Monogamy constraints on entanglement of four-qubit pure states

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We report a set of monogamy constraints on one-tangle, two-tangles, three-tangles and four-way correlations of a general four-qubit pure state. It is found that given a two-qubit marginal state ρ of a four qubit pure state $|\Psi_4\rangle$, the non-Hermitian matrix $\rho\tilde{\rho}$ where $\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y)$, contains information not only about the entanglement properties of the two-qubits in state ρ but also about three tangles involving the selected pair as well as four-way correlations of the pair of qubits in $|\Psi_4\rangle$. To extract information about tangles of a four-qubit state $|\Psi_4\rangle$, the coefficients in the characteristic polynomial of matrix $\rho\tilde{\rho}$ are analytically expressed in terms of 2×2 matrices of state coefficients. Four-tangles distinguish between different types of entangled four-qubit pure states.

I. INTRODUCTION

Entanglement is not only a necessary ingredient for processing quantum information [1] but also has important applications in other areas such as quantum field theory [2], statistical physics [3], and quantum biology [4]. Multipartite entanglement is a resource for multiuser quantum information tasks. Bipartite entanglement is well understood as there is concise result to entanglement classification problem. For bipartite systems, the notion of maximally entangled states is independent of the specific quantification of entanglement. However, since the mathematical structure of multipartite states is much more complex than that of bipartite states, the characterization of multipartite entanglement is a far more challenging task [5]. Even the identification of maximally entangled states in multi-party systems is highly non-trivial.

Walter et al. [6] used an algebraic geometry approach to show that single particle states are a rich source of information on multiparticle entanglement. In a recent letter [7], we have shown that two-qubit subsystems of an N-qubit state contain information about the correlations beyond two-qubit entanglement. In this context, four-qubit pure states offer an interesting case study, since a good part of residual correlations can be identified as contributions from seven four-tangles as defined in this article. One of the key features of multipartite correlations that separates quantum-ness from classicality is monogamy of entanglement. Monogamy of quantum entanglement refers to shareability of entanglement in a composite quantum system. Monogamy relation for entanglement of three-qubit states, known as CKW inequality, was reported in a seminal paper by Coffman, Kundu, and Wootters [8]. Recent efforts to find monogamy relations satisfied by tangles of four-qubit states include refs. [9–14]. A detailed analysis of residual correlations for four-qubit pure states, yields monogamy constraints, reported in this article.

One-tangle is known to quantify the entanglement of a single qubit with the rest of the composite system in an N-qubit pure state, whereas two-tangle (or concurrence as defined in ref. [15, 16]) is a measure of entanglement of two qubits. One tangle, defined as $\tau_{1|2...N} = 2(1 - \text{Tr}(\rho^2))$, quantifies essentially the mixedness of single-qubit marginal state ρ . Likewise, mixedness of a two-qubit marginal state of an N-qubit pure state is due to 2-way, 3-way, ..., N-way correlations of two qubits with N - 2 qubits. In [7], it has been shown, analytically, that two-tangle can be written as the difference of two terms, where the first term contributes to one-tangle while the second term is a function of degree 8, 12 and 16 local unitary invariant functions of state coefficients. Since two-tangle and the first term are calculable quantities, the difference gives quantitative information about correlations beyond two-way correlations. Reported monogamy constraints are functional relations satisfied by entanglement of a single qubit to the rest of the system (one-tangle), the entanglement of two-qubit marginal states (two-tangles), entanglement of three-qubit marginal states due to three-way correlations (three-tangles), and the residual correlations written as functions of four-qubit unitary invariant functions of state coefficients. By identifying quantitatively the contributions of three-tangles and four-tangles to correlations beyond two-tangles). By identifying quantitatively the contributions of three-tangles and four-tangles to correlations beyond two-tangles, and the residual correlations written as functions of three-tangles and four-tangles to correlations beyond two-tangles, it is possible to know how entanglement is distributed in subsystems of the four-qubit pure state. Monogamy of entanglement has potential

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applications in areas of physics such as quantum key distribution [17–19], classification of quantum states [20–22], frustrated spin systems [23, 24], and even black-hole physics [25].

