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Multipartite entanglement measure and complete monogamy relation

by

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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 literatures are not complete. We establish here a strict framework for defining multipartite entanglement measure (MEM): apart from the postulates of bipartite measure [i.e., vanishing on separable and nonincreasing under local operations and classical communication (LOCC)], a genuine 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 genuine MEM (an MEM is called a genuine 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, respectively. We show that (i) the extensions of EoF, concurrence, tangle, and Tsallis q-entropy of entanglement are genuine MEMs, (ii) multipartite extensions of Rényi α-entropy of entanglement, negativity and the convex-roof extension of negativity are unified MEMs but not genuine 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 by-product, we find out a class of states that satisfy the additivity of EoF. We also find a class of tripartite states that one part can maximally entangled with other two parts simultaneously according to the definition of maximally entangled mixed state (MEMS) in [Quantum Inf. Comput. 12, 0063 (2012)]. Consequently, we improve the definition of maximally entangled state (MES) and prove that there is no MEMS and 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 [3, 4], concurrence [5–7], tangle [8], relative entropy of entanglement [9, 10], negativity [11, 12], geometric measure [13–15], squashed entanglement [16, 17], the conditional entanglement of mutual information [18], three-tangle [19], the generalizations of concurrence [20, 21], and the α-entanglement entropy [22], etc. However, apart from the α-entanglement entropy, all other measures are either only defined on the bipartite case or just discussed with only the axioms of the bipartite case.

One of the most important issues closely related to entanglement measure is the monogamy relation of entanglement [23], 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 [24–26] but also in other area of physics, such as no-signaling theories [34], condensed matter physics [27–29], statistical mechanics [24], and even black-hole physics [30]. Particularly, it is the crucial property that guarantees quantum key distribution secure [23, 31]. 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, 32–53] 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 [32, Theorem 6] and squashed entanglement [32, Theorem 8] and all the other measures that defined by the convex-roof extension are monogamous [52]. But all these monogamy relations are discussed via the bipartite measures of entanglement: only the relation between $A|BC$, AB and AC are revealed, the global correlation in ABC and the correlation contained in part BC is 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 CKW is not "complete". We thus

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need to explore a complete monogamy relation which can exhibit the entanglement between ABC, AB, AC and BC in extenso.

The phenomenon becomes much more complex when moving from the bipartite case to the multipartite case [22, 54–56]. 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 MEM and bipartite ones, which requires a "unified" way (i.e., the unification condition) to define entanglement measures. In [22], Szalay developed the two kinds of indicator functions for characterizing mulitpartite entanglement based on the complex lattice-theoretic structure of partial separability classification for multipartite states. But the second kind in fact can not quantify entanglement effectively and the unification condition was not considered as a necessary requirement of MEM. The purpose of this paper is to give, concisely, "richer" postulates in defining a genuine 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 bipartite entanglement measure and the associated monogamy relation in Sec. II, and explore the additional postulates for multipartite entanglement measures in Sec. III. Sec. 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 tripartite case, and discuss their complete monogamy property. Particularly, we find a class of states that are additive under the tripartite entanglement of formation. Sec. VI mainly discusses what is the maximally entangled state. We give a new definition of maximally entangled state by means of its extension. Finally, in Sec. VII, we summarize our main findings and conclusions.

II. REVIEWING OF THE BIPARTITE ENTANGLEMENT MEASURE

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

- (E-1) $E(\rho) = 0$ if ρ is separable;
- (E-2) E cannot increase under LOCC, i.e., $E(\Phi(\rho)) \leqslant E(\rho)$ for any LOCC Φ [(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 can not 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 $E(\sigma') \leq E(\rho)$.

Almost all measures of entanglement studied in literature (although not all [58]) 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 $E(\sigma') \leq E(\rho)$ becomes

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

That is, LOCC can not increase entanglement on average. An entanglement measure E is said to be an entanglement monotone [57] 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 [57, Theorem 2] showed that E_F, defined as Eqs. (2) and (3), is an entanglement monotone iff 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, ρ_2, and any $\lambda \in [0, 1]$. Very recently, Guo and Gour [52] 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

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

we have that $E_F(\rho^{AC})=0$, or equivalently (for continuous measures [51]), there exists some $\alpha>0$ such that

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

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

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

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

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

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

for mixed state, where the minimum is taken over all pure-state decomposition $\{p_i,|\psi_i\rangle\}$ 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 subscription 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 mixed state, they are defined by the convex-roof extension as Eq. (2). The negativity [11, 12] is defined by

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

where T_x denotes the transpose with respect to the subsystem X, $\|\cdot\|_{\mathrm{Tr}}$ 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

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

where p_js are the eigenvalues of ρ is strictly concave if $g''(p)<0$ for all $0<p<1$ [52]. This includes the quantum Tsallis q-entropy [59–61] T_q with $q>0$ and the Rényi α-entropy [62–64] 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 literatures so far, such as E_f, C, τ, N_F, Tsallis q-entropy of entanglement ($q>0$) and Rényi $\alpha-$ entropy of entanglement ($0<\alpha<1$), etc., are monogamous [52].

III. POSTULATES FOR MULTIPARTITE ENTANGLEMENT MEASURE

A. Multipartite entanglement monotone

We now turn to 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 literatures [20, 21, 54] if it satisfies:

- **(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

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

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 bipartite entanglement monotone proposed in Ref. [57], we give at first a necessary-sufficient criterion of tripartite entanglement monotone (TEM):

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

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

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

$$h^{(3)}\left(\rho^A\otimes\rho^B\otimes\rho^C\right) \geqslant \sum_k p_k h^{(3)}\left(\sigma_k^A\otimes\sigma_k^B\otimes\sigma_k^C\right) \tag{12}$$

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 iff $h^{(3)}$ is LOCC-concave. Apparently, $E^{(3)}(\rho)=h^{(3)}\left(\rho^A\otimes\rho^B\otimes\rho^C\right)$ and $E^{(3)}(\sigma_k)=h^{(3)}\left(\sigma_k^A\otimes\sigma_k^B\otimes\sigma_k^C\right)$ 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

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

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 show 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 achieve that

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

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 ii) above reduces to Eq. (4) for bipartite case. That is, for bipartite case, concavity is equivalent to LOCC-concavity, but it is unknown whether it also true for tripartite case.

