}S(\rho^A\otimes\rho^B)$	✓	✓	✓ [60]	✓	✓
$C^{(3)}$	$[3-\mathrm{Tr}(\rho^A)^2-\mathrm{Tr}(\rho^B)^2-\mathrm{Tr}(\rho^C)^2]^{\frac{1}{2}}$	$[2-\mathrm{Tr}(\rho^A)^2-\mathrm{Tr}(\rho^B)^2]^{\frac{1}{2}}$	✓	✓	✓ [60]	✓	✓
$\tau^{(3)}$	$3-\mathrm{Tr}(\rho^A)^2-\mathrm{Tr}(\rho^B)^2-\mathrm{Tr}(\rho^C)^2$	$2-\mathrm{Tr}(\rho^A)^2-\mathrm{Tr}(\rho^B)^2$	✓	✓	✓ [60]	✓	✓
$T_q^{(3)}$	$\frac{1}{2}[T_q(\rho^A)+T_q(\rho^B)+T_q(\rho^C)]$	$\frac{1}{2}[T_q(\rho^A)+T_q(\rho^B)]$	✓	✓	✓ [60]	✓	✓
$R_\alpha^{(3)}$	$\frac{1}{2}R_\alpha(\rho^A\otimes\rho^B\otimes\rho^C)$	$\frac{1}{2}R_\alpha(\rho^A\otimes\rho^B)$	✓	×	✓ [60]	?	×
$N_F^{(3)}$	$\mathrm{Tr}^2\sqrt{\rho^A}+\mathrm{Tr}^2\sqrt{\rho^B}+\mathrm{Tr}^2\sqrt{\rho^C}-3$	$\mathrm{Tr}^2\sqrt{\rho^A}+\mathrm{Tr}^2\sqrt{\rho^B}-2$	✓	×	✓ [60]	✓	?
$N^{(3)}$	$\Vert\rho^{T_a}\Vert_{\rm Tr}+\Vert\rho^{T_b}\Vert_{\rm Tr}+\Vert\rho^{T_c}\Vert_{\rm Tr}-3$	$\Vert\rho^{T_a}\Vert_{\rm Tr}+\Vert\rho^{T_b}\Vert_{\rm Tr}-2$	✓	×	?	✓	?
$E_{\rm sq}^{(3)}$ [17]	$\frac{1}{2}\inf I(A:B:C\vert E)$	$\frac{1}{2}\inf I(A:B\vert E)$	✓	✓	✓ [41]	✓	?
$E_I^{(3)}$ [18]	$\frac{1}{2}\inf[I(AA':BB':CC')-I(A':B':C')]$	$\frac{1}{2}\inf[I(AA':BB')-I(A':B')]$	✓	✓	?	?	?
$E_r^{(3)}$ [9]	$\inf_\sigma S(\rho^{ABC}\Vert\sigma_{\rm sep}^{ABC})$	$\inf_\sigma S(\rho^{AB}\Vert\sigma_{\rm sep}^{AB})$	✓	?	?	?	?
$E_G^{(3)}$ [15]	$1-\sup_\phi\vert\langle\psi\vert\phi\rangle^{ABC}\vert^2$	$1-\sup_\phi\vert\langle\psi\vert\phi\rangle^{AB}\vert^2$	✓	?	?	?	?

this paper. The notations $E_F^{(m)}$ and $E_F^{(m-k)}$ with capital F in the subscript denote other general convex-roof extended measures.)

Note that, for $|\psi\rangle\in\mathcal{H}^{AB}$, $\tau(|\psi\rangle)$ and $N(|\psi\rangle)$ can be rewritten as

$$\tau(|\psi\rangle)=2-\mathrm{Tr}(\rho^A)^2-\mathrm{Tr}(\rho^B)^2,$$
$$N(|\psi\rangle)=\tfrac{1}{4}(\mathrm{Tr}^2\sqrt{\rho^A}+\mathrm{Tr}^2\sqrt{\rho^B}-2).$$

We thus give the definitions for any $|\psi\rangle\in\mathcal{H}^{ABC}$ as

$$\tau^{(3)}(|\psi\rangle)=3-\mathrm{Tr}(\rho^A)^2-\mathrm{Tr}(\rho^B)^2-\mathrm{Tr}(\rho^C)^2, \quad (34)$$

$$C^{(3)}(|\psi\rangle)=\sqrt{\tau^{(3)}(|\psi\rangle)}, \quad (35)$$

$$N^{(3)}(|\psi\rangle)=\mathrm{Tr}^2\sqrt{\rho^A}+\mathrm{Tr}^2\sqrt{\rho^B}+\mathrm{Tr}^2\sqrt{\rho^C}-3 \quad (36)$$

for pure states and define them by the convex-roof extensions for the mixed states (in order to coincide with the bipartite case, we denote by $\tau^{(3)}$, $C^{(3)}$, and $N_F^{(3)}$ the convex-roof extensions):

$$\tau^{(3)}(\rho^{ABC})=\min_{\{p_i,|\psi_i\rangle\}}\sum_i p_i\tau^{(3)}(|\psi_i\rangle\langle\psi_i|),$$

$$C^{(3)}(\rho^{ABC})=\min_{\{p_i,|\psi_i\rangle\}}\sum_i p_iC^{(3)}(|\psi_i\rangle\langle\psi_i|),$$

$$N_F^{(3)}(\rho^{ABC})=\min_{\{p_i,|\psi_i\rangle\}}\sum_i p_iN^{(3)}(|\psi_i\rangle\langle\psi_i|),$$

where the minimum is taken over all pure-state decompositions $\{p_i,|\psi_i\rangle\}$ of ρ^{ABC}. Observe that

$$N^{(3)}(|\psi\rangle)=\Vert\rho^{T_a}\Vert_{\rm Tr}+\Vert\rho^{T_b}\Vert_{\rm Tr}+\Vert\rho^{T_c}\Vert_{\rm Tr}-3$$

for pure state $\rho=|\psi\rangle\langle\psi|\in\mathcal{S}^{ABC}$; we define

$$N^{(3)}(\rho)=\Vert\rho^{T_a}\Vert_{\rm Tr}+\Vert\rho^{T_b}\Vert_{\rm Tr}+\Vert\rho^{T_c}\Vert_{\rm Tr}-3 \quad (37)$$

for mixed states $\rho\in\mathcal{S}^{ABC}$. By definition, all these tripartite measures are unified (see Table I). It is worth mentioning here that $E^{(3)}$ is not unique in general for a given $E^{(2)}$ for bipartite states; e.g., we also can define

$$\tau'^{(3)}(|\psi\rangle^{ABC})=2[1-\sqrt{\mathrm{Tr}(\rho^A)^2}\sqrt{\mathrm{Tr}(\rho^B)^2}\sqrt{\mathrm{Tr}(\rho^C)^2}] \quad (38)$$

for the tripartite system. $\tau'^{(3)}$ does not obey condition E4: It is easy to see that the two-qubit state σ^{BC} with spectra $\{87/128, 37/128, 1/32, 0\}$ as in Eq. (41) leads to $\mathrm{Tr}(\sigma^B)^2\mathrm{Tr}(\sigma^C)^2<\mathrm{Tr}(\sigma^{BC})^2$ [the existence of such state is guaranteed by the result in Ref. [81]; also see Eq. (41) below].

