P H Y S I C A L   R E V I E W   L E T T E R S

# General Monogamy Relation for the Entanglement of Formation in Multiqubit Systems

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We prove exactly that the squared entanglement of formation, which quantifies the bipartite entanglement, obeys a general monogamy inequality in an arbitrary multiqubit mixed state. Based on this kind of exotic monogamy relation, we are able to construct two sets of useful entanglement indicators: the first one can detect all genuine multiqubit entangled states even in the case of the two-qubit concurrence and $n$-tangles being zero, while the second one can be calculated via quantum discord and applied to multipartite entanglement dynamics. Moreover, we give a computable and nontrivial lower bound for multiqubit entanglement of formation.

For multipartite quantum systems, one of the most important properties is that entanglement is monogamous [1], which implies that a quantum system entangled with another system limits its entanglement with the remaining others [2]. For entanglement quantified by the squared concurrence [3], Coffman, Kundu, and Wootters (CKW) proved the first quantitative relation [4] for three-qubit states, and Osborne and Verstraete proved the corresponding relation for $N$-qubit systems, which reads [5]

$$C^2_{A_1|A_2\cdots A_N} - C^2_{A_1A_2} - C^2_{A_1A_3} - \cdots - C^2_{A_1A_N} \geq 0. \quad (1)$$

Similar inequalities were also generalized to Gaussian systems [6,7] and squashed entanglement [8,9]. As is known, the monogamy property can be used for characterizing the entanglement structure in many-body systems [4,10]. A genuine three-qubit entanglement measure named "three-tangle" was obtained via the monogamy relation of squared concurrence in three-qubit pure states [4]. However, for three-qubit mixed states, there exists a special kind of entangled state that has neither two-qubit concurrence nor three-tangle [11]. There also exists a similar case for $N$-qubit mixed states [12]. To reveal this critical entanglement structure other exotic monogamy relations beyond the squared concurrence may be needed.

On the other hand, from a practical viewpoint, to calculate the entanglement measures that appeared in the monogamy relation is basic. Unfortunately, except for the two-qubit case [3], this task is extremely hard (or almost impossible) for mixed states due to the convex roof extension of pure state entanglement [13]. Quantum correlation beyond entanglement (e.g., the quantum discord [14,15]) has recently attracted considerable attention, and various efforts have been made to connect quantum discord to quantum entanglement [16]. It is natural to ask whether

or not the calculation method for quantum discord can be utilized to characterize the entanglement structure and entanglement distribution in multipartite systems.

In this Letter, by analyzing the entanglement distribution in multiqubit systems, we prove exactly that the squared entanglement of formation (SEF) [3] is monogamous in an arbitrary multiqubit mixed state. Furthermore, based on the exotic monogamy relation, we construct two sets of useful indicators overcoming the flaws of concurrence, where the first one can detect all genuine multiqubit entangled states and be utilized in the case when the concurrence and $n$-tangles are zero, while the second one can be calculated via quantum discord and applied to a practical dynamical procedure. Finally, we give a computable and nontrivial lower bound for multiqubit entanglement of formation.

*General monogamy inequality for squared entanglement of formation.*—The entanglement of formation in a bipartite mixed state $\varrho_{AB}$ is defined as [13,17],

$$E_f(\varrho_{AB}) = \min \sum_i p_i E_f(|\psi^i\rangle_{AB}), \quad (2)$$

where the minimum runs over all the pure state decompositions $\{p_i, |\psi^i\rangle_{AB}\}$, and $E_f(|\psi^i\rangle_{AB}) = S(\rho_A^i)$ is the von Neumann entropy of subsystem $A$. For a two-qubit mixed state $\rho_{AB}$, Wootters derived an analytical formula [3]

$$E_f(\rho_{AB}) = h\left(\frac{1 + \sqrt{1 - C^2_{AB}}}{2}\right), \quad (3)$$

where $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$ is the binary entropy and $C_{AB} = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}$ is the concurrence with the decreasing nonnegative $\lambda_i$s being the eigenvalues of the matrix $\rho_{AB}(\sigma_y \otimes \sigma_y)\rho^*_{AB}(\sigma_y \otimes \sigma_y)$.