Monogamy constraints are closely related to classification of entangled states. Four-tangles, when used to label the entanglement classes of ref. [26] along with three-tangles and two-tangles unambiguously distinguish between different types of entanglement due to four-way correlations. In the case of four-qubit states, information from single particle states [6] already points to different entanglement types in four-qubit pure states, however, information from two-qubit subsystems quantifies the entanglement of the states due to four-way correlations in each class.

Two-tangle, one-tangle, three-tangle and necessary unitary invariants are defined in Section II through Section VI, with our main results presented in Sections VII, VIII and IX. Analysis of tangles of a four-qubit GHZ state and Cluster state are in Sections X and XI. Monogamy of four-qubit correlations in a special subset of four-qubit states $L_{a,ia,(ia)_2}$ is discussed in section XII. Tangle based classification of four-qubit states is discussed in section XIII. Section XIV on entanglement transfer using a simple circuit model illustrates how two-way correlations of a pair of qubits leaks into environment through successive interactions of one of the qubits of the pair. Concluding remarks follow in section XV.

II. DEFINITION OF TWO-TANGLE

Two-tangle or concurrence, a well known measure of two-qubit entanglement [15, 16] is an entanglement monotone. A generic two-qubit pure state in computational basis reads as

$$|\Psi_{12}\rangle = \sum_{i_1, i_2} a_{i_1 i_2} |i_1 i_2\rangle; \quad (i_m = 0, 1),$$
(1)

where $a_{i_1i_2}$ are the state coefficients. The indices i_1 and i_2 refer to the state of qubits A_1 and A_2 , respectively. Entanglement of qubit A_1 with A_2 is quantified by two-tangle defined as

$$\tau_{1|2}(|\Psi_{12}\rangle) = 2 |a_{00}a_{11} - a_{10}a_{01}|.$$
(2)

Consider the action of a unitary transformation $U^j = \frac{1}{\sqrt{1+|x|^2}} \begin{bmatrix} 1 & -x^* \\ x & 1 \end{bmatrix}$ on qubit A_j . We can verify that

$$U^{1}\tau_{1|2}(|\Psi_{12}\rangle) = U^{2}\tau_{1|2}(|\Psi_{12}\rangle) = \tau_{1|2}(|\Psi_{12}\rangle).$$
(3)

Two-tangle of a mixed state $\rho = \sum_{i} p_i \left| \phi_{12}^{(i)} \right\rangle \left\langle \phi_{12}^{(i)} \right|$ is constructed through convex roof extension as

$$\tau_{1|2}\left(\rho\right) = 2 \min_{\left\{p_{i},\phi_{12}^{(i)}\right\}} \sum_{i} p_{i} \left| a_{00}^{(i)} a_{11}^{(i)} - a_{10}^{(i)} a_{01}^{(i)} \right|.$$

$$\tag{4}$$

Specifically, two-tangle [15, 16] of a two-qubit state ρ_{12} is given by

$$\tau_{1|2}\left(\rho\right) = \max\left(0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\right),\tag{5}$$

where $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ are the eigenvalues of non-Hermitian matrix $\rho \tilde{\rho}$ with $\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y)$. Here * denotes complex conjugation in the standard basis and σ_y is the Pauli matrix. In the most general case, the characteristic polynomial of $\rho \tilde{\rho}$ has the form

$$x^4 - x^3 n_4 + x^2 n_8 - x n_{12} + n_{16} = 0 ag{6}$$

where the coefficients n_d are given by

$$n_4 = tr\left(\rho\widetilde{\rho}\right); n_8\left(\rho\right) = \frac{1}{2}\left(\left(tr\rho\widetilde{\rho}\right)^2 - tr\left(\rho\widetilde{\rho}\right)^2\right); \tag{7}$$

$$n_{12} = \frac{1}{6} \left(\left(tr\rho\widetilde{\rho} \right)^3 - 3tr\left(\rho\widetilde{\rho}\right)tr\left(\rho\widetilde{\rho}\right)^2 + 2tr\left(\rho\widetilde{\rho}\right)^3 \right); \tag{8}$$

$$n_{16} = \det\left(\rho\widetilde{\rho}\right).\tag{9}$$

Matrix elements of a two-qubit mixed state ρ are degree-two functions of state coefficients of the pure state from which ρ has been obtained. As such a given coefficient $n_d(\rho)$ is a unitary invariant function of state coefficients of the pure state of which ρ is a part. The subscript d refers to the degree of the invariant. Defining $C(\rho) = \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}$, we can verify that for $C(\rho) = \pm |C(\rho)|$ the coefficient n_4 satisfies the relation

$$n_4 = |C(\rho)|^2 + \sqrt{4n_8 + 8\sqrt{n_{16}} \pm 8\sqrt{f_{16}}},\tag{10}$$

where $f_{16} \ge 0$ is defined as

$$f_{16} = \sqrt{n_{16}} |C(\rho)|^2 \left(n_4 - |C(\rho)|^2 \right) + n_{12} |C(\rho)|^2 , \qquad (11)$$