Since the Tsallis q entropy is subadditive if and only if $q>1$, i.e.,

$$T_q(\rho^{AB})\leqslant T_q(\rho^A)+T_q(\rho^B),\ q>1,\ \rho^{A,B}=\mathrm{Tr}_{B,A}\rho^{AB},$$

where

$$T_q(\rho):=(1-q)^{-1}[\mathrm{Tr}(\rho^q)-1]$$

is the Tsallis q entropy, but not additive [i.e., $T_q(\rho\otimes\sigma)\neq T_q(\rho)+T_q(\sigma)$ in general] in general [76], we can define the tripartite Tsallis q entropy of entanglement by

$$T_q^{(3)}(|\psi\rangle):=\tfrac{1}{2}[T_q(\rho^A)+T_q(\rho^B)+T_q(\rho^C)],\quad q>1 \quad (39)$$

for pure state $|\psi\rangle\in\mathcal{H}^{ABC}$, and then define this by the convex-roof extension for mixed states. The Rényi entropy is additive [82], i.e.,

$$R_\alpha(\rho\otimes\sigma)=R_\alpha(\rho)+R_\alpha(\sigma),$$

and we thus define the tripartite Rényi α entropy of entanglement by

$$R_\alpha^{(3)}(|\psi\rangle):=\tfrac{1}{2}R_\alpha(\rho^A\otimes\rho^B\otimes\rho^C),\ 0<\alpha<1 \quad (40)$$

for the pure state and by the convex-roof extension for mixed states, where

$$R_\alpha(\rho):=(1-\alpha)^{-1}\ln(\mathrm{Tr}\rho^\alpha)$$

is the Rényi α entropy.

B. Monogamy of these extended measures

We can easily show that $E_f^{(3)}$, $\tau^{(3)}$, and $C^{(3)}$ satisfy condition E4′ and, furthermore, the theorem below is true.

Theorem 5. $E_f^{(3)}$, $\tau^{(3)}$, $C^{(3)}$, $T_q^{(3)}$, $N_F^{(3)}$, and $N^{(3)}$ are completely monogamous TEMs. $E_f^{(3)}$, $\tau^{(3)}$, $C^{(3)}$, and $T_q^{(3)}$ are complete TEMs while $R_\alpha^{(3)}$, $N_F^{(3)}$, and $N^{(3)}$ are unified TEMs but not complete TEMs.

Proof. The unification condition for all these quantities is clear from the definition. We show at first that $E_f^{(3)}$, $\tau^{(3)}$, $C^{(3)}$, and $T_q^{(3)}$ satisfy condition E4′. The cases of $E_f^{(3)}$ and $T_q^{(3)}$ are obvious since $S(\rho^{AB}) \leqslant S(\rho^A) + S(\rho^B)$ and $T_q(\rho^{AB}) \leqslant T_q(\rho^A) + T_q(\rho^B)$ (note that $q > 1$). For the case of $\tau^{(3)}$, we have $\tau^{(3)}(|\psi\rangle^{ABC}) \geqslant \tau^{(2)}(|\psi\rangle^{A|BC})$ since (see Theorem 2 in Ref. [83])

$$1 + \mathrm{Tr}(\rho^{BC})^2 \geqslant \mathrm{Tr}(\rho^B)^2 + \mathrm{Tr}(\rho^C)^2.$$

Therefore the case of $C^{(3)}$ is also true.

The complete monogamy of $E_f^{(3)}$, $\tau^{(3)}$, $C^{(3)}$, and $T_q^{(3)}$ is clear by Theorem 1. For any $\rho^{ABC} \in \mathcal{S}^{ABC}$, if $N^{(3)}(\rho^{ABC}) = N^{(2)}(\rho^{AB})$, i.e., $\|\rho_{ABC}^{T_a}\|_{\mathrm{Tr}} + \|\rho_{ABC}^{T_b}\|_{\mathrm{Tr}} + \|\rho_{ABC}^{T_c}\|_{\mathrm{Tr}} - 3 = \|\rho_{AB}^{T_a}\|_{\mathrm{Tr}} + \|\rho_{AB}^{T_b}\|_{\mathrm{Tr}} - 2$, then $\|\rho_{ABC}^{T_c}\|_{\mathrm{Tr}} = 1$, which implies that $\rho^{AB|C}$ is a positive partial transpose (PPT) state, and therefore ρ^{AC} and ρ^{BC} are PPT states. Thus $N^{(3)}$ and $N_F^{(3)}$ are completely monogamous.

For any $E^{(3)} \in \{E_f^{(3)}, \tau^{(3)}, C^{(3)}, T_q^{(3)}, R_\alpha^{(3)}, N_F^{(3)}\}$ and any pure state $|\psi\rangle^{ABC} \in \mathcal{H}^{ABC}$, we have

$$\begin{aligned} &E^{(3)}(|\psi\rangle^{ABC}) \\ &\quad = \tfrac{1}{2}[E^{(2)}(|\psi\rangle^{A|BC}) + E^{(2)}(|\psi\rangle^{AB|C}) + E^{(2)}(|\psi\rangle^{B|AC})], \end{aligned}$$

which indicates that $E^{(3)}$ is a TEM from the fact that $E^{(2)}$ is an entanglement monotone. Similarly, one can show that $N^{(3)}$ is also a TEM.

Recall that mixed two-qubit state ρ^{AB} with spectrum $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \lambda_4 \geqslant 0$ and marginal states ρ^A and ρ^B exist if and only if the minimal eigenvalues λ_A and λ_B of the marginal states satisfy the following inequalities [81]:

$$\begin{cases} \min(\lambda_A, \lambda_B) \geqslant \lambda_3 + \lambda_4, \\ \lambda_A + \lambda_B \geqslant \lambda_2 + \lambda_3 + 2\lambda_4, \\ |\lambda_A - \lambda_B| \leqslant \min(\lambda_1 - \lambda_3, \lambda_2 - \lambda_4). \end{cases} \tag{41}$$

Based on this result, we can find counterexamples, which shows that $N_F^{(3)}$ violates condition E4′ (thus $N^{(3)}$ also violates condition E4′). Specifically, we take the following two-qubit state ρ^{BC} with spectrum {327/512, 37/128, 37/512, 0} and two marginal states, i.e., ρ^B and ρ^C having spectra {7/8, 1/8} and {3/4, 1/4}, respectively. Then

$$1 + \mathrm{Tr}^2(\sqrt{\rho^{BC}}) > \mathrm{Tr}^2(\sqrt{\rho^B}) + \mathrm{Tr}^2(\sqrt{\rho^C}).$$

If we take another two-qubit state σ^{BC} such that σ^{BC}, σ^B, and σ^C have spectra {87/128, 37/128, 1/32, 0}, {7/8, 1/8} and {3/4, 1/4}, then

$$1 + \mathrm{Tr}^2(\sqrt{\sigma^{BC}}) < \mathrm{Tr}^2(\sqrt{\sigma^B}) + \mathrm{Tr}^2(\sqrt{\sigma^C}).$$

Namely, $N_F^{(3)}$ and $N^{(3)}$ violate condition E4′ for pure states. $R_\alpha^{(3)}$ violates condition E4′ since the Rényi α entropy is not subadditive except for $\alpha = 0$ or 1 [84]. ■

From the proof of Theorem 5, we can conclude that if $E_F^{(3)}$ satisfies condition E4′ where the equality holds if and only if $\rho^{BC} = \rho^B \otimes \rho^C$ for $|\psi\rangle^{ABC} = |\phi\rangle^{AB_1}|\eta\rangle^{B_2C}$ then it is completely monogamous, but not necessarily tightly completely monogamous as in (28).