A key result of this work is to show exactly that the bipartite entanglement quantified by the squared entanglement of formation $E_f^2$ obeys a general monogamy inequality in an arbitrary $N$-qubit mixed state, i.e.,

$$E_f^2(\rho_{A_1|A_2,...,A_n}) - E_f^2(\rho_{A_1A_2}) - \cdots - E_f^2(\rho_{A_1A_n}) \geq 0, \quad (4)$$

where $E_f^2(\rho_{A_1|A_2,...,A_n})$ quantifies the entanglement in the partition $A_1|A_2, ..., A_n$ (hereafter, $n = N$ for qubit cases), and $E_f^2(\rho_{A_1A_j})$ quantifies the one in the two-qubit system $A_1A_j$. Under two assumptions, a qualitative analysis on three-qubit pure states was given in Ref. [18]. Before showing the general inequality, we first give the two propositions, whose analytical proofs are presented in the Supplemental Material [19].

*Proposition I*: The squared entanglement of formation $E_f^2(C^2)$ in two-qubit mixed states varies monotonically as a function of the squared concurrence $C^2$.

*Proposition II*: The squared entanglement of formation $E_f^2(C^2)$ is convex as a function of the squared concurrence $C^2$.

We now analyze the monogamy property of $E_f^2$ in an $N$-qubit pure state $|\psi\rangle_{A_1A_2,...,A_n}$. According to the Schmidt decomposition [20], the subsystem $A_2A_3, ..., A_n$ is equal to a logic qubit $A_{2,...,n}$. Thus, the entanglement $E_f(A_1|A_2, ..., A_n)$ can be evaluated using Eq. (3), leading to

$$
\begin{aligned}
&E_f^2(C^2_{A_1|A_2,...,A_n}) \\
&\geq E_f^2(C^2_{A_1A_2} + \cdots + C^2_{A_1A_n}) \\
&\geq E_f^2(C^2_{A_1A_2}) + E_f^2(C^2_{A_1A_3}) + \cdots + E_f^2(C^2_{A_1A_n}), \quad (5)
\end{aligned}
$$

where we have used the two propositions, with the details presented in Ref. [19].

At this stage, most importantly, we prove that the squared entanglement of formation $E_f^2$ is monogamous in an arbitrary $N$-qubit mixed state $\rho_{A_1A_2,...,A_n}$. In this case, the analytical Wootters formula in Eq. (3) cannot be applied to $E_f(\rho_{A_1|A_2,...,A_n})$, since the subsystem $A_2A_3, ..., A_n$ is not a logic qubit in general. But we can still use the convex roof extension of pure state entanglement as shown in Eq. (2). Therefore, we have

$$E_f(\rho_{A_1|A_2,...,A_n}) = \min \sum_i p_i E_f(|\psi^i\rangle_{A_1|A_2,...,A_n}), \quad (6)$$

where the minimum runs over all the pure state decompositions $\{p_i, |\psi^i\rangle\}$. We assume that the optimal decomposition for Eq. (6) takes the form

$$\rho_{A_1A_2,...,A_n} = \sum_{i=1}^m p_i |\psi^i\rangle_{A_1A_2,...,A_n} \langle\psi^i|. \quad (7)$$

Under this decomposition, we have

$$E_f(\rho_{A_1|A_2,...,A_n}) = \sum_i p_i E_f(|\psi^i\rangle_{A_1|A_2,...,A_n}) = \sum_i E1_i,$$

$$E_f'(\rho_{A_1A_j}) = \sum_i p_i E_f(\rho^i_{A_1A_j}) = \sum_i Ej_i, \quad (8)$$

where $E_f'(\rho_{A_1A_j})$ is the average entanglement of formation under the specific decomposition in Eq. (7) and the parameter $j \in [2, n]$. Then we can derive the following monogamy inequality,

$$
\begin{aligned}
&E_f^2(\rho_{A_1|A_2,...,A_n}) - \sum_j E_f'^2(\rho_{A_1A_j}) \\
&= \left(\sum_i E1_i\right)^2 - \sum_j \left(\sum_i Ej_i\right)^2 \\
&= \sum_i \left(E1_i^2 - \sum_j Ej_i^2\right) \\
&+ 2\sum_i \sum_{k=i+1} \left(E1_iE1_k - \sum_j Ej_iEj_k\right) \geq 0, \quad (9)
\end{aligned}
$$

where, in the second equation, the first term is non-negative because the $E_f^2$ is monogamous in pure state components, and the second term is also non-negative from a rigorous analysis shown in the Supplemental Material [19], justifying the monogamous relation. On the other hand, for the two-qubit entanglement of formation, the following relation is satisfied

$$E_f(\rho_{A_1A_j}) \leq E_f'(\rho_{A_1A_j}), \quad (10)$$

since $E_f'(\rho_{A_1A_j})$ is a specific average entanglement under the decomposition in Eq. (7), which is greater than $E_f(\rho_{A_1A_j})$ in general. Combining Eqs. (9) and (10), we can derive the monogamy inequality of Eq. (4), such that we have completed the whole proof showing that the squared entanglement $E_f^2$ is monogamous in $N$-qubit mixed states.