To obtain Eq. (10) we used the expressions for the coefficients n_d (d = 4, 8, 12, 16) in terms of eigenvalues of matrix $(\rho \tilde{\rho})$ and the condition $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$. Derivation of Eq. (10) is given in Appendix A. Since by definition $\tau_{1|2}(\rho) = \max(0, C(\rho))$, we may rewrite Eq. (10) as

$$n_4 - \tau_{1|2}^2(\rho) = \sqrt{4n_8 + \chi_{12}^\pm},\tag{12}$$

where

$$\chi_{12}^{+} = 8\sqrt{n_{16}} + 8\sqrt{f_{16}},\tag{13}$$

and

$$\chi_{12}^{-} = 8\sqrt{n_{16}} - 8\sqrt{f_{16}} + 2n_4 |C(\rho)|^2 - |C(\rho)|^4.$$
(14)

This is an important relation between coefficients n_d and two-tangle.

III. TWO-TANGLES AND ONE-TANGLE OF AN N-QUBIT PURE STATE

Expressions for one-tangle as well as polynomial coefficients of degree four and eight in terms of state coefficients of an N-qubit pure state are written down, in this section. A general N-qubit pure state in computational basis reads as

$$|\Psi_{12...N}\rangle = \sum_{i_1, i_2, \dots, N} a_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle; \ i_m = 0, 1.$$
(15)

Here $a_{i_1i_2...i_N}$ are complex state coefficients and the indices $i_1, i_2, ..., i_N$ refer to the state of qubits at locations $A_1, A_2,..., A_N$, respectively. State of qubit pair A_1A_j is $\rho_{1j} = Tr_{2,...,j-1,j+1,...N}(|\Psi_{12...N}\rangle \langle \Psi_{12...N}|)$ with matrix elements given by

$$(\rho_{1j})_{i_1 i_j k_1 k_j} = \sum_I a_{i_1 i_j I} a^*_{k_1 k_j I}, \tag{16}$$

where index $I = \{i_2 i_3 \dots i_{j-1} i_{j+1} \dots i_N\}$ with associated value $I_v \equiv \sum_{\substack{m=2\\m \neq j}}^N 2^{m-2} i_m$. Writing the characteristic polynomial

for $\rho_{1j}\tilde{\rho}_{1j}$ it is found that for qubit pair A_1A_j in state ρ_{1j} ,

$$n_4(\rho_{1j}) = 2\sum_{I \le J} |D_{1jIJ} + D_{1jJI}|^2, \qquad (17)$$

where

$$D_{1jIJ} = a_{0(i_j=0)I} a_{1(i_j=1)J} - a_{1(i_j=0)J} a_{0(i_j=1)I}.$$
(18)

A simplified notation I < J is being used when $I_v < J_v$. The functions $(D_{1jIJ} + D_{1jJI})$ are invariant with respect to unitary transformations on the focus qubit and qubit j and depending on the value of I and J represent a sum of determinants of 2-way, 3-way,..., N-way matrices of dimension 2. One-tangle defined as $\tau_{1|2...N} = 4 \det(\rho_1)$ where

 $\rho_1 = Tr_{A_2...A_N}(|\Psi_{12...N}\rangle \langle \Psi_{12...N}|)$ and $(\rho_1)_{i_1k_1} = \sum_{i_j,I} a_{i_1i_jI} a^*_{k_1i_jI}$ quantifies the entanglement of qubit A_1 with rest of the system. One can verify that

$$\tau_{1|2...N} = 4 \sum_{j=2}^{N} \left(\sum_{I} |D_{1jII}|^2 + \sum_{I < J} |D_{1jIJ}|^2 \right).$$
(19)

Comparing Eq. (17) and Eq. (19), we obtain

$$\tau_{1|2...N} = \sum_{j=2}^{N} \left(n_4 \left(\rho_{1j} \right) - X_{1j} \right), \tag{20}$$

where the quantity X_{1j} defined as

$$X_{1j} = 2\sum_{I < J} \left(D_{1jIJ} D_{1jJI}^* + D_{1jIJ}^* D_{1jJI} \right),$$
(21)

represents coherences. The sum of coherences, $\sum_{j=2}^{N} X_{1j}$, turns out to be zero for N-odd and is equal to sum of unitary invariants of degree two for N-even.