Proposition 4. $E_f^{(3)}$, $C^{(3)}$, $\tau^{(3)}$, and $T_q^{(3)}$ are tightly completely monogamous.

Proof. Since $S(\rho^{BC}) \leqslant S(\rho^B) + S(\rho^C)$ holds for any pure state $|\psi\rangle \in \mathcal{H}^{ABC}$, $E_f^{(3)}(ABC) \geqslant E_f^{(2)}(A|BC)$ for any $\rho \in \mathcal{S}^{ABC}$. In addition, $\rho^{BC} = \rho^B \otimes \rho^C$ provided $E_f^{(3)}(|\psi\rangle^{ABC}) = E_f^{(2)}(|\psi\rangle^{A|BC})$. Thus $E_f^{(3)}$ is tightly completely monogamous by Theorem 4. Observe that

$$\begin{aligned} \tau^{(3)}(|\psi\rangle^{ABC}) &= 3 - [\mathrm{Tr}(\rho^A)^2 + \mathrm{Tr}(\rho^B)^2 + \mathrm{Tr}(\rho^C)^2] \\ &\geqslant 2 - [\mathrm{Tr}(\rho^A)^2 + \mathrm{Tr}(\rho^{BC})^2] \\ &= \tau^{(2)}(|\psi\rangle^{A|BC}) \end{aligned}$$

since $1 + \mathrm{Tr}(\rho^{BC})^2 \geqslant \mathrm{Tr}(\rho^B)^2 + \mathrm{Tr}(\rho^C)^2$ (see Theorem 2 in Ref. [83]). By Proposition 4.5 in Ref. [85], we can get the following result (i.e., Lemma 2; see the Appendix for details): for any bipartite state $\rho \in \mathcal{S}^{AB}$, $1 + \mathrm{Tr}(\rho^2) = \mathrm{Tr}(\rho^A)^2 + \mathrm{Tr}(\rho^B)^2$ if and only if $\rho = \rho^A \otimes \rho^B$ with $\min\{\mathrm{rank}(\rho^A), \mathrm{rank}(\rho^B)\} = 1$. This guarantees that

$$1 + \mathrm{Tr}(\rho^{BC})^2 = \mathrm{Tr}(\rho^B)^2 + \mathrm{Tr}(\rho^C)^2$$

if and only if ρ^B or ρ^C is pure. For the Tsallis entropy, we have [76]

$$T_q(\rho \otimes \sigma) = T_q(\rho) + T_q(\sigma) \tag{42}$$

if and only if either ρ or σ is pure. By Theorem 4, $C^{(3)}$, $\tau^{(3)}$, and $T_q^{(3)}$ are tightly completely monogamous. ■

We conjecture that $R_\alpha^{(3)}$ is not tightly completely monogamous since $R_\alpha(\rho^{AB}) = R_\alpha(\rho^A) + R_\alpha(\rho^B)$ may not imply $\rho^{AB} = \rho^A \otimes \rho^B$ necessarily. Whether $N_F^{(3)}$ and $N^{(3)}$ are tightly completely monogamous is still unknown.

For $E \in \{E_f^{(3)}, C^{(3)}, \tau^{(3)}, T_q^{(3)}\}$, with some abuse of notations, by Proposition 2, Eq. (28) holds if and only if

$$E^{\alpha_1}(\rho^{ABC}) \geqslant E^{\alpha_1}(\rho^{A|BC}) + E^{\alpha_1}(\rho^{BC})$$

for some $\alpha_1 > 0$. In addition,

$$E^{\alpha_2}(\rho^{A|BC}) \geqslant E^{\alpha_2}(\rho^{AB}) + E^{\alpha_2}(\rho^{AC})$$

for some $\alpha_2 > 0$ from Theorem 1 in Ref. [59]. Taking $\alpha = \max\{\alpha_1, \alpha_2\}$, we have that

$$\begin{aligned} E^\alpha(\rho^{ABC}) &\geqslant E^\alpha(\rho^{A|BC}) + E^\alpha(\rho^{BC}) \\ &\geqslant E^\alpha(\rho^{AB}) + E^\alpha(\rho^{AC}) + E^\alpha(\rho^{BC}) \end{aligned}$$

holds for these E.

C. Additivity of the entanglement of formation

As a byproduct of the tripartite entanglement of formation $E_f^{(3)}$, we discuss in this section the additivity of this measure. Recall that the additivity of the entanglement formation $E_f^{(2)}$ is a long-standing open problem which was conjectured to be true [86] and then disproved by Hastings in 2009 [87]. We always expect intuitively that the measure of entanglement should be additive in the sense of [88]

$$E(\rho^{AB}\otimes\sigma^{A'B'}) = E(\rho^{AB}) + E(\sigma^{A'B'}), \tag{43}$$

where $E(\rho^{AB}\otimes\sigma^{A'B'}) := E(\rho^{AB}\otimes\sigma^{A'B'})$ up to the partition $AA'|BB'$. Equation (43) means that, from the resource-based point of view, sharing two particles from the same preparing device is exactly "twice as useful" to Alice and Bob as having just one. By now, we know that the squashed entanglement [16] and the conditional entanglement of mutual information [18] are additive. Although EoF is not additive for all states, construction of additive states for EoF is highly expected [89]. In what follows, we present a class of states such that $E_f^{(2)}$ is additive (and thus for such class of states we have $E_f^{(2)} = E_c$ [86], where E_c denotes the entanglement cost), and present, analogously, a class of states such that $E_f^{(3)}$ is additive.

Theorem 6.