*Two kinds of multipartite entanglement indicator.*— Lohmayer et al. [11] studied a kind of mixed three-qubit states composed of a Greenberger-Horne-Zeilinger(GHZ) state and a $W$ state

$$\rho_{ABC} = p|\text{GHZ}_3\rangle\langle\text{GHZ}_3| + (1-p)|W_3\rangle\langle W_3|, \quad (11)$$

where $|\text{GHZ}_3\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$, $|W_3\rangle = (|100\rangle + |010\rangle + |001\rangle)/\sqrt{3}$, and the parameter $p$ ranges in [0, 1]. They found that when the parameter $p \in (p_c, p_0)$, with $p_c \simeq 0.292$ and $p_0 \simeq 0.627$, the mixed state $\rho_{ABC}$ is entangled but without two-qubit concurrence and three-tangle. The three-tangle quantifies the genuine tripartite entanglement and is defined as [4] $\tau(\rho_{ABC}) = \min \sum_i p_i[C^2_{A|BC}(|\psi^i_{ABC}\rangle) - C^2_{AB}(\rho^i_{AB}) - C^2_{AC}(\rho^i_{AC})]$. It is still an unsolved problem of how to characterize the

entanglement structure in this kind of states, although an explanation via the enlarged purification system was given [12].

Based on the monogamy inequality of $E_f^2$ in pure states, we can introduce a kind of indicator for multipartite entanglement in an $N$-qubit mixed state $\rho_{A_1 A_2,\ldots,A_n}$ as

$$\tau_{\text{SEF}}^{(1)}(\rho_N^{A_1}) = \min \sum_i p_i [E_f^2(|\psi^i\rangle_{A_1|A_2,\ldots,A_n}) - \sum_{j\neq 1} E_f^2(\rho_{A_1 A_j}^i)], \quad (12)$$

where the minimum runs over all the pure state decompositions $\{p_i, |\psi^i\rangle_{A_1 A_2,\ldots,A_n}\}$. This indicator can detect the genuine three-qubit entanglement in the mixed state specified in Eq. (11). After some analysis, we can get the optimal pure state decomposition for the three-qubit mixed state

$$\rho_{ABC} = \frac{\alpha}{3} \sum_{j=0}^2 |\psi^j(p_0)\rangle\langle\psi^j(p_0)| + (1-\alpha)|W_3\rangle\langle W_3|, \quad (13)$$

where the pure state component $|\psi^j(p_0)\rangle = \sqrt{p_0}|\text{GHZ}_3\rangle - e^{(2\pi i/3)j}\sqrt{1-p_0}|W_3\rangle$ and the parameter $\alpha = p/p_0$ with $p < p_0 \simeq 0.627$. Then the indicator is

$$\tau_{\text{SEF}}^{(1)}(\rho_{ABC}^A) = \alpha\tau_{\text{SEF}}^{(1)}(|\psi^0(p_0)\rangle) + (1-\alpha)\tau_{\text{SEF}}^{(1)}(|W\rangle)$$
$$= \alpha s_p + (1-\alpha)s_w, \quad (14)$$

where $s_p \simeq 0.217061$ and $s_w \simeq 0.238162$. In Fig. 1, we plot the entanglement indicators $\tau_{\text{SEF}}^{(1)}$, $E_f^2(AB) + E_f^2(AC)$, and $E_f^2(A|BC)$ in comparison to the indicators $\tau$, $C_{AB}^2 + C_{AC}^2$, and $C_{A|BC}^2$ calculated originally in Ref. [11]. As seen from Fig. 1, although the three-tangle $\tau$ is zero when $p \in (0, p_0)$, the nonzero $\tau_{\text{SEF}}^{(1)}$ indicates the existence of the genuine three-qubit entanglement. This point may also be understood as a fact that the three-tangle $\tau$ indicates merely the GHZ-type entanglement while the newly introduced indicator $\tau_{\text{SEF}}^{(1)}$ can detect *all* genuine three-qubit entangled states.