The coefficient $n_8(\rho_{1j})$, written in terms of state coefficients reads as

$$n_8(\rho_{1j}) = \sum_{I,J,K,L} \left| \begin{array}{c} (D_{1jIJ} + D_{1jJI}) (D_{1jKL} + D_{1jLK}) \\ - (D_{1jIL} + D_{1jLI}) (D_{1jKJ} + D_{1jJK}) \end{array} \right|^2.$$
(22)

While the coefficient $n_4(\rho_{1j})$ is a sum of squares of moduli of two-qubit invariants, the coefficient $n_8(\rho_{1j})$ is a sum of squares of three-qubit invariants.

IV. TANGLES OF A THREE-QUBIT PURE STATE AND MONOGAMY OF ENTANGLEMENT

For a three-qubit system, the entanglement measures are known to satisfy CKW inequality [8]. In this section, we establish the relation between coefficients $n_d(\rho)$ and entanglement measures of a three-qubit pure state

$$|\Psi_{123}\rangle = \sum_{i_1, i_2, i_3} a_{i_1 i_2 i_3} |i_1 i_2 i_3\rangle, \quad (i_m = 0, 1).$$
⁽²³⁾

Using the notation of ref. [27], the determinants of negativity fonts for the state $|\Psi_{123}\rangle$ are defined as $D_{(A_3)_{i_3}}^{00} = a_{00i_3}a_{11i_3} - a_{10i_3}a_{01i_3}$ (two-way), $D_{(A_2)_{i_2}}^{00} = a_{0i_20}a_{1i_21} - a_{1i_20}a_{0i_21}$ (two-way), and $D^{00i_3} = a_{00i_3}a_{11i_3+1} - a_{10i_3}a_{01i_3+1}$ (three-way). This set of determinants is the same as that obtained by substituting j = 2, 3 and $I \equiv \{0, 1\}$, in Eq. (18). For example, taking A_1 as focus qubit $D_{12i_3i_3+1} = D_{13i_2i_2+1} = D^{00i_3}$. One-tangle, defined as $\tau_{1|23} (|\Psi_{123}\rangle) = 4 \det(\rho_1)$ where $\rho_1 = Tr_{A_2A_3}(|\Psi_{123}\rangle \langle \Psi_{123}|)$, quantifies the entanglement of qubit A_1 with qubits A_2 and A_3 . Three tangle [8] of $|\Psi_{123}\rangle$ is equal to four times the modulus of a unitary invariant polynomial of degree four that is

$$\tau_{1|2|3}\left(|\Psi_{123}\rangle\right) = 4\left|I_{3,4}\left(|\Psi_{123}\rangle\right)\right|,\tag{24}$$

where

$$I_{3,4}(|\Psi_{123}\rangle) = (D^{000} + D^{001})^2 - 4D^{00}_{(A_3)_0}D^{00}_{(A_3)_1} = (D^{000} - D^{001})^2 - 4D^{00}_{(A_2)_0}D^{00}_{(A_2)_1}.$$
(25)

Three-tangle of the mixed state ρ_{123} is defined as the average of pure state three-tangles, minimized over all complex decompositions $\left\{p_i, \left|\phi_{123}^{(i)}\right\rangle\right\}$ of ρ_{123} that is

$$\tau_{1|2|3}\left(\rho_{123}\right) = \min_{\left\{p_{i}, \left|\phi_{123}^{(i)}\right\rangle\right\}} \sum_{i} p_{i} \tau_{1|2|3}\left(\left|\phi_{123}^{(i)}\right\rangle\right).$$
(26)

Here p_i is the probability of finding the normalized three-qubit state $|\phi_{123}^{(i)}\rangle$ in the mixed state ρ_{123} .