B. Unification condition for 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 couple 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 bi-separable 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

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

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 in 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 be instead by $h(\rho^A)$ since any bipartite pure state has Schmidt decomposition, which guarantees that the eigenvalues of ρ^A coincide with that 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 multiparite case, the unification condition requires 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 $X \neq A$, $X, Y, Z \in \{A, B, C\}$]. 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 (E3). Hereafter, we always assume that $E^{(3)}$ is a unified measure unless otherwise specified.

We need note here that, although the analytic formulas for $E^{(2)}$ and $E^{(3)}$ can not be uniquely determined each other, 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 multipartite entanglement measure

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

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

For any given $\rho^{ABC} \in \mathcal{S}^{ABC}$, $E^{(3)}(\rho^{ABC})$ extract 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 $|\psi\rangle^{ABC}$ that 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 $\mathcal{H}^B$ [50–52]. 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 in Sec. VI). We thus need additionally the following *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 nonnegative function $E^{(3)}$, as a "genuine" tripartite entanglement measure, not only need obey the conditions (E1)-(E2) but also need satisfy the conditions (E3) and (E4). One can easily check that the triparite squashed entanglement and the tripartite conditional entanglement of mutual information are genuine entanglement monotones [i.e., they also satisfy (E3)-(E4)], but the k-ME concurrence [20] violates (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).

Remark 2. Postulate (E4) is in consistence with the multipartite monotonic indicator functions of the first kind [see Eq. (87) in Ref. [22]]. From the arguments in this paper, the multipartite monotonic indicator functions of the second kind in Ref. [22] is meaningless for defining MEM.

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

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

where

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

$I(A:B|E)$ is 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 ${\rm Tr}_E(\rho^{ABCE}) = \rho^{ABC}$. In Ref. [17], the tripartite squashed entanglement, denoted by $E^q_{\rm sq}$, is defined by $E^q_{\rm sq}(\rho^{ABC}) := \inf I(A:B:C|E)$. Observe that

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

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

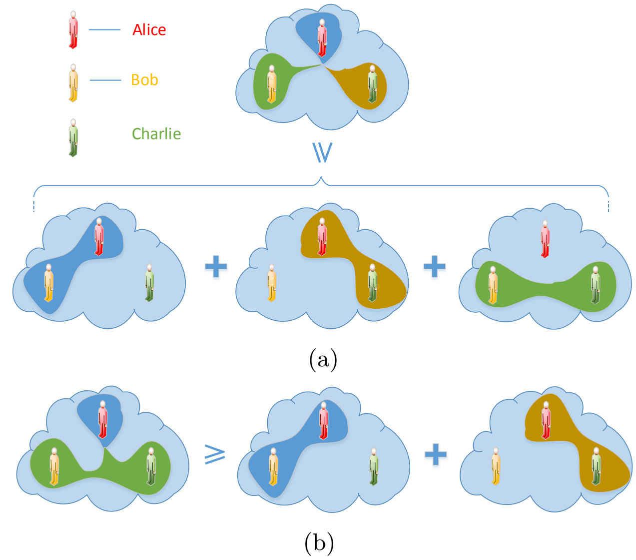

FIG. 1: (color online). Schematic picture of the monogamy relation under (a) the unified tripartite entanglement measure and (b) the bipartite entanglement measure, respectively.

IV. COMPLETE MONOGAMY RELATION FOR MULTIPARTITE MEASURE

A. Complete monogamy relation for unified MEM

Since there is no bipartite cut among the subsystems when we consider the genuine MEM, we thus, following the spirit of the bipartite case proposed in [51], 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 subsystem 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 can not be entangled with part C additionally. While the monogamy relation up to bipartite measures is not "complete" (we can call it "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 is *completely* *monogamous*. The difference between these two kinds of monogamy relations, i.e., Eq. (6) and Eq. (19) (see below) [or equivalently, Eq. (5) and Eq. (18)], is illustrated in Fig. 1. By the proof of Theorem 1 in [51], the following theorem is obvious.

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*

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

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

As the monogamy exponent α in Eq. (6) for bipartite measure, we call the smallest possible value for α satisfies Eq. (19) in a given dimension $d = \dim \mathcal{H}^{ABC}$, the *monogamy exponent* associated with a unified measure $E^{(3)}$, and 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 [51]. 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 satisfying 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 Eq. (10). By replacing $E_f(A|BC)$, $E_f(A|B)$ with $E_F^{(3)}$, $E_F^{(2)}$ in Theorem 3 in Ref. [51] respectively, we can conclude that, if $E_F^{(3)}$ is completely monogamous on pure tripartite states in $\mathcal{H}^{ABC}$, then it is also completely monogamous on tripartite mixed states acting on $\mathcal{H}^{ABC}$.

The first disentangling theorem was investigated in Ref. [50] with respect to bipartite negativity. Very recently, Guo and Gour showed in Ref. [51] that, the disentangling theorem is valid for any bipartite entanglement monotone on 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. [51], that the Lemma 3 below is valid.