(i) Let $\rho^{AB}\otimes\sigma^{A'B'}$ be a state in $\mathcal{S}^{AA'BB'}$. If there exists an optimal ensemble $\{p_i, |\psi_i\rangle^{AA'BB'}\}$ for E_f, i.e., $E_f(\rho^{AB}\otimes\sigma^{A'B'}) = \sum_i p_i E(|\psi_i\rangle^{AA'BB'})$, such that any pure state $|\psi_i\rangle^{AA'BB'}$ is a product state, i.e., $|\psi_i\rangle^{AA'BB'} = |\phi_i\rangle^{AB}|\varphi_i\rangle^{A'B'}$ for some pure state $|\phi_i\rangle^{AB}\in\mathcal{H}^{AB}$ and $|\varphi_i\rangle^{A'B'}\in\mathcal{H}^{A'B'}$, then we have

$$E_f^{(2)}(AB\otimes A'B') = E_f^{(2)}(AB) + E_f^{(2)}(A'B'). \tag{44}$$

(ii) Let $\rho^{ABC}\otimes\sigma^{A'B'C'}$ be a state in $\mathcal{S}^{AA'BB'CC'}$. If there exists an optimal ensemble $\{p_i, |\psi_i\rangle^{AA'BB'CC'}\}$ for $E_f^{(3)}$ such that any pure state $|\psi_i\rangle^{AA'BB'CC'}$ is a product state, i.e., $|\psi_i\rangle^{AA'BB'CC'} = |\phi_i\rangle^{ABC}|\varphi_i\rangle^{A'B'C'}$ for some pure state $|\phi_i\rangle^{ABC}\in\mathcal{H}^{ABC}$ and $|\varphi_i\rangle^{A'B'C'}\in\mathcal{H}^{A'B'C'}$, then we have

$$E_f^{(3)}(ABC\otimes A'B'C') = E_f^{(3)}(ABC) + E_f^{(3)}(A'B'C'). \tag{45}$$

Proof. We only discuss the additivity of $E_f^{(3)}$; the case of E_f can be followed analogously. For pure states $|\phi\rangle^{ABC}\in\mathcal{H}^{ABC}$ and $|\varphi\rangle^{A'B'C'}\in\mathcal{H}^{A'B'C'}$, this is clear since

$$\begin{aligned}
&E_f^{(3)}(|\phi\rangle\langle\phi|^{ABC}\otimes|\varphi\rangle\langle\varphi|^{A'B'C'})\\
&= \tfrac{1}{2}[S(|\phi\rangle\langle\phi|^{ABC}\otimes|\varphi\rangle\langle\varphi|^{A'B'C'}\|\rho^{AA'}\otimes\rho^{BB'}\otimes\rho^{CC'})]\\
&= \tfrac{1}{2}[S(\rho^{AA'}) + S(\rho^{BB'}) + S(\rho^{CC'})]\\
&= \tfrac{1}{2}[S(\rho^{A}) + S(\rho^{B}) + S(\rho^{C}) + S(\sigma^{A'})\\
&\quad + S(\sigma^{B'}) + S(\sigma^{C'})]\\
&= \tfrac{1}{2}[S(|\phi\rangle\langle\phi|^{ABC}\|\rho^{A}\otimes\rho^{B}\otimes\rho^{C})\\
&\quad + S(|\varphi\rangle\langle\varphi|^{A'B'C'}\|\sigma^{A'}\otimes\sigma^{B'}\otimes\sigma^{C'})]\\
&= E_f^{(3)}(\rho^{ABC}) + E_f^{(3)}(\sigma^{A'B'C'}),
\end{aligned}$$

where $\rho^{xx'} = \mathrm{Tr}_{\overline{xx'}}(|\phi\rangle\langle\phi|^{ABC}\otimes|\varphi\rangle\langle\varphi|^{A'B'C'})$, $\rho^{x} = \mathrm{Tr}_{\bar{x}}(|\phi\rangle\langle\phi|^{ABC})$, and $\sigma^{x'} = \mathrm{Tr}_{\bar{x}'}(|\varphi\rangle\langle\varphi|^{A'B'C'})$.

Assume that both ρ^{ABC} and $\sigma^{A'B'C'}$ are mixed. Let $\{p_i, |\psi_i\rangle^{AA'BB'CC'}\}$ be the optimal ensemble satisfying

$$E_f^{(3)}(\rho^{ABC}\otimes\sigma^{A'B'C'}) = \sum_i p_i E_f^{(3)}(|\psi_i\rangle^{AA'BB'CC'}).$$

Then

$$\begin{aligned}
&\sum_i p_i E_f^{(3)}(|\psi_i\rangle^{AA'BB'CC'})\\
&\quad = \sum_i p_i\big[E_f^{(3)}(|\phi_i\rangle^{ABC}) + E_f^{(3)}(|\varphi_i\rangle^{A'B'C'})\big]\\
&\quad \geqslant E_f^{(3)}(\rho^{ABC}) + E_f^{(3)}(\sigma^{A'B'C'})
\end{aligned}$$

since by assumption we have

$$|\psi_i\rangle^{AA'BB'CC'} = |\phi_i\rangle^{ABC}|\varphi_i\rangle^{A'B'C'}.$$

On the other hand, let $\{t_i, |\phi_i\rangle^{ABC}\}$ and $\{q_j, |\varphi_j\rangle^{A'B'C'}\}$ be the optimal ensembles satisfying

$$\begin{aligned}
E_f^{(3)}(\rho^{ABC}) &= \sum_i t_i E_f^{(3)}(|\phi_i\rangle^{ABC}),\\
E_f^{(3)}(\sigma^{A'B'C'}) &= \sum_j q_j E_f^{(3)}(|\varphi_j\rangle^{A'B'C'}).
\end{aligned}$$

Writing $|\psi_{ij}\rangle^{AA'BB'CC'} = |\phi_i\rangle^{ABC}|\varphi_j\rangle^{A'B'C'}$ reveals that

$$\begin{aligned}
&E_f^{(3)}(\rho^{ABC}) + E_f^{(3)}(\sigma^{A'B'C'})\\
&\quad = \sum_i t_i E_f^{(3)}(|\phi_i\rangle^{ABC}) + \sum_j q_j E_f^{(3)}(|\varphi_j\rangle^{A'B'C'})\\
&\quad = \sum_{i,j} t_i q_j E_f^{(3)}(|\psi_{ij}\rangle^{AA'BB'CC'})\\
&\quad \geqslant E_f^{(3)}(\rho^{ABC}\otimes\sigma^{A'B'C'}).
\end{aligned}$$

The case that ρ^{ABC} is pure while $\sigma^{A'B'C'}$ is mixed can be proved similarly. ■

Particularly, if ρ^{AB} or $\sigma^{A'B'}$ (respectively, ρ^{ABC} or $\sigma^{A'B'C'}$) is pure, then $\rho^{AB}\otimes\sigma^{A'B'}$ (respectively, $\rho^{ABC}\otimes\sigma^{A'B'C'}$) is additive under $E_f^{(3)}$ (respectively, $E_f^{(2)}$). Together with the result of Hastings in Ref. [87], we conclude that the state $\rho^{AB}\otimes\sigma^{A'B'}$ (respectively, $\rho^{ABC}\otimes\sigma^{A'B'C'}$) that violates the additivity (43) definitely has an optimal pure-state decomposition in which some pure states are not product states up to the partition $AB|A'B'$ (respectively, $ABC|A'B'C'$). Our approach is far different from that of Ref. [89], in which it is shown that a state with range in the entanglement-breaking space is always additive.