$$n_8(\rho_{1j}) = \frac{1}{16} \tau_{1|2|3}^2(|\Psi_{123}\rangle), \quad n_{12}(\rho_{1j}) = n_{16}(\rho_{1j}) = 0, \tag{27}$$

and

$$\tau_{1|23}\left(|\Psi_{123}\rangle\right) = n_4\left(\rho_{12}\right) + n_4\left(\rho_{13}\right). \tag{28}$$

From Eq. (12), the two-tangle of the state ρ_{1j} reads as

$$\tau_{1|j}^{2}(\rho_{1j}) = n_{4}(\rho_{1j}) - \frac{1}{2}\tau_{1|2|3}(|\Psi_{123}\rangle); \quad (j = 2, 3).$$
⁽²⁹⁾

Substituting the value of coefficients $n_4(\rho_{1j})$ from Eq (29) into Eq. (28), the tangles for $|\Psi_{123}\rangle$ satisfy the constraint (CKW inequality):

$$\tau_{1|23}\left(|\Psi_{123}\rangle\right) = \tau_{1|2}^{2}\left(\rho_{12}\right) + \tau_{1|3}^{2}\left(\rho_{13}\right) + \tau_{1|2|3}\left(|\Psi_{123}\rangle\right). \tag{30}$$

In other words, with qubit A_1 as focus qubit the sum of two-tangles and three-way correlations in $|\Psi_{123}\rangle$ is equal to $\tau_{1|23}(|\Psi_{123}\rangle)$. Analogous relations can be found by taking A_2 or A_3 as the focus qubit. It implies that stronger the entanglement of a qubit pair in a three-qubit pure state, the weaker is entanglement of the pair with the rest of the system. This also implies that if three-way correlations are maximal that is $\tau_{1|2|3}(|\Psi_{123}\rangle) = 1 = \tau_{1|23}(|\Psi_{123}\rangle)$, then $\tau_{1|2}^2(\rho_{12}) = \tau_{1|3}^2(\rho_{13}) = 0$.

V. ONE-TANGLE OF A FOUR-QUBIT PURE STATE

In this section, we consider the case where two-qubit state is a marginal state of four-qubit composite system in a pure state. An understanding of distribution of quantum correlations in a pure state with more than three qubits is a fascinating challenge. Our main objective is to find the relation between one-tangle of the state with qubit A_1 as the focus qubit, coefficients $n_4(\rho_{1j})$ and $n_8(\rho_{1j})$ (j = 2 to 4). To facilitate the calculation, the formalism of determinants of negativity fonts is used to express $n_4(\rho_{1j})$ and $n_8(\rho_{1j})$ in terms of two-qubit, three-qubit and four-qubit unitary invariant combinations of state coefficients. For more on definition and physical meaning of determinants of negativity fonts, please refer to section (VI) of ref. [27]. A general four-qubit pure state reads as

$$|\Psi_{1234}\rangle = \sum_{i_1, i_2, i_3, i_4} a_{i_1 i_2 i_3 i_4} |i_1 i_2 i_3 i_4\rangle, \quad (i_m = 0, 1),$$
(31)

where the state coefficients $a_{i_1i_2i_3i_4}$ are complex numbers. The indices i_1 , i_2 , i_3 , i_4 refer, respectively, to the state of qubits A_1 , A_2 , A_3 , and A_4 . Taking qubit A_1 as the focus qubit, for the purpose of this article the determinants of negativity fonts of $|\Psi_{1234}\rangle$ are defined as $D^{00}_{(A_3)_{i_3}(A_4)_{i_4}} = a_{00i_3i_4}a_{11i_3i_4} - a_{10i_3i_4}a_{01i_3i_4}$ (two-way), $D^{00}_{(A_2)_{i_2}(A_4)_{i_4}} = a_{0i_20i_4}a_{1i_21i_4} - a_{1i_20i_4}a_{0i_21i_4}$ (two-way), $D^{00}_{(A_2)_{i_2}(A_3)_{i_3}} = a_{0i_2i_30}a_{1i_2i_31} - a_{1i_2i_30}a_{0i_2i_31}$ (two-way), $D^{00i_4}_{(A_4)_{i_4}} = a_{00i_3i_4}a_{11i_3,i_4\oplus 1} - a_{10i_3i_4}a_{01i_3,i_4\oplus 1}$ (three-way), $D^{00i_4}_{(A_2)_{i_2}} = a_{0i_20i_4}a_{1i_21i_4\oplus 1} - a_{1i_20i_4}a_{0i_21i_4\oplus 1}$ (three-way), $D^{00i_4}_{(A_3)_{i_3}} = a_{00i_3i_4}a_{11i_3,i_4\oplus 1} - a_{10i_3i_4}a_{01i_3,i_4\oplus 1}$ (three-way), $D^{00i_4}_{(A_2)_{i_2}} = a_{0i_20i_4}a_{1i_21i_4\oplus 1} - a_{1i_20i_4}a_{0i_21i_4\oplus 1}$ (three-way), and $D^{00i_3i_4} = a_{00i_3i_4}a_{11,i_3\oplus 1,i_4\oplus 1} - a_{10i_3i_4}a_{01,i_3\oplus 1,i_4\oplus 1}$ (four-way). All these determinants correspond to the set of D_{1jIJ} obtained by substituting j = (2,3,4) and $I \equiv \{00, 10, 01, 11\}$, in Eq. (18). To understand what does the determinant of a four-way negativity font represent, consider the state