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

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

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

Theorem 4. *Let $E^{(3)}$ be a unified TEM for which $h^{(2)}$, induced from $h^{(3)}$ as defined in (11), is strictly concave. Then, if ρ^{ABC} is a tripartite state and $E_F^{(3)}(\rho^{ABC}) = E_F^{(2)}(\rho^{AB})$, then*

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

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

$$|\psi\rangle^{ABC} = |\phi\rangle^{AB}|\eta\rangle^{C}. \quad (22)$$

Proof. By Lemma 3, we can derive that if ρ^{ABC} be a pure tripartite state satisfying the disentangling condition (18), then

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

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,

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

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 $\rho_j^{A,B} := \mathrm{Tr}_{B,A}|\psi_j\rangle\langle\psi_j|^{AB}$, we conclude that if Eq. (18) holds then we must have

$$\sum_{j=1}^{n} p_j h^{(2)}(\rho_j^{A} \otimes \rho_j^{B}) = h^{(2)}(\rho^{A} \otimes \rho^{B}).$$

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

$$\rho_j^{A} = \rho^{A}, \ \rho_j^{B} = \rho^{B}, \quad j = 1, ..., n. \quad (23)$$

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

Comparing with Theorem in Ref. [52], we can see that the strict concavity of $h^{(2)}$ for tripartite case is stronger than that of bipartite case, which leads to that the sate satisfying the tripartite disentangling condition just 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 m-partite case, $m \geqslant 4$, we can easily derive the following disentangling conditions with the same spirit as that of 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

$$E^{(4)}(\rho^{ABCD}) = E^{(2)}(\rho^{AB}) \tag{24}$$

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

$$E^{(4)}(\rho^{ABCD}) = E^{(3)}(\rho^{ABC}) \tag{25}$$

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 complement of the Theorem in Ref. [52].

Theorem 5. *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,*

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

and in turn iff

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

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 $|\psi\rangle^{AB_1} \in \mathcal{H}^{AB_1}$, $|\psi\rangle^{B_1C} \in \mathcal{H}^{B_1C}$; 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 $\rho^A = \sum_i \left(\lambda_i^A\right)^2 |\psi_i\rangle\langle\psi_i|^A$ and $\mathrm{rank}(\rho^C) = n$ with spectrum decomposition $\rho^C = \sum_j \left(\lambda_j^C\right)^2 |\psi_j\rangle\langle\psi_j|^C$. 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 $|\psi\rangle^{B_2C} = \sum_j \lambda_j^C |y_j\rangle^{B_2} |\psi_i\rangle^C$up to local unitary operator U^B. It is now clear that $E(\rho^{AB}) = E(|\psi\rangle^{A|BC})$.

Together with Theorem in [52], we get

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

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 GHZ state, then ρ^{AC} is separable but $\rho^{AC} \neq \rho^A \otimes \rho^C$ and $E^{(2)}(\rho^{AB}) = 0 < E^{(2)}(|\psi\rangle^{A|BC})$. □

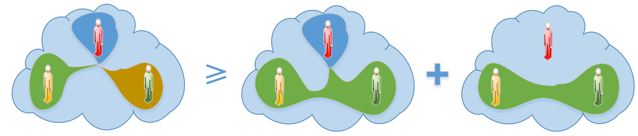

FIG. 2: (color online). Schematic picture of the tight monogamy relation.

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

Proposition 6. *$E_{\mathrm{sq}}^{(3)}$ is completely monogamous, i.e.,*

$$E_{\mathrm{sq}}^{(3)}\left(\rho^{ABC}\right) \geqslant E_{\mathrm{sq}}\left(\rho^{AB}\right) + E_{\mathrm{sq}}\left(\rho^{AC}\right) + E_{\mathrm{sq}}\left(\rho^{BC}\right) \tag{26}$$

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

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

The proof is completed. □

Moreover, if there exists a optimal extension ρ^{ABCE} such that $E_{\mathrm{sq}}^{(3)}(\rho^{ABC}) = \frac{1}{2}I(A:B:C|E)$, then ρ^{ABC} the tripartite disentangling condition (18) with respect to $E_{\mathrm{sq}}^{(3)}$ iff ρ^{ABEC} is a Markov state [65], 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 genuine MEM

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

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

$$E^{(3)}(\rho^{ABC}) = E^{(2)}(\rho^{A|BC}) \tag{27}$$

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

As one may expect, we show below that, the tightly complete monogamy Eq. (27) is stronger than the complete monogamy relation Eq. (18) in general.

Theorem 7. *Let $E^{(3)}$ be a genuine 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

$$E^{(2)}(\rho^{AB}) = E^{(2)}(|\psi\rangle^{A|BC}) = E^{(3)}(|\psi\rangle^{ABC}) \tag{28}$$

since $E^{(2)}(\rho^{AB}) \leqslant E^{(2)}(\rho^{A|BC}) \leqslant E^{(3)}(\rho^{ABC})$ holds for any state ρ^{ABC}. It follows from the assumption that ρ^{BC} is separable. Together with Theorem 5, we can conclude that

$$|\psi\rangle^{ABC} = |\psi\rangle^{AB}|\psi\rangle^{C}. \tag{29}$$

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

By Definition 2, the following can be easily checked.

Theorem 8. *Let $E_F^{(3)}$, defined as in Eq. (10), be a unified TEM for which h, as defined in (11), satisfies (E4′) with the equality holds iff $\rho^{BC} = \rho^B \otimes \rho^C$. Then $E_F^{(3)}$ is tightly completely monogamous.*

V. EXTENDING BIPARTITE MEASURES TO GENUINE MULTIPARTITE MEASURES

A. Tripartite extension of bipartite measures

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

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

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

$$\begin{aligned} E^{(3)}(|\psi\rangle) &:= \frac{1}{2}\left[S\left(|\psi\rangle\langle\psi|\|\rho^A \otimes \rho^B \otimes \rho^C\right)\right] \\ &= \frac{1}{2}\left[S(\rho^A) + S(\rho^B) + S(\rho^C)\right] \end{aligned} \tag{30}$$

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

$$E_f^{(3)}\left(\rho^{ABC}\right) = \min_{\{p_i,|\psi_i\rangle\}} \sum_i p_i E^{(3)}(|\psi_i\rangle) \tag{31}$$

for mixed state $\rho^{ABC} \in \mathcal{S}^{ABC}$. $E_f^{(3)}$ coincides with the α-entanglement entropy defined in Ref. [22].