VI. MAXIMALLY ENTANGLED STATE AND THE MONOGAMY RELATION

A. Original definition of the maximally entangled state

The MES, as a crucial quantum resource in quantum information processing tasks such as quantum teleportation [90–92], superdense coding [93,94], quantum computation [95], and quantum cryptography [96], has been explored considerably [97–112]. For a bipartite system with state space $\mathcal{H}^{AB} = \mathcal{H}^A\otimes\mathcal{H}^B$, $\dim\mathcal{H}^A = m$, $\dim\mathcal{H}^B = n$ $(m\leqslant n)$, a pure state $|\psi\rangle^{AB}$ is called a maximally entangled state if and only if $\rho^A = \frac{1}{m}I^A$ [113], where ρ^A is the reduced state of $\rho^{AB} = |\psi\rangle\langle\psi|^{AB}$ with respect to subsystem A. Equivalently, $|\psi\rangle^{AB}$ is an MES if and only if

$$|\psi\rangle^{AB} = \frac{1}{\sqrt{m}}\sum_{i=1}^{m}|i\rangle^A|i\rangle^B, \tag{46}$$

where $\{|i\rangle^A\}$ is an orthonormal basis of $\mathcal{H}^A$ and $\{|i\rangle^B\}$ is an orthonormal set of $\mathcal{H}^B$. An MES $|\psi\rangle^{AB}$ always archives the maximal amount of entanglement for a certain entanglement measure [102] (such as entanglement of formation [3,4] and concurrence [5–7]). For example, the well-known Einstein-Podolsky-Rosen states are maximally entangled pure states.

It was proved in Ref. [114] that any MES in a $d\otimes d$ system is pure. Later, Li *et al.* showed in Ref. [102] that the maximal entanglement can also exist in mixed states for $m\otimes n$ systems with $n\geqslant 2m$ (or $m\geqslant 2n$). A necessary and sufficient condition of the mixed maximally entangled state (MMES) was proposed [102]: an $m\otimes n$ ($n\geqslant 2m$) bipartite mixed state ρ^{AB} is maximally entangled if and only if

$$\rho^{AB} = \sum_{k=1}^{r} p_k|\psi_k\rangle\langle\psi_k|^{AB}, \quad \sum_k p_k = 1,\ p_k\geqslant 0, \tag{47}$$

where $|\psi_k\rangle^{AB}$s are maximally entangled pure states with

$$|\psi_k\rangle^{AB} = \frac{1}{\sqrt{m}}\sum_{i=0}^{m-1}|i\rangle^A|i_k\rangle^B, \tag{48}$$

$\{|i\rangle^A\}$ is an orthonormal basis of $\mathcal{H}^A$, and $\{|i_k\rangle^B\}$ is an orthonormal set of $\mathcal{H}^B$, satisfying $\langle i_s|j_t\rangle^B = \delta_{ij}\delta_{st}$. Let $\mathcal{H}^{B'}$ be the subspace spanned by $\{|i_k\rangle^B : i = 0, 1, \ldots, m-1, k = 1, 2, \ldots, r\}$. Then there exists a unitary operator $U^{B'}$ acting on $\mathcal{H}^{B'}$ such that

$$U^{B'}|i_k\rangle^B = |i\rangle^{B_1}|k\rangle^{B_2},$$

where

$$\mathcal{H}^{B_1} := \mathrm{span}\{|i\rangle^{B_1} : i = 0, 1, \ldots, m-1\}$$

and

$$\mathcal{H}^{B_2} = \mathrm{span}\{|k\rangle^{B_2} : k = 1, 2, \ldots, r\}.$$

That is, the MMES ρ^{AB} can be rewritten as

$$\rho^{AB} = |\psi_+\rangle\langle\psi_+|^{AB_1}\otimes\left(\sum_{k=1}^{r}p_k|k\rangle\langle k|^{B_2}\right), \tag{49}$$

up to some local unitary on part B, where

$$|\psi_+\rangle^{AB_1} = \frac{1}{\sqrt{m}}\sum_{i=0}^{m-1}|i\rangle^A|i\rangle^{B_1}$$

is the maximally pure state in $\mathcal{H}^{AB_1}$, $\sum_k p_k = 1$, $p_k\geqslant 0$. The main purpose of this section is to show that ρ^{AB} in Eq. (47) [or equivalently in Eq. (49)] is not a complete MES physically; there does not exist a mixed MES in any bipartite system.

B. Incompatibility of the MMES and the monogamy law

We begin with the fact that it seems that entanglement can be freely shared.

Theorem 7. Let ρ^{ABC} be a state acting on $\mathcal{H}^{ABC}$ with $2\dim\mathcal{H}^A\leqslant\dim\mathcal{H}^B$. If $\rho^{AB} = \mathrm{Tr}_C\rho^{ABC}$ is a mixed state as in Eq. (47), then ρ^{AC} is a product state but ρ^{BC} is not necessarily separable.

Proof. We assume with no loss of generality that ρ^{AB} has the form as in Eq. (49) for some subspaces $\mathcal{H}^{B_1}$ and $\mathcal{H}^{B_2}$ of $\mathcal{H}^B$. If $|\psi\rangle^{ABC}$ is a state with reduced state ρ^{AB}, then it is straightforward that

$$|\phi\rangle^{ABC} = |\psi_+\rangle^{AB_1}|\psi\rangle^{B_2C} \tag{50}$$

with

$$|\psi\rangle^{B_2C} = \sum_k\sqrt{p_k}|k\rangle^{B_2}|k\rangle^C, \tag{51}$$

where $\{|k\rangle^C\}$ is an orthonormal set in $\mathcal{H}^C$. It is easy to see that $\rho^{AC} = \rho^A\otimes\rho^C$ and ρ^{BC} is entangled.

If ρ^{ABC} is a mixed state with reduced state ρ^{AB} as an assumption, we let

$$E_f(\rho^{A|BC}) = \sum_{s=1}^{l}q_sE_f(|\phi_s\rangle\langle\phi_s|^{A|BC}).$$

It follows that

$$E_f(|\phi_s\rangle\langle\phi_s|^{A|BC}) = E_f\left(\rho_s^{AB}\right)$$

since $\ln m\geqslant E_f(A|BC)\geqslant E_f(AB)$ for any ρ^{ABC} and $\sum_s q_sE_f(\rho_s^{AB})\geqslant E_f(\rho^{AB}) = \ln m$, where $m = \dim\mathcal{H}^A$, $\rho_s^{AB} = \mathrm{Tr}_C|\phi_s\rangle\langle\phi_s|^{ABC}$. By the theorem in Ref. [60], together with the assumption of ρ^{AB}, we have

$$|\phi_s\rangle^{ABC} = |\psi_+\rangle^{AB_1}|\phi_s\rangle^{B_2C},$$

where $|\psi_+\rangle^{AB_1}\in\mathcal{H}^A\otimes\mathcal{H}^{B_1}$ and $|\phi_s\rangle^{B_2C}\in\mathcal{H}^{B_2}\otimes\mathcal{H}^C$. We now can obtain that

$$\rho^{ABC} = |\psi_+\rangle\langle\psi_+|^{AB_1}\otimes\rho^{B_2C}, \tag{52}$$

where

$$\rho^{B_2C} = \sum_s q_s|\phi_s\rangle\langle\phi_s|^{B_2C} \tag{53}$$

with

$$|\phi_s\rangle^{B_2C} = \sum_{k=1}^{r}\sqrt{p_k}\left|e_k^{(s)}\right\rangle^{B_2}\left|f_k^{(s)}\right\rangle^C. \tag{54}$$