For three-qubit mixed states, a state $\varrho_{ABC}$ is called genuine tripartite entangled if any decomposition into pure states $\varrho_{ABC} = \sum_i p_i |\psi_{ABC}^i\rangle\langle\psi_{ABC}^i|$ contains at least one genuine tripartite-entangled component $|\psi_{ABC}^i\rangle \neq |\phi_1\rangle \otimes |\phi_2\rangle$, with $|\phi_1\rangle$ and $|\phi_2\rangle$ corresponding to the states of a single qubit or a couple of qubits [1]. For the tripartite entanglement indicator $\tau_{\text{SEF}}^{(1)}(\varrho_{ABC}^A)$, we have the following lemma, and the proof can be found in the Supplemental Material [19].

*Lemma 1.*—For three-qubit mixed states, the multipartite entanglement indicator $\tau_{\text{SEF}}^{(1)}(\varrho_{ABC}^A)$ is zero if and only if the quantum state is biseparable, i.e., $\varrho_{ABC} = \sum_j p_j \rho_{AB}^j \otimes \rho_C^j + \sum_j q_j \rho_{AC}^j \otimes \rho_B^j + \sum_j r_j \rho_A^j \otimes \rho_{BC}^j$.
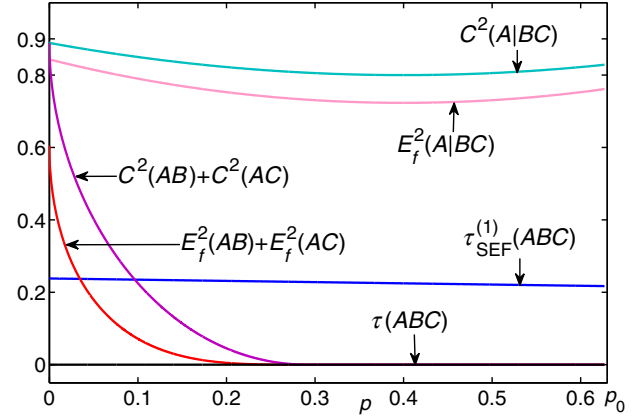


FIG. 1 (color online). Entanglement indicators $\tau_{\text{SEF}}^{(1)}$, $E_f^2(AB) + E_f^2(AC)$, and $E_f^2(A|BC)$ in comparison with the indicators $\tau$, $C_{AB}^2 + C_{AC}^2$, and $C_{A|BC}^2$ in Ref. [11], where the nonzero $\tau_{\text{SEF}}^{(1)}$ detects the genuine three-qubit entanglement in the region.

When the three-qubit mixed state $\varrho_{ABC}$ is genuine tripartite entangled, its optimal pure state decomposition contains at least one three-qubit entangled component. According to the lemma, we obtain that $\tau_{\text{SEF}}^{(1)}(\varrho_{ABC}^A)$ is surely nonzero.

For $N$-qubit mixed states, when the indicator $\tau_{\text{SEF}}^{(1)}(\rho_N^{A_1})$ in Eq. (12) is zero, we can prove that there exists *at most* two-qubit entanglement in the partition $A_1|A_2,\ldots,A_n$ (see lemmas b and c in Ref. [19]), and we further have the following lemma.

*Lemma 2.*—In $N$-qubit mixed states, the multipartite entanglement indicator

$$\tau_{\text{SEF}}^{(1)}(\rho_N) = \min \sum_j p_j \frac{\sum_{l=1}^n \tau_{\text{SEF}}^{(1)}(|\psi^j\rangle_N^{A_l})}{N} \quad (15)$$

is zero if and only if the quantum state is $(N/2)$ separable in the form $\rho_{A_1 A_2,\ldots,A_n} = \sum_{i_1,\ldots,i_n=1}^n \sum_j p_j^{\{i_1,\ldots,i_n\}} \rho_{A i_1 A i_2}^j \otimes \cdots \otimes \rho_{A i_{k-1} A i_k}^j \otimes \cdots \otimes \rho_{A i_{n-1} A i_n}^j$, which has at most two-qubit entanglement with the superscript $\{i_1,\ldots,i_n\}$ being all permutations of the $N$ qubits.

According to lemma 2, whenever an $N$-qubit state contains genuine multiqubit entanglement, the indicator $\tau_{\text{SEF}}^{(1)}(\rho_N)$ is surely nonzero. Thus, this quantity can serve as a genuine multiqubit entanglement indicator in $N$-qubit mixed states. The analytical proof of this lemma and its application to an $N$-qubit mixed state (without two-qubit concurrence and $n$-tangles) are presented in the Supplemental Material [19].