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

$$E^{(3-2)}(|\psi\rangle) := \frac{1}{2}\min_{\sigma\in\mathcal{P}_3^2(|\psi\rangle)} S\left(|\psi\rangle\langle\psi|\|\sigma\right). \tag{32}$$

For any mixed state $\rho \in \mathcal{S}^{ABC}$, the entanglement 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 by $E_f^{(3)}$ throughout this paper. The notation $E_F^{(m)}$, $E_F^{(m-k)}$ with capital F in the subscription denotes 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

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

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

$$\begin{aligned} \tau^{(3)}(|\psi\rangle) &= 3 - \mathrm{Tr}\left(\rho^A\right)^2 - \mathrm{Tr}\left(\rho^B\right)^2 - \mathrm{Tr}\left(\rho^C\right)^2, && (33) \\ C^{(3)}(|\psi\rangle) &= \sqrt{\tau^{(3)}(|\psi\rangle)}, && (34) \\ N^{(3)}(|\psi\rangle) &= \mathrm{Tr}^2\sqrt{\rho^A} + \mathrm{Tr}^2\sqrt{\rho^B} + \mathrm{Tr}^2\sqrt{\rho^C} - 3 && (35) \end{aligned}$$

for pure states and define by the convex-roof extension 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, respectively):

$$\begin{aligned} \tau^{(3)}\left(\rho^{ABC}\right) &= \min_{\{p_i,|\psi_i\rangle\}} \sum_i p_i \tau^{(3)}(|\psi_i\rangle\langle\psi_i|), \\ C^{(3)}\left(\rho^{ABC}\right) &= \min_{\{p_i,|\psi_i\rangle\}} \sum_i p_i C^{(3)}(|\psi_i\rangle\langle\psi_i|), \\ N_F^{(3)}(\rho^{ABC}) &= \min_{\{p_i,|\psi_i\rangle\}} \sum_i p_i N^{(3)}\left(|\psi_i\rangle\langle\psi_i|\right), \end{aligned}$$

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

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

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

$$N^{(3)}(\rho) = \|\rho^{T_a}\|_{\mathrm{Tr}} + \|\rho^{T_b}\|_{\mathrm{Tr}} + \|\rho^{T_c}\|_{\mathrm{Tr}} - 3 \tag{36}$$

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

$$\tau'^{(3)}(|\psi\rangle^{ABC}) = 2\left[1 - \sqrt{\mathrm{Tr}\left(\rho^A\right)^2}\sqrt{\mathrm{Tr}\left(\rho^B\right)^2}\sqrt{\mathrm{Tr}\left(\rho^C\right)^2}\right] \tag{37}$$

TABLE I: Comparing 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, 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 $E_r^{(3)}$, tripartite geometric measure of entanglement $E_G^{(3)}$ and the three-tangle τ_{ABC}. M denotes $E^{(2)}$ is monogamous, CM denotes $E^{(3)}$ is completely monogamous and TCM denotes $E^{(3)}$ is tightly completely monogamous in the following.

$E^{(3)}$	$E^{(3)}$ 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
$E_f^{(3)}$	$\frac12 S(\rho^A\otimes\rho^B\otimes\rho^C)$	$\frac12 S(\rho^A\otimes\rho^B)$	✓	✓	✓ [52]	✓	✓
$C^{(3)}$	$[3-\mathrm{Tr}\left(\rho^A\right)^2-\mathrm{Tr}\left(\rho^B\right)^2-\mathrm{Tr}\left(\rho^C\right)^2]^{\frac12}$	$[2-\mathrm{Tr}\left(\rho^A\right)^2-\mathrm{Tr}\left(\rho^B\right)^2]^{\frac12}$	✓	✓	✓ [52]	✓	✓
$\tau^{(3)}$	$3-\mathrm{Tr}\left(\rho^A\right)^2-\mathrm{Tr}\left(\rho^B\right)^2-\mathrm{Tr}\left(\rho^C\right)^2$	$2-\mathrm{Tr}\left(\rho^A\right)^2-\mathrm{Tr}\left(\rho^B\right)^2$	✓	✓	✓ [52]	✓	✓
$T_q^{(3)}$	$\frac12[T_q(\rho^A)+T_q(\rho^B)+T_q(\rho^C)]$	$\frac12[T_q(\rho^A)+T_q(\rho^B)]$	✓	✓	✓ [52]	✓	✓
$R_\alpha^{(3)}$	$\frac12 R_\alpha(\rho^A\otimes\rho^B\otimes\rho^C)$	$\frac12 R_\alpha(\rho^A\otimes\rho^B)$	✓	×	✓ [52]	✓	×
$N_F^{(3)}$	$\mathrm{Tr}^2\sqrt{\rho^A}+\mathrm{Tr}^2\sqrt{\rho^B}+\mathrm{Tr}^2\sqrt{\rho^C}-3$	$\mathrm{Tr}^2\sqrt{\rho^A}+\mathrm{Tr}^2\sqrt{\rho^B}-2$	✓	×	✓ [52]	✓	×
$N^{(3)}$	$\Vert\rho^{T_a}\Vert_{\rm Tr}+\Vert\rho^{T_b}\Vert_{\rm Tr}+\Vert\rho^{T_c}\Vert_{\rm Tr}-3$	$\Vert\rho^{T_a}\Vert_{\rm Tr}+\Vert\rho^{T_b}\Vert_{\rm Tr}-2$	✓	×	?	✓	×
$E_{\rm sq}^{(3)}$ [17]	$\frac12\inf I(A:B:C\vert E)$	$\frac12\inf I(A:B\vert E)$	✓	✓	✓ [32]	✓	?
$E_I^{(3)}$ [18]	$\frac12\inf[I(AA':BB':CC')-I(A':B':C')]$	$\frac12\inf[I(AA':BB')-I(A':B')]$	✓	✓	?	?	?
$E_r^{(3)}$ [9]	$\inf_\sigma S(\rho^{ABC}\Vert\sigma_{sep}^{ABC})$	$\inf_\sigma S(\rho^{AB}\Vert\sigma_{sep}^{AB})$	✓	?	?	?	?
$E_G^{(3)}$ [15]	$1-\sup_\phi\vert\langle\psi\vert\phi\rangle^{ABC}\vert^2$	$1-\sup_\phi\vert\langle\psi\vert\phi\rangle^{AB}\vert^2$	✓	?	?	?	?
$\tau_{ABC}^{(3)}$ [19]	$C_{A\vert BC}^2-C_{AB}^2-C_{AC}^2$	×	×	×	–	–	–