Together with the form of ρ^{AB} as supposed, we have $|e_k^{(s)}\rangle^{B_2} = |k\rangle^{B_2}$. It is clear that ρ^{AC} is a product state and ρ^{BC} is entangled in general in such a case. ■

By the argument in the proof above, we find that, in the state space $\mathcal{H}^{ABC}$, even ρ^{AB} achieves the maximal entanglement between part A and part B (i.e., it is a maximally entangled state according to Ref. [102]), and ρ^{AC} and ρ^{BC} are far from each other (the former one is a product state and the latter one can be entangled). Furthermore, by the arguments above, if $p_k\equiv\frac{1}{r}$, $k = 1, 2, \ldots, r$, then $\rho^{BC} = \mathrm{Tr}_A|\psi\rangle\langle\psi|^{ABC}$ as in Eq. (51) is also an MES according to Ref. [102]. In such a case

$$|\psi\rangle^{BAC} = \sum_{i,k}\frac{1}{mr}(|i\rangle^{B_1}|k\rangle^{B_2})\otimes(|i\rangle^A|k\rangle^C) \tag{55}$$

is a maximally entangled pure state with respect to the cutting $B|AC$. Let $|f_k^{(s)}\rangle^C$ as in Eq. (54). If $\dim H^C\geqslant lr$, we let

$$\left|f_k^{(s)}\right\rangle^C = |k\rangle^{C_1}|s\rangle^{C_2}, \tag{56}$$

for some orthonormal sets $\{|k\rangle^{C_1}: k = 1, \ldots, r\}$ and $\{|s\rangle^{C_2}: s = 1, 2, \ldots, l\}$ in $\mathcal{H}^C$, where

$$\mathcal{H}^{C_1} := \text{span}\{|k\rangle^{C_1} : k = 1, \ldots, r\}$$

and

$$\mathcal{H}^{C_2} = \text{span}\{|s\rangle^{C_2} : s = 1, 2 \ldots, l\}.$$

Then ρ^{B_2C} in Eq. (53) is an MMES according to Ref. [102] whenever $p_k \equiv \frac{1}{r}$. That is, if ρ^{AB} is an MMES in the sense of Ref. [102], it is possible that ρ^{BC} is also an MMES in the sense of Ref. [102]. In fact,

$$\rho^{BAC} = \sum_{s=1}^{l} \frac{1}{l} |\phi_s\rangle\langle\phi_s|^{BAC} \tag{57}$$

with

$$|\phi_s\rangle^{BAC} = \sum_{i,k} \frac{1}{rm} (|i\rangle^{B_1}|k\rangle^{B_2}) \otimes (|i\rangle^{A}|k\rangle^{C_1}|s\rangle^{C_2}) \tag{58}$$

is an MES with respect to the cutting $B|AC$ according to Ref. [102]. Namely, B can maximally entangled with A and C simultaneously.

However, this fact contradicts with the monogamy law of entanglement [19,34,41–61]: entanglement cannot be freely shared among many parties. In particular, if two parties A and B are maximally entangled, then neither of them can share entanglement with a third party C.

It is clear that for both $|\phi\rangle^{ABC}$ in Eq. (50) [or (55)] and ρ^{ABC} in Eq. (52) [or (57)] the disentangling conditions (5) and (18) are valid (we take $E^{(2)} = E_f^{(2)} = E_f$ and $E^{(3)} = E_f^{(3)}$ here). In fact, we have the following.

(1) $E_f^{(2)}(|\psi\rangle^{A|BC}) = E_f^{(2)}(\rho^{AB})$ and $E_f^{(2)}(\rho\rangle^{AC}) = 0$.
(2) $E_f^{(2)}(|\psi\rangle^{B|AC}) = E_f^{(2)}(\rho^{AB}) + E_f^{(2)}(\rho^{BC})$.
(3) $E_f^{(2)}(|\psi\rangle^{C|AB}) = E_f^{(2)}(\rho^{BC})$ and $E_f^{(2)}(\rho^{AC}) = 0$.
(4) $E_f^{(3)}(|\psi\rangle^{ABC}) = E_f^{(2)}(\rho^{AB}) + E_f^{(2)}(\rho^{BC})$.
(5) $E_f^{(2)}(\rho^{A|BC}) = E_f^{(2)}(\rho^{AB})$ and $E_f^{(2)}(\rho\rangle^{AC}) = 0$.
(6) $E_f^{(2)}(\rho^{B|AC}) = E_f^{(2)}(\rho^{AB}) + E_f^{(2)}(\rho^{BC})$.
(7) $E_f^{(2)}(\rho^{C|AB}) = E_f^{(2)}(\rho^{BC})$ and $E_f^{(2)}(\rho^{AC}) = 0$.
(8) $E_f^{(3)}(\rho^{ABC}) = E_f^{(2)}(\rho^{AB}) + E_f^{(2)}(\rho^{BC})$.

That is, the above examples in Eqs. (55) and (57) indicate that, while part B and part A are maximally entangled, part B and part C can also be maximally entangled, which is not consistent with the monogamy law of entanglement on one hand and indicates that they satisfy the monogamy inequality on the other hand. So, why does this incompatible phenomenon which seems a contradiction occur? Is the monogamy law not true, or is the maximally entangled state not a "genuine" MES? We show below that the maximally entangled state should be defined by its tripartite extension with the unified entanglement measure and the monogamy of entanglement should be characterized by the complete monogamy relation under the unified entanglement measure. That is, the multipartite entanglement and the monogamy of entanglement cannot be revealed completely by means of the bipartite measures.

C. When is a state an MES?

We remark here that both the monogamy relation with respect to the bipartite measure as in Eq. (5) and the complete monogamy relation as in Eq. (18) support the monogamy law of entanglement. Although the states in Eqs. (55) and (57) are MMESs according to Ref. [102], we have

$$E_f^{(3)}(\rho^{ABC}) = \ln(mr) > E_f^{(2)}(\rho^{AB}) = \ln m. \tag{59}$$

That is, all these monogamy relations support the monogamy law of entanglement. In other words, the monogamy relations above are compatible with the monogamy law. We thus believe that the monogamy law is true.