$$|\Psi\rangle = a_{0000} |0000\rangle + a_{1000} |1000\rangle + a_{0111} |0111\rangle + a_{1111} |1111\rangle, \qquad (32)$$

with $D^{0000} = a_{0000}a_{1111} - a_{1000}a_{0111}$. It is easily verified that taking negativity of partial transpose of $|\Psi\rangle$ with respect to qubit A_1 as the entanglement measure, the entanglement of qubit A_1 with the three remaining qubits due to four-way correlations is $4 |D^{0000}|$.

Matrix elements of the state $\rho_{12} = Tr_{A_3A_4}(|\Psi_{1234}\rangle \langle \Psi_{1234}|)$ are given by

$$(\rho_{12})_{i_1 i_2 j_1 j_2} = \sum_{i_3 i_4} a_{i_1 i_2 i_3 i_4} a^*_{j_1 j_2 i_3 i_4}.$$
(33)

We use Eq. (33) to express the characteristic polynomial of $\rho_{12}\rho_{12}$ in terms of state coefficients of $|\Psi_{1234}\rangle$ and identify the coefficient $n_4(\rho_{12})$. Similarly one can obtain the coefficients $n_4(\rho_{13})$ and $n_4(\rho_{14})$ from the states $\rho_{13} = Tr_{A_2A_4}(|\Psi_{1234}\rangle \langle \Psi_{1234}|)$ and $\rho_{14} = Tr_{A_2A_3}(|\Psi_{1234}\rangle \langle \Psi_{1234}|)$, respectively. Expression for $n_4(\rho_{1j})$ (j = 2 to 4) in terms of determinants of negativity fonts is given by Eq. (B14) in subsection B2 of Appendix B.

One-tangle, $\tau_{1|234}(|\Psi_{1234}\rangle) = 4 \det(\rho_1)$ with $\rho_1 = Tr_{A_2A_3A_4}(|\Psi_{1234}\rangle\langle\Psi_{1234}|)$, quantifies the entanglement of qubit A_1 with qubits $A_2A_3A_4$. Using Eq. (20), it is easily verified that one-tangle satisfies the relation,

$$\tau_{1|234} = \sum_{j=2}^{4} n_4\left(\rho_{1j}\right) - \frac{1}{2} \left(\tau_{1|2|3|4}^{(0)}\right)^2.$$
(34)

In Eq. (34), the four-qubit tangle $\tau_{1|2|3|4}^{(0)}$ is defined as

$$\tau_{1|2|3|4}^{(0)} = 2 \left| D^{0000} + D^{0011} - D^{0010} - D^{0001} \right|.$$
(35)

It is known to detect GHZ-like entanglement of a four-qubit state, vanishes on a W-like state of four qubits, however, fails to vanish on product of two-qubit entangled states. Four-qubit invariant of degree two

$$I_{4,2} = D^{0000} + D^{0011} - D^{0010} - D^{0001}$$
(36)

is the same as degree-two invariant H of ref. [28].