for tripartite system. $\tau'^{(3)}$ does not obey (E4): It is easy to see that, the two-qubit state σ^{BC} with spectra $\{87/128, 37/128, 1/32, 0\}$ as Eq. (40) leads to $\mathrm{Tr}(\sigma^B)^2\mathrm{Tr}(\sigma^C)^2<\mathrm{Tr}(\sigma^{BC})^2$ (the existing of such state is guaranteed by result in [66], also see Eq. (40) below).

Since the Tsallis q-entropy is subadditive iff $q>1$, 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 [61], we can define tripartite Tsallis q-entropy of entanglement by

$$T_q^{(3)}(|\psi\rangle):=\frac12\left[T_q(\rho^A)+T_q(\rho^B)+T_q(\rho^C)\right],\ q>1 \quad (38)$$

for pure state $|\psi\rangle\in\mathcal{H}^{ABC}$, and then define by the convex-roof extension for mixed states. The Rényi entropy is additive [67], i.e.,

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

we thus define tripartite Rényi α-entropy of entanglement by

$$R_\alpha^{(3)}(|\psi\rangle):=\frac12 R_\alpha(\rho^A\otimes\rho^B\otimes\rho^C),\ 0<\alpha<1 \quad (39)$$

for 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

Notice in particular that, if $E_F^{(3)}$ is a TEM defined as in Eqs.(10) and (11), then item (E4) is equivalent to **(E4′)**: $h(\rho^A\otimes\rho^B\otimes\rho^C)\geqslant h(\rho^A\otimes\rho^{BC})$, $\forall\ |\psi\rangle\in\mathcal{H}^{ABC}$. We can show that $E_f^{(3)}$, $\tau^{(3)}$ and $C^{(3)}$ satisfy (E4′), and furthermore, the theorem below is true.

Theorem 9. *$E_f^{(3)}$, $\tau^{(3)}$, $C^{(3)}$, $T_q^{(3)}$, $R_\alpha^{(3)}$, $N_F^{(3)}$ and $N^{(3)}$ are completely monogamous TEMs. $E_f^{(3)}$, $\tau^{(3)}$, $C^{(3)}$, and $T_q^{(3)}$ are genuine TEMs while $R_\alpha^{(3)}$, $N_F^{(3)}$ and $N^{(3)}$ are unified TEMs but not genuine TEMS.*

Proof. The unification condition for all these quantities are clear from definition. The complete monogamy of $E_f^{(3)}$, $\tau^{(3)}$, $C^{(3)}$, $T_q^{(3)}$, $R_\alpha^{(3)}$ and $N_F^{(3)}$ are clear by Theorem 4. For any $\rho^{ABC}\in\mathcal{S}^{ABC}$, if $N^{(3)}(\rho^{ABC})=N^{(2)}(\rho^{AB})$, i.e., $\Vert\rho_{ABC}^{T_a}\Vert_{\rm Tr}+\Vert\rho_{ABC}^{T_b}\Vert_{\rm Tr}+\Vert\rho_{ABC}^{T_c}\Vert_{\rm Tr}-3=\Vert\rho_{AB}^{T_a}\Vert_{\rm Tr}+\Vert\rho_{AB}^{T_b}\Vert_{\rm Tr}-2$, then $\Vert\rho_{ABC}^{T_c}\Vert_{\rm Tr}=1$ which implies that $\rho^{A|BC}$ is a PPT state, and therefore ρ^{AC} and ρ^{BC} are PPT states. 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

$$\begin{aligned} & E^{(3)}(|\psi\rangle^{ABC}) \\ = & \frac12[E^{(2)}(|\psi\rangle^{A|BC})+E^{(2)}(|\psi\rangle^{AB|C})+E^{(2)}(|\psi\rangle^{B|AC})], \end{aligned}$$

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

We now show that $E_f^{(3)}$, $\tau^{(3)}$, $C^{(3)}$ and $T_q^{(3)}$ satisfy (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 [68, Theorem 2]

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

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

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, ρ^B exists if and only if the minimal eigenvalues λ_A, λ_B of the marginal states satisfying the following inequalities [66]:

$$\begin{cases} \min(\lambda_A, \lambda_B) \geqslant \lambda_3 + \lambda_4, \\ \lambda_A + \lambda_B \geqslant \lambda_2 + \lambda_3 + 2\lambda_4, \\ |\lambda_A - \lambda_B| \leqslant \min(\lambda_1 - \lambda_3, \lambda_2 - \lambda_4). \end{cases} \tag{40}$$

Based on this result, we can find counterexamples, which shows that $N_F^{(3)}$ violates (E4′) (then $N^{(3)}$ violates (E4′), either). 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 $N^{(3)}$ violates E4′ for pure states. $R_\alpha^{(3)}$ violates E4′ since the Renyi α-entropy is not subadditive except for $\alpha = 0$ or 1 [69]. □

From the proof of Theorem 9, we can conclude that if $E_F^{(3)}$ satisfies (E4′) with the equality holds iff $\rho^{BC} = \rho^B \otimes \rho^C$ for $|\psi\rangle^{ABC} = |\phi\rangle^{AB_1}|\eta\rangle^{B_2C}$, then it is completely monogamous, but not necessarily tightly completely monogamous as (27).