In general, the calculation of the indicators defined in Eqs. (12) and (15) is very difficult due to the convex roof extension. Here, based on the monogamy property of $E_f^2$ in mixed states, we can also introduce an alternative multipartite entanglement indicator as

$$\tau_{\mathrm{SEF}}^{(2)}(\rho_N^{A_1}) = E_f^2(\rho_{A_1|A_2,\ldots,A_n}) - \sum_{j \neq 1} E_f^2(\rho_{A_1 A_j}), \qquad (16)$$

which detects the multipartite entanglement (under the given partition) not stored in pairs of qubits (although this quantity is not monotone under local operations and classical communication [19]). From the Koashi-Winter formula [8], the multiqubit entanglement of formation can be calculated by a purified state $|\psi\rangle_{A_1 A_2,\ldots,A_n R}$, with $\rho_{A_1 A_2,\ldots,A_n} = \mathrm{tr}_R |\psi\rangle\langle\psi|$,

$$E_f(A_1|A_2,\ldots,A_n) = D(A_1|R) + S(A_1|R), \qquad (17)$$

where $S(A_1|R) = S(A_1 R) - S(R)$ is the quantum conditional entropy with $S(x)$ being the von Neumann entropy, and the quantum discord $D(A_1|R)$ is defined as [14,15]

$$D_{A_1|R} = \min_{\{E_k^R\}} \sum_k p_k S(A_1|E_k^R) - S(A_1|R), \qquad (18)$$

with the minimum running over all the positive operator-valued measures and the measurement being performed on subsystem $R$. Recent studies on quantum correlation provide some effective methods [21–29] for calculating the quantum discord, which can be used to quantify the indicator in Eq. (16). For all partitions, we may introduce a partition-independent indicator $\tau_{\mathrm{SEF}}^{(2)}(\rho_N) = \sum_{i=1}^n \tau_{\mathrm{SEF}}^{(2)}(\rho_N^{A_i})/N$.

We now apply the indicator $\tau_{\mathrm{SEF}}^{(2)}$ to a practical dynamical procedure of a composite system which is composed of two entangled cavity photons being affected by the dissipation of two individual $N$-mode reservoirs. The interaction of a single cavity-reservoir system is described by the Hamiltonian [30] $\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a} + \hbar\sum_{k=1}^N \omega_k \hat{b}_k^\dagger \hat{b}_k + \hbar\sum_{k=1}^N g_k(\hat{a}\hat{b}_k^\dagger + \hat{b}_k\hat{a}^\dagger)$. When the initial state is $|\Phi_0\rangle = (\alpha|00\rangle + \beta|11\rangle)_{c_1 c_2}|00\rangle_{r_1 r_2}$ with the dissipative reservoirs being in the vacuum state, the output state of the cavity-reservoir system has the form [30]

$$|\Phi_t\rangle = \alpha|0000\rangle_{c_1 r_1 c_2 r_2} + \beta|\phi_t\rangle_{c_1 r_1}|\phi_t\rangle_{c_2 r_2}, \qquad (19)$$