On the other hand, for pure state $|\psi\rangle^{AB} \in \mathcal{S}^{AB}$, if it is maximally entangled, then any tripartite extension $|\psi\rangle^{ABC}$ (i.e., $|\psi\rangle^{AB} = \text{Tr}_C|\psi\rangle\langle\psi|^{ABC}$) must admit the form of $|\psi\rangle^{ABC} = |\psi\rangle^{AB}|\eta\rangle^C$, that is, both A and B cannot be entangled with C whenever A and B are maximally entangled. And in such a case we have $E^{(2)}(|\psi\rangle^{AB}) = E^{(3)}(|\psi\rangle^{ABC})$ for $E^{(2,3)} = E_f^{(2,3)}$. That is, a maximal entanglement does not depend on whether a third part is added; a maximal amount of entanglement remains in any extended system. Namely, for the maximally entangled state, the maximal entanglement cannot increase when we add a new part. Therefore, we give the following definition.

Definition 3. Let ρ^{AB} be a state in $\mathcal{S}^{AB}$ with $\dim \mathcal{H}^A = m \leqslant \dim \mathcal{H}^B$. Then ρ^{AB} is an MES if and only if (i)

$$E_f^{(2)}(\rho^{AB}) = \ln m \tag{60}$$

and (ii) for any extension ρ^{ABC} of ρ^{AB} (i.e., $\rho^{AB} = \text{Tr}_C\rho^{ABC}$) we have

$$E_f^{(3)}(\rho^{ABC}) = E_f^{(2)}(\rho^{AB}). \tag{61}$$

By this definition, the states in Eqs. (55) and (57) are not MESs since $E_f^{(3)}(\rho^{ABC}) > E_f^{(2)}(\rho^{AB})$. Note that this definition of MESs is compatible with the monogamy law and makes the concept of MESs more clear: if ρ^{AB} is an MES, then by the monogamy of $E_f^{(3)}$ we immediately obtain that both ρ^{AC} and ρ^{BC} are separable. This also indicates that the complete monogamy relation can reflect the monogamy law more effectively. From Theorem 7, we obtain our main result.

Theorem 8. There is no MMES in any bipartite quantum system.

In fact, we can also show that there is no multipartite MMES since any extension of MMES would increase entanglement from the new part. Note that the states in Eqs. (55) and (57) are really maximal to some extent; we thus propose the following definition.

Definition 4. Let $\dim \mathcal{H}^{ABC}$ be a tripartite state space with $\dim \mathcal{H}^A = m$ and $\dim \mathcal{H}^B = n \geqslant 2m$. If $\rho^{AB} \in \mathcal{S}^{AB}$ admits the form of Eq. (47), we call it an MMES up to part A. If $p_k \equiv \frac{1}{r}$ in Eq. (47) additionally, then ρ^{AB} is an MMES up to part B.

That is, the definition of the MMES in [102] is in fact an MMES up to part A with the assumption that $\dim \mathcal{H}^B \geqslant 2 \dim \mathcal{H}^A$. It is clear that ρ^{B_2C} in Eq. (53) with $|f_k^{(s)}\rangle^C$ as in Eq. (56) is an MMES up to part B_2 whenever $p_k \equiv \frac{1}{r}$, and if $q_s \equiv \frac{1}{l}$ additionally then ρ^{B_2C} is an MMES up to part C. We can easily check that, if ρ^{AB} is an MMES up to part A, then $\rho^A = \frac{1}{m}I^A$, and if ρ^{AB} is an MMES up to part B, then $\rho^A=\frac{1}{m}I^A$ and $\rho^B=\frac{1}{mr}I^{B_1B_2}$ for some subspace $\mathcal{H}^{B_1B_2}$ of $\mathcal{H}^B$. In addition, we can conclude that the maximally entangled state must reach the maximal entanglement for a well-defined entanglement measure (such as entanglement of formation, concurrence, and negativity) but there do exist states that are not genuine maximally entangled states (e.g., the MMES up to part A) that also achieve the maximal amount of entanglement. Namely, the MMES up to one subsystem is an MES mathematically but not physically.

VII. CONCLUSION AND DISCUSSION

We established a "fine grained" framework for defining a complete MEM and proposed the associated complete monogamy formula. In our framework, together with the complete monogamy formula, we can explore multipartite entanglement more efficiently. We not only can investigate the distribution of entanglement in more detail than the previous monogamy relation but also can verify whether the previous bipartite measures of entanglement are "good" measures. By justification, we found that EoF, concurrence, tangle, Tsallis q entropy of entanglement, and squashed entanglement are better than Rényi α entropy of entanglement, negativity, and relative entropy of entanglement. In addition, we improved the definition of maximally entangled states and showed that for any bipartite quantum system the only maximally entangled state is the maximally entangled pure state. We can conclude that the property of the bipartite state is more clear when it is regarded as a reduced state of its extension, namely, the quantum system is always not closed, and it should be studied in a bigger picture. The most tripartite measures by now support both the monogamy law of entanglement and the additional protocols of multipartite entanglement measures and the associated complete monogamy relation we proposed. Especially, the maximally entangled state is highly consistent with our scenario. We believe that our results present tools and insights into investigating multipartite entanglement and other multipartite correlation beyond entanglement.

As a byproduct, interestingly, we found a class of states that are additive with respect to the entanglement of formation, which would shed light on the problem of the classical communication capacity of the quantum channel [86,115].

However, we still do not know (i) whether the tripartite conditional entanglement of mutual information is completely monogamous and tightly complete monogamous, (ii) whether the tripartite squashed entanglement is tightly completely monogamous, and (iii) whether the tripartite relative entropy of entanglement and the tripartite geometric measure are complete multipartite entanglement measures (also see Table I). We conjecture that the answers to these questions are affirmative.

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APPENDIX: PROOF OF LEMMA 2

By modifying the proof of Proposition 4.5 in Ref. [85], we can get the following lemma, which is necessary in order to prove $C^{(3)}$ and $\tau^{(3)}$ are tightly monogamous. In the proof of Lemma 1, we replace the notation ρ^X and I^X by ρ_X and I_X, respectively, for simplicity of notations.

Lemma 2. For any bipartite state $\rho_{AB}\in\mathcal{S}^{AB}$, we have

$$1+\max\left\{\mathrm{Tr}\left(\rho_A^2\right),\mathrm{Tr}\left(\rho_B^2\right)\right\}\mathrm{Tr}\left(\rho_{AB}^2\right)\geqslant\mathrm{Tr}\left(\rho_A^2\right)+\mathrm{Tr}\left(\rho_B^2\right),\tag{A1}$$

where $\rho_{A,B}=\mathrm{Tr}_{B,A}\rho_{AB}$. Moreover, $1+\mathrm{Tr}(\rho_{AB}^2)=\mathrm{Tr}(\rho_A^2)+\mathrm{Tr}(\rho_B^2)$ if and only if $\rho_{AB}=\rho_A\otimes\rho_B$ with $\min\{\mathrm{rank}(\rho_A),\mathrm{rank}(\rho_B)\}=1$.