Proposition 10. *$E_f^{(3)}$, $C^{(3)}$, $\tau^{(3)}$ and $T_q^{(3)}$ are tightly completely monogamous while $R_\alpha^{(3)}$, $N_F^{(3)}$ and $N^{(3)}$ are not tightly completely monogamous.*

Proof. $R_\alpha^{(3)}$, $N_F^{(3)}$ and $N^{(3)}$ are not tightly completely monogamous since they do not satisfy item (E4). 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 8. Observe that

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

since $1 + \mathrm{Tr}(\rho^{BC})^2 \geqslant \mathrm{Tr}(\rho^B)^2 + \mathrm{Tr}(\rho^C)^2$ [68, Theorem 2]. By Proposition 4.5 in Ref. [70], we can get the following result (i.e., Lemma 14, see in the Appendix for detail): 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 [61]

$$T_q(\rho \otimes \sigma) = T_q(\rho) + T_q(\sigma) \tag{41}$$

if and only if either of ρ, σ is pure. By Theorem 8, $C^{(3)}$, $\tau^{(3)}$ and $T_q^{(3)}$ are tightly completely monogamous. □

For $E \in \{E_f^{(3)}, C^{(3)}, \tau^{(3)}, T_q^{(3)}\}$, with some abuse of notations, by Proposition 2, Eq. (27) holds iff

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

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

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

for some $\alpha_2 > 0$ from Theorem 1 in Ref. [51]. Taking $\alpha = \max\{\alpha_1, \alpha_2\}$, we have

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

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 this measure. Recall that, the additivity of the entanglement formation $E_f^{(2)}$ is a long standing open problem which is conjectured to be true [71] and then disproved by Hastings in 2009 [72]. We always expect intuitively that the measure of entanglement should be additive in the sense of [73]

$$E\left(\rho^{AB} \otimes \sigma^{A'B'}\right) = E\left(\rho^{AB}\right) + E\left(\sigma^{A'B'}\right), \tag{42}$$

where $E(\rho^{AB} \otimes \sigma^{A'B'}) := E(\rho^{AB} \otimes \sigma^{A'B'})$ up to the partition $AA'|BB'$. Eq. (42) 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 [74]. In what follows, we present a new class of states such that $E_f^{(2)}$ is additive (and thus for such class of states, we have $E_f^{(2)} = E_c$ [71], E_c denotes the entanglement cost), and present, analogously, a class of states such that $E_f^{(3)}$ is additive.

Theorem 11. *(i) Let $\rho^{AB}\otimes\sigma^{A'B'}$ be a state in $\mathcal{S}^{AA'BB'}$. If there exists a 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*

$$E_f^{(2)}(AB\otimes A'B') = E_f^{(2)}(AB) + E_f^{(2)}(A'B'). \quad (43)$$

(ii) Let $\rho^{ABC}\otimes\sigma^{A'B'C'}$ be a state in $\mathcal{S}^{AA'BB'CC'}$. If there exists a 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

$$E_f^{(3)}(ABC\otimes A'B'C') = E_f^{(3)}(ABC) + E_f^{(3)}(A'B'C'). \quad (44)$$

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 $|\varphi\rangle^{A'B'C'}\in\mathcal{H}^{A'B'C'}$, it is clear since

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

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

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 that satisfying

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

Then

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

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 that satisfying

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

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

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

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

Particularly, if ρ^{AB} or $\sigma^{A'B'}$ (resp. ρ^{ABC} or $\sigma^{A'B'C'}$) is pure, then $\rho^{AB}\otimes\sigma^{A'B'}$ (resp. $\rho^{ABC}\otimes\sigma^{A'B'C'}$) is additive under $E_f^{(3)}$ (resp. $E_f^{(2)}$). Together with the result of Hastings in Ref. [72], we conclude that, the state $\rho^{AB}\otimes\sigma^{A'B'}$ (resp. $\rho^{ABC}\otimes\sigma^{A'B'C'}$) that violates the additivity (42) definitely have a optimal pure-state decomposition in which some pure states are not product state up to the partition $AB|A'B'$ (resp. $ABC|A'B'C'$). Our approach is far different from that of Re. [74], in which it is shown that, if a state with range in the entanglement-breaking space is always additive.

VI. MAXIMALLY ENTANGLED STATE & THE MONOGAMY RELATION

A. The original definition of maximally entangled state

The *maximally entangled state* (MES), as a crucial quantum resource in quantum information processing tasks such as quantum teleportation [75–77], superdense coding [78, 79], quantum computation [80] and quantum cryptography [81], has been explored considerably [82–97]. For a bipartite system with state space $\mathcal{H}^{AB} = \mathcal{H}^A \otimes \mathcal{H}^B$, $\dim \mathcal{H}^A = m$, $\dim \mathcal{H}^B = n$ $(m \le n)$, a pure state $|\psi\rangle^{AB}$ is called a maximally entangled state if and only if $\rho^A = \frac{1}{m} I^A$ [98], 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

$$|\psi\rangle^{AB} = \frac{1}{\sqrt{m}} \sum_{i=1}^{m} |i\rangle^A |i\rangle^B, \tag{45}$$

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 [87] (such as entanglement of formation [3, 4], and concurrence [5–7]). For example, the well-known EPR states are maximally entangled pure states.