where $|\phi_t\rangle = \xi(t)|10\rangle + \chi(t)|01\rangle$ with the amplitudes being $\xi(t) = \exp(-\kappa t/2)$ and $\chi(t) = [1 - \exp(-\kappa t)]^{1/2}$. As quantified by the concurrence, the entanglement dynamical property was addressed in Refs. [30,31], but the multipartite entanglement analysis is mainly based on some specific bipartite partitions in which each party can be regarded as a logic qubit. When one of the parties is not equivalent to a logic qubit, the characterization for multipartite entanglement structure is still an open problem. For example, in the dynamical procedure, although the monogamy relation $C_{c_1|c_2 r_1}^2 - C_{c_1 c_2}^2 - C_{c_1 r_1}^2$ is satisfied, the entanglement $C_{c_1|c_2 r_1}^2$ is unavailable so far because subsystem $c_2 r_1$ is a four-level system and the convex roof extension is needed. Fortunately, in this case, we can utilize the presented indicator $\tau_{\mathrm{SEF}}^{(2)}(\rho_{c_1 c_2 r_1}^{c_1}) = E_f^2(c_1|c_2 r_1) - E_f^2(c_1 c_2) - E_f^2(c_1 r_1)$ to indicate the genuine tripartite
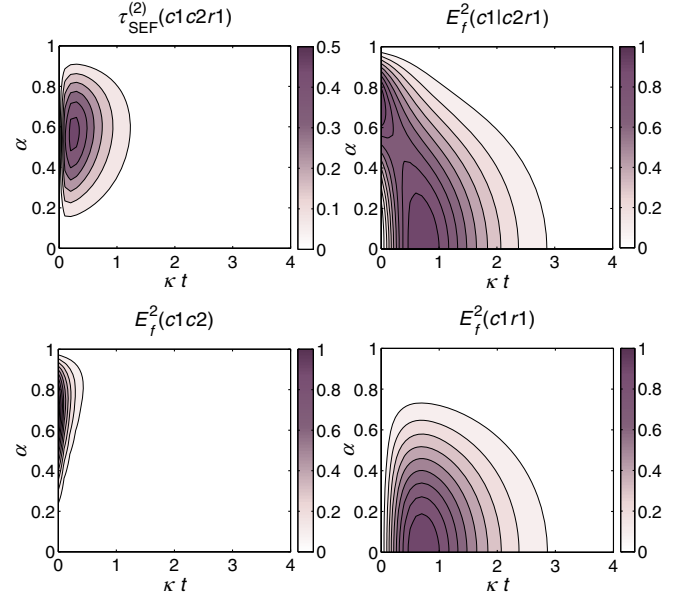


FIG. 2 (color online). The indicator $\tau_{\mathrm{SEF}}^{(2)}(\rho_{c_1 c_2 r_1}^{c_1})$ and its entanglement components as functions of the time evolution $\kappa t$ and the initial amplitude $\alpha$, which detects the tripartite entanglement area and illustrates the entanglement distribution in the dynamical procedure.

entanglement, where $E_f(c_1|c_2 r_1)$ can be obtained via the quantum discord $D_{c_1|r_2}$ [19]. This indicator detects the genuine tripartite entanglement which does not come from two-qubit pairs. In Fig. 2, the indicator and its entanglement components are plotted as functions of the time evolution $\kappa t$ and the initial amplitude $\alpha$, where the nonzero $\tau_{\mathrm{SEF}}^{(2)}(c_1 c_2 r_1)$ actually detects the tripartite entanglement area and the bipartite components of $E_f^2$ characterize the entanglement distribution in the dynamical procedure. By analyzing the multipartite entanglement structure, we can know how the initial cavity photon entanglement transfers in the multipartite cavity-reservoir system, which provides the necessary information to design an effective method for suppressing the decay of cavity photon entanglement.

*Discussion and conclusion.*—The entanglement of formation is a well-defined measure for bipartite entanglement and has the operational meaning in entanglement preparation and data storage [2]. Unfortunately, it does not satisfy the usual monogamy relation. As an example, its monogamy score for the three-qubit $W$ state is $E_f(A|BC) - E_f(AB) - E_f(AC) = -0.1818$. In this Letter, we show exactly that the squared entanglement $E_f^2$ is monogamous, which mends the gap of the entanglement of formation. Furthermore, in comparison to the monogamy of concurrence, the newly introduced indicators can really detect all genuine multiqubit entangled states and extend the territory of entanglement dynamics in many-body systems. In addition, via the established monogamy relation in Eq. (4), we can obtain

$$E_f(\rho_{A_1|A_2,\ldots,A_n}) \geq \sqrt{E_f^2(\rho_{A_1A_2}) + \cdots + E_f^2(\rho_{A_1A_n})}, \quad (20)$$

which provides a nontrivial and computable lower bound for the entanglement of formation.

In summary, we have not only proven exactly that the squared entanglement of formation is monogamous in $N$-qubit mixed states, but also provided a set of useful tools for characterizing the entanglement in multiqubit systems, overcoming some flaws of the concurrence. Two kinds of indicators have been introduced: the first one can detect all genuine multiqubit entangled states and solve the critical outstanding problem in the case of the two-qubit concurrence and $n$-tangles being zero, while the second one can be calculated via quantum discord and applied to a practical dynamical procedure of cavity-reservoir systems when the monogamy of concurrence loses its efficacy. Moreover, the computable lower bound can be utilized to estimate the multiqubit entanglement of formation.

*Note added.*—Recently, by using the same assumptions as those made in Ref. [18], a similar idea on the monogamy of squared entanglement of formation was presented in Ref. [32], but the claimed monogamy for mixed states was not proven in that paper [33], in contrast to what we have done in the present work.

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