Proof. Without loss of generality, we assume that $\mathrm{Tr}(\rho_B^2)\geqslant\mathrm{Tr}(\rho_A^2)$. Let $\mathrm{spec}(\rho_A)=\{x_1,x_2,\ldots\}$ and $\mathrm{spec}(\rho_B)=\{y_1,y_2,\ldots\}$. For any real number κ, we see that

$$\begin{aligned}&\mathrm{Tr}\left(\rho_A^2\right)+\mathrm{Tr}\left(\rho_B^2\right)\\&\quad=\mathrm{Tr}[(\rho_A\otimes I_B+I_A\otimes\rho_B)\rho_{AB}]\\&\quad=\kappa+\mathrm{Tr}[(\rho_A\otimes I_B+I_A\otimes\rho_B-\kappa I_{AB})\rho_{AB}]\\&\quad\leqslant\kappa+\mathrm{Tr}[(\rho_A\otimes I_B+I_A\otimes\rho_B-\kappa I_{AB})_+\rho_{AB}],\end{aligned}$$

i.e.,

$$\mathrm{Tr}\left(\rho_A^2\right)+\mathrm{Tr}\left(\rho_B^2\right)\leqslant\kappa+\mathrm{Tr}(Z_\kappa\rho_{AB}),$$

where $Z_k=(\rho_A\otimes I_B+I_A\otimes\rho_B-\kappa I_{AB})_+$, the positive part of the operator $\rho_A\otimes I_B+I_A\otimes\rho_B-\kappa I_{AB}$. Furthermore, we have

$$\mathrm{Tr}\left(\rho_A^2\right)+\mathrm{Tr}\left(\rho_B^2\right)\leqslant\kappa+\mathrm{Tr}\left(Z_\kappa^2\right)\mathrm{Tr}\left(\rho_{AB}^2\right).$$

It suffices to show

$$\min\left\{\kappa+\mathrm{Tr}\left(Z_\kappa^2\right)\mathrm{Tr}\left(\rho_{AB}^2\right)\right\}\leqslant1+\mathrm{Tr}\left(\rho_{AB}^2\right).\tag{A2}$$

Consider now the function

$$f_\kappa(a)=\sum_j(y_j+a-\kappa)_+^2=\|(\mathbf{y}+a-\kappa)_+\|_2^2,$$

where $\mathbf{y}+a-\kappa:=(y_1+a-\kappa,y_2+a-\kappa,\ldots)$. This function is convex and

$$f_\kappa(\kappa)=\|\mathbf{y}\|_2^2=\mathrm{Tr}\left(\rho_B^2\right)\leqslant1.$$

If we assume that $\kappa\geqslant\max_j y_j=\|\mathbf{y}\|=\|\rho_B\|_\infty$, then

$$f_\kappa(0)=0.$$

Hence, under this assumption, we conclude that the convex function is below the straight line through (0,0), $(\kappa,\mathrm{Tr}(\rho_B^2))$, the equation of which is given by $y=\frac{\mathrm{Tr}(\rho_B^2)}{\kappa}x$. It follows from the above discussion that

$$f_\kappa(a)\leqslant\frac{\mathrm{Tr}\left(\rho_B^2\right)}{\kappa}a,\quad a\in[0,\kappa].$$

Thus, if $\kappa \geqslant \|\rho_B\|_\infty$, apparently all $x_i \in [0, \kappa]$; then

$$\mathrm{Tr}\big(Z_\kappa^2\big) = \|Z_\kappa\|_2^2 = \sum_{i,j}^{d}(x_i + y_j - \kappa)_+^2 = \sum_i f_\kappa(x_i)$$

$$\leqslant \sum_i \frac{\mathrm{Tr}\big(\rho_B^2\big)}{\kappa} x_i = \frac{1}{\kappa}\mathrm{Tr}\big(\rho_B^2\big).$$

Therefore, for any $\kappa \geqslant \max\{\|\rho_A\|_\infty, \|\rho_B\|_\infty\}$, we have

$$\mathrm{Tr}\big(\rho_A^2\big) + \mathrm{Tr}\big(\rho_B^2\big) \leqslant \kappa + \frac{1}{\kappa}\mathrm{Tr}\big(\rho_B^2\big)\mathrm{Tr}\big(\rho_{AB}^2\big).$$

Next we consider the function

$$g(\kappa) = \kappa + \frac{1}{\kappa}\mathrm{Tr}\big(\rho_B^2\big)\mathrm{Tr}\big(\rho_{AB}^2\big),$$

where

$$\kappa \geqslant \max\{\|\rho_A\|_\infty, \|\rho_B\|_\infty\} := \kappa_0.$$

It is easy to see that g is strictly convex and it has a global minimum at

$$\kappa_{\min} := \|\rho_B\|_2\|\rho_{AB}\|_2$$

with a minimum value $g_{\min} := 2\kappa_{\min}$. Clearly, g is strictly decreasing in the interval $(0, \kappa_{\min}]$ and strictly increasing in $[\kappa_{\min}, 1]$.

(i) If $\kappa_{\min} < \kappa_0$, then

$$\min\{g(\kappa) : \kappa \geqslant \kappa_0\} = \kappa_0 + \frac{1}{\kappa_0}\kappa_{\min}^2.$$

(ii) If $\kappa_{\min} \geqslant \kappa_0$, then

$$\min\{g(\kappa) : \kappa \geqslant \kappa_0\} = 2\kappa_{\min}.$$

In summary, we get that

$$\min\{g(\kappa) : \kappa \geqslant \kappa_0\} = \begin{cases} \kappa_0 + \frac{1}{\kappa_0}\kappa_{\min}^2, & \text{if } \kappa_{\min} < \kappa_0, \\ 2\kappa_{\min}, & \text{if } \kappa_{\min} \geqslant \kappa_0. \end{cases}$$

Therefore, since $\kappa_0 \leqslant 1$, we finally get that

$$\mathrm{Tr}\big(\rho_A^2\big) + \mathrm{Tr}\big(\rho_B^2\big) \leqslant \min\{g(\kappa) : \kappa \geqslant \kappa_0\} \leqslant 1 + \kappa_{\min}^2$$

$$\leqslant 1 + \mathrm{Tr}\big(\rho_{AB}^2\big).$$

If $\mathrm{Tr}(\rho_A^2) + \mathrm{Tr}(\rho_B^2) = 1 + \mathrm{Tr}(\rho_{AB}^2)$, then

$$1 + \mathrm{Tr}\big(\rho_B^2\big)\mathrm{Tr}\big(\rho_{AB}^2\big) = 1 + \mathrm{Tr}\big(\rho_{AB}^2\big).$$

Thus ρ_B is a pure state. Similarly, by the symmetry of A and B, we can also conclude that, if $\mathrm{Tr}(\rho_A^2) \geqslant \mathrm{Tr}(\rho_B^2)$, then

$$\mathrm{Tr}\big(\rho_A^2\big) + \mathrm{Tr}\big(\rho_B^2\big) \leqslant 1 + \mathrm{Tr}\big(\rho_A^2\big)\mathrm{Tr}\big(\rho_{AB}^2\big).$$

In such a case, we see that

$$1 + \mathrm{Tr}\big(\rho_A^2\big)\mathrm{Tr}\big(\rho_{AB}^2\big) = 1 + \mathrm{Tr}\big(\rho_{AB}^2\big) \tag{A3}$$

implies ρ_A is pure. ∎

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