It is proved in Ref. [99] that any MES in a $d \otimes d$ system is pure. Later, Li *et al.* showed in Ref. [87] that the maximal entanglement can also exist in mixed states for $m \otimes n$ systems with $n \ge 2m$ (or $m \ge 2n$). A necessary and sufficient condition of MEMS is proposed [87]: An $m \otimes n$ $(n \ge 2m)$ bipartite mixed state ρ^{AB} is maximally entangled if and only if

$$\rho^{AB} = \sum_{k=1}^{r} p_k |\psi_k\rangle\langle\psi_k|^{AB}, \quad \sum_k p_k = 1,\ p_k \ge 0, \tag{46}$$

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

$$|\psi_k\rangle^{AB} = \frac{1}{\sqrt{m}} \sum_{i=0}^{m-1} |i\rangle^A |i_k\rangle^B, \tag{47}$$

$\{|i\rangle^A\}$ 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 that 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

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

and

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

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

$$\rho^{AB} = |\psi_+\rangle\langle\psi_+|^{AB_1} \otimes \left(\sum_{k=1}^{r} p_k |k\rangle\langle k|^{B_2} \right), \tag{48}$$

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 $\mathcal{H}^{AB_1}$, $\sum_k p_k = 1$, $p_k \ge 0$. The main purpose of this section is to show that ρ^{AB} in Eq. (46) [or equivalently in Eq. (48)] is not a genuine MEMS physically, there does not exist mixed MES in any bipartite systems.

B. The incompatibility of MEMS and the monogamy law

We begin with the following fact, which seems that entanglement can be freely shared.

Theorem 12. *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. (46), 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. (48) 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

$$|\phi\rangle^{ABC} = |\psi_+\rangle^{AB_1} |\psi\rangle^{B_2C} \tag{49}$$

with

$$|\psi\rangle^{B_2C} = \sum_k \sqrt{p_k} |k\rangle^{B_2} |k\rangle^C, \tag{50}$$

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 assumption, we let

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

It follows that

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

since $\ln m \geqslant E_f(A|BC) \geqslant E_f(AB)$ for any ρ^{ABC} and $\sum_s q_s E_f(\rho_s^{AB}) \geqslant E_f(\rho^{AB}) = \ln m$, where $m = \dim\mathcal{H}^A$, $\rho_s^{AB} = \mathrm{Tr}_C |\phi_s\rangle\langle\phi_s|^{ABC}$. By Theorem in Ref. [52], 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

$$\rho^{ABC} = |\psi_+\rangle\langle\psi_+|^{AB_1} \otimes \rho^{B_2C}, \tag{51}$$

where

$$\rho^{B_2C} = \sum_s q_s |\phi_s\rangle\langle\phi_s|^{B_2C} \tag{52}$$

with

$$|\phi_s\rangle^{B_2C} = \sum_{k=1}^{r} \sqrt{p_k} |e_k^{(s)}\rangle^{B_2} |f_k^{(s)}\rangle^C. \tag{53}$$

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 out 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. [87]), 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. (50) is also an MES according to Ref. [87]. In such a case

$$|\psi\rangle^{BAC} = \sum_{i,k} \frac{1}{mr} \left(|i\rangle^{B_1}|k\rangle^{B_2}\right) \otimes \left(|i\rangle^{A}|k\rangle^{C}\right) \tag{54}$$

is a maximally entangled pure state with respect to the cutting $B|AC$. Let $|f_k^{(s)}\rangle^C$ as in Eq. (53). If $\dim H^C \geqslant lr$, we let

$$|f_k^{(s)}\rangle^C = |k\rangle^{C_1}|s\rangle^{C_2}, \tag{55}$$

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

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

and

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

Then ρ^{B_2C} in Eq. (52) is an MEMS according to Ref. [87] whenever $p_k \equiv \frac{1}{r}$. That is, if ρ^{AB} is an MEMS in the sense of Ref. [87], it is possible that ρ^{BC} is also an MEMS in the sense of Ref. [87]. In fact,

$$\rho^{BAC} = \sum_{s=1}^{l} \frac{1}{l} |\phi_s\rangle\langle\phi_s|^{BAC} \tag{56}$$

with

$$|\phi_s\rangle^{BAC} = \sum_{i,k} \frac{1}{rm} \left(|i\rangle^{B_1}|k\rangle^{B_2}\right) \otimes \left(|i\rangle^{A}|k\rangle^{C_1}|s\rangle^{C_2}\right) \tag{57}$$

is an MEMS with respect to the cutting $B|AC$ according to Ref. [87]. Namely, B can maximally entangle with A and C simultaneously.

However, this fact contradicts with the monogamy law of entanglement [19, 32–53]: 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. (49) [or (54)] and ρ^{ABC} in Eq. (51) [or (56)], 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

- $E_f^{(2)}(|\psi\rangle^{A|BC}) = E_f^{(2)}(\rho^{AB})$ and $E_f^{(2)}(\rho)^{AC}) = 0$.
- $E_f^{(2)}(|\psi\rangle^{B|AC}) = E_f^{(2)}(\rho^{AB}) + E_f^{(2)}(\rho^{BC})$.
- $E_f^{(2)}(|\psi\rangle^{C|AB}) = E_f^{(2)}(\rho^{BC})$ and $E_f^{(2)}(\rho^{AC}) = 0$.
- $E_f^{(3)}(|\psi\rangle^{ABC}) = E_f^{(2)}(\rho^{AB}) + E_f^{(2)}(\rho^{BC})$.
- $E_f^{(2)}(\rho^{A|BC}) = E_f^{(2)}(\rho^{AB})$ and $E_f^{(2)}(\rho)^{AC}) = 0$.
- $E_f^{(2)}(\rho^{B|AC}) = E_f^{(2)}(\rho^{AB}) + E_f^{(2)}(\rho^{BC})$.
- $E_f^{(2)}(\rho^{C|AB}) = E_f^{(2)}(\rho^{BC})$ and $E_f^{(2)}(\rho^{AC}) = 0$.
- $E_f^{(3)}(\rho^{ABC}) = E_f^{(2)}(\rho^{AB}) + E_f^{(2)}(\rho^{BC})$.

That is, the above examples in Eq. (54) and Eq. (56) 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 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 "genuinely" 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 mixed state an MEMS?