VI. THREE-TANGLES OF A FOUR-QUBIT STATE AND UNITARY INVARIANTS OF DEGREE EIGHT

To decipher the nature of correlations represented by $n_4(\rho_{1j})$ and $n_8(\rho_{1j})$, we write the characteristic polynomial of matrix $\rho_{1j}\rho_{1j}$ in terms of the state coefficients of $|\Psi_{1234}\rangle$ and identify the coefficients $n_4(\rho_{1j})$, $n_8(\rho_{1j})$, $n_{12}(\rho_{1j})$ and $n_{16}(\rho_{1j})$. A rather lengthy analytical calculation reveals that when two-qubit state ρ_{1j} is a marginal state of $|\Psi_{1234}\rangle$ then the coefficient $n_4(\rho_{1j})$ is a sum of squares of moduli of two-qubit invariants while the coefficient $n_8(\rho_{1j})$ is a sum of stree-qubit invariants. Expressions for $n_4(\rho_{1j})$ (Eq. (B14)) and $n_8(\rho_{1j})$ (Eq. (B15)) are given in subsection B 2 of Appendix B. The coefficient $n_8(\rho_{1j})$ can, in turn, be rewritten as a sum of four-qubit unitary invariant combinations of three-qubit invariants. This section deals with the relation between the three-tangle of a given triple in a four-qubit pure state and the corresponding four-qubit invariant. It is shown in the following section, that the coefficient $n_8(\rho_{1j})$, $\{j = 2, 3, 4\}$, is a function of two of the three-tangles $\tau_{1|j|k}(\rho_{1jk})$, $\{k = 2, 3, 4 : k \neq j\}$ and four-tangles.

It has been shown in our earlier works that given a three-qubit marginal state of a four-qubit state, the upper bound on three-tangle [29] depends on a specific unitary invariant [27] of the pure four-qubit state and genuine four-tangle of the state [27, 30]. Using the definition of three-tangle of a mixed state (Eq. (26)), we identify the four-qubit invariant which contains the three-tangle of a mixed state. For the state $|\Psi_{1234}\rangle$, the three-qubit invariants corresponding to $I_{3,4}(|\Psi_{123}\rangle)$ (Eq. (25)) read as

$$I_{A_4}^{4,0} = \left(D_{(A_4)_0}^{000} + D_{(A_4)_0}^{001}\right)^2 - 4D_{(A_3)_0(A_4)_0}^{00} D_{(A_3)_1(A_4)_0}^{00}.$$
(37)

and

$$I_{A_4}^{0,4} = \left(D_{(A_4)_1}^{000} + D_{(A_4)_1}^{001}\right)^2 - 4D_{(A_3)_0(A_4)_1}^{00} D_{(A_3)_1(A_4)_1}^{00}.$$
(38)

Here superscript in $I_{A_4}^{4,0}$ indicates that it is a three-qubit invariant of degree (4 + 0) that is each term is a product of four of the state coefficients, all of which have $i_4 = 0$, and none of them contains a state coefficient with $i_4 = 1$. Likewise, $I_{A_4}^{0,4}$ is a three-qubit invariant with each term being a product of four state coefficients all of which have $i_4 = 1$. The superscript contains information about the transformation properties of the invariant under the action of a unitary $U^4 = \frac{1}{\sqrt{1+|x|^2}} \begin{bmatrix} 1 & -x^* \\ x & 1 \end{bmatrix}$ on qubit A_4 . One can verify that $I_{A_4}^{4,0} \left(U^4 | \Psi_{1234} \rangle \right)$ is a function of three-qubit invariants contained in the set $\left\{ I_{A_4}^{4-m,m} : m = 0, 4 \right\}$. Here superscript in element $I_{A_4}^{4-m,m}$ indicates that it is a three-qubit invariant of degree four such that each term is a product of (4 - m) state coefficients with $i_4 = 0$, and m state coefficient with $i_4 = 1$.

The form of elements of the set in terms of determinants of negativity fonts is given in subsection B 3 of Appendix B. Four-qubit invariant that quantifies the three-way and genuine four-way correlations [27] of triple $A_1A_2A_3$, reads as

$$N_{4,8}^{(123)} = \left| I_{A_4}^{4,0} \right|^2 + 4 \left| I_{A_4}^{3,1} \right|^2 + 6 \left| I_{A_4}^{2,2} \right|^2 + 4 \left| I_{A_4}^{1,3} \right|^2 + \left| I_{A_4}^{0,4} \right|^2, \tag{39}$$

whereas the degree-eight invariant that measures genuine four-way entanglement of the state $|\Psi_{1234}\rangle$ is given by

$$I_{4,8} = 3\left(I_{A_4}^{2,2}\right)^2 - 4I_{A_4}^{3,1}I_{A_4}^{1,3} + I_{A_4}^{4,0}I_{A_4}^{0,4}.$$
(40)

First subscript in $N_{4,8}^{(123)}$ or $I_{4,8}$ indicates that it is a four-qubit invariant while the second subscript indicates the degree of the invariant.