We remark here that, both the monogamy relation with respect to 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. (54) and (56) are MEMs according to Ref. [87], we have

$$E_f^{(3)}(\rho^{ABC}) = \ln(mr) > E_f^{(2)}(\rho^{AB}) = \ln m. \tag{58}$$

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., $|\psi\rangle^{AB} = \mathrm{Tr}_C|\psi\rangle\langle\psi|^{ABC}$) must admit the form of $|\psi\rangle^{ABC} = |\psi\rangle^{AB}|\eta\rangle^C$, that is, both A and B cannot 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, it remains maximal amount of entanglement 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 MEM if and only if i)*

$$E_f^{(2)}(\rho^{AB}) = \ln m \tag{59}$$

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

$$E_f^{(3)}(\rho^{ABC}) = E_f^{(2)}(\rho^{AB}). \tag{60}$$

By this definition, the states in Eqs. (54) and (56) are not MEMs since $E_f^{(3)}(\rho^{ABC}) > E_f^{(2)}(\rho^{AB})$. Note that this definition of MEM is compatible with the monogamy law and makes the concept of MEM more clearly: 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 reflects the monogamy law more effectively. From Theorem 12, we obtain our main result:

Theorem 13. *There is no MEMS in any bipartite quantum system.*

In fact, we can also show that there is no multipartite MEMS since any extension of MEMS would increase entanglement from the new part. Note that the states in Eq. (54) and Eq. (56) 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. (46), we call it an MEMS up to part A. If $p_k \equiv \frac{1}{r}$ in Eq. (46) additionally, then ρ^{AB} is an MEMS up to part B.*

That is, the definition of MEMS in [87] is in fact an MEMS 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. (52) with $|f_k^{(s)}\rangle^C$ as in Eq. (55) is an MEMS 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 MEMS up to part C. We can easily check that, if ρ^{AB} is an MEMS up to part A, then $\rho^A = \frac{1}{m} I^A$, and if ρ^{AB} is an MEMS 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 well-defined entanglement measure (such as entanglement of formation, concurrence, negativity, etc.) but there do exist states that are not genuine maximally entangled state (eg. the MEMS up to part A) also achieves the maximal amount of entanglement. Namely, the MEMS up to one subsystem is an MES mathematically but not physically.

VII. CONCLUSION AND DISCUSSION

We established a “fine grained” framework for defining genuine MEM and proposed the associated complete monogamy formula. In our framework, together with the complete monogamy formula, we can explore mulitipartite 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 bipartite state is more clear when it is regarded as a reduced state of its extension, namely, quantum system is always not closed, 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 new tools and new insights into investigating multipartite entanglement and other multipartite correlation beyond entanglement.

As a by-product, interestingly, we found a class of states that are additive with respect to the entanglement of formation, which would shed new light on the problem of the classical communication capacity of the quantum channel [71, 100].

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 genuine multipartite entanglement measures (also see in Table I). We conjecture that the answers to theses questions are affirmative.

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Appendix: Proof of Lemma 14

By modifying the proof of Proposition 4.5 in Ref. [70], 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 14. *For any bipartite state $\rho_{AB} \in \mathcal{S}^{AB}$, we have*

$$\begin{aligned} & 1+\max\left\{\mathrm{Tr}\left(\rho_A^2\right), \mathrm{Tr}\left(\rho_B^2\right)\right\}\mathrm{Tr}\left(\rho_{AB}^2\right) \\ \geqslant\ & \mathrm{Tr}\left(\rho_A^2\right)+\mathrm{Tr}\left(\rho_B^2\right), \end{aligned} \tag{A.1}$$

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

Proof. Without loss of generality, we assume that $\mathrm{Tr}\left(\rho_B^2\right) \geqslant \mathrm{Tr}\left(\rho_A^2\right)$. 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

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

i.e.,

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

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

$$\min\left\{\kappa + \mathrm{Tr}\left(Z_\kappa^2\right)\mathrm{Tr}\left(\rho_{AB}^2\right)\right\} \leqslant 1+\mathrm{Tr}\left(\rho_{AB}^2\right). \tag{A.2}$$

Consider now the function

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

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

$$f_\kappa(\kappa) = \|\boldsymbol{y}\|_2^2 = \mathrm{Tr}\left(\rho_B^2\right) \leqslant 1.$$

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

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

Hence, under this assumption, we conclude that the convex function is below the straight line through $(0,0)$, $(\kappa, \mathrm{Tr}\left(\rho_B^2\right))$, whose equation is given by $y = \frac{\mathrm{Tr}\left(\rho_B^2\right)}{\kappa}x$. 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

$$\begin{aligned} \mathrm{Tr}\left(Z_\kappa^2\right) &= \|Z_\kappa\|_2^2 = \sum_{i,j}^d (x_i+y_j-\kappa)_+^2 = \sum_i f_\kappa(x_i) \\ &\leqslant \sum_i \frac{\mathrm{Tr}\left(\rho_B^2\right)}{\kappa}x_i = \frac{1}{\kappa}\mathrm{Tr}\left(\rho_B^2\right). \end{aligned}$$

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

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

Next we consider the function

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

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 on the interval $(0,\kappa_{\min}]$ and strictly increasing on $[\kappa_{\min}, 1]$.

(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

$$\begin{aligned} \mathrm{Tr}\left(\rho_A^2\right)+\mathrm{Tr}\left(\rho_B^2\right) &\leqslant \min\{g(\kappa) : \kappa \geqslant \kappa_0\} \leqslant 1+\kappa_{\min}^2 \\ &\leqslant 1+\mathrm{Tr}\left(\rho_{AB}^2\right). \end{aligned}$$

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

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

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

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

In such a case, we see that

$$1 + \mathrm{Tr}\left(\rho_A^2\right) \mathrm{Tr}\left(\rho_{AB}^2\right) = 1 + \mathrm{Tr}\left(\rho_{AB}^2\right) \tag{A.3}$$

implies ρ_A is pure. $\square$

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