On the other hand, for the mixed state $\rho_{123} = Tr_{A_4}(|\Psi_{1234}\rangle\langle\Psi_{1234}|) = \sum_{i=0,1} p_i \left|\phi_{123}^{(i)}\rangle\langle\phi_{123}^{(i)}\right|$, the three tangle (Eq. (26)) is given by

$$\left[\tau_{1|2|3}\left(\rho_{123}\right)\right]^{\frac{1}{2}} = 2 \min_{\left\{p_{i}, \left|\phi_{123}^{\left(i\right)}\right\rangle\right\}} \left\{ \left|I_{A_{4}}^{4,0}\right|^{\frac{1}{2}} + \left|I_{A_{4}}^{0,4}\right|^{\frac{1}{2}} \right\}.$$
(41)

It is known from ref. [29] that the upper bound on $\tau_{1|2|3}(\rho_{123})$, is given by

$$\tau_{1|2|3}^{up}\left(\rho_{123}\right) = \sqrt{16N_{4,8}^{(123)} - \frac{1}{6}\left(\tau_{1|2|3|4}^{(1)}\right)^2},\tag{42}$$

where $\tau_{1|2|3|4}^{(1)} = \sqrt{16 |12I_{4,8}|}$ is the genuine four-tangle defined in refs. [27, 30].

In general, for a selection of three qubits $A_1A_jA_k$, where j = 2 to 4 and k = 2 to 4, with the appropriate set of three-qubit invariants $\left\{I_{A_i}^{4-m,m}\left(|\Phi_i\rangle\right): m = 0, 4, i \neq j \neq k\right\}$, degree-eight invariant $N_{4,8}^{(1jk)}$ and three-tangle $\tau_{1|j|k}\left(\rho_{1jk}\right)$ satisfy the inequality

$$\sqrt{16N_{4,8}^{(1jk)} - \frac{1}{6} \left(\tau_{1|2|3|4}^{(1)}\right)^2} \ge \tau_{1|j|k} \left(\rho_{1jk}\right).$$
(43)

In case $\tau_{1|j|k}(\rho_{1jk}) = 0$, $16N_{4,8}^{(1jk)} = \frac{1}{6} \left(\tau_{1|2|3|4}^{(1)}\right)^2$. Expressions for $N_{4,8}^{(1jk)}$ and $\tau_{1|2|3|4}^{(1)}$ are given in subsection B4 of Appendix B.

VII. WHAT DOES COEFFICIENT $n_8(\rho_{1j})$ REPRESENT?

An analytical calculation reveals that for the two-qubit state, $\rho_{12} = Tr_{A_3A_4}(|\Psi_{1234}\rangle \langle \Psi_{1234}|)$, the coefficient $n_8(\rho_{12})$ is a sum of four-qubit invariants. Two of these four-qubit invariants are $N_{4,8}^{(123)}$ and $N_{4,8}^{(124)}$. The coefficient $n_8(\rho_{12})$ also contains contribution from $|3(I_{4,2})^2 - P_{12}|$, where $P_{1j}, (j = 2 \text{ to } 4)$ are already known from earlier works on polynomial invariants [31]. Subscripts on P_{1j} refer to the pair of qubits A_1A_j . The invariant P_{1j} is non zero if the qubit pair A_1A_j is entangled to the rest of the system in the four-qubit pure state $|\Psi_{1234}\rangle$. Detailed form of these invariants in terms of determinants of negativity fonts is given in subsection B 5 of appendix B. It is easily verified that $P_{1j}, (j = 2 \text{ to } 4)$ are not independent invariants because

$$P_{12} + P_{13} + P_{14} = 3 \left(I_{4,2} \right)^2. \tag{44}$$

The exact expression for coefficient $n_8(\rho_{12})$ reads as

$$n_{8}(\rho_{12}) = N_{4,8}^{(123)} + N_{4,8}^{(124)} + \frac{1}{24} \left| 3 \left(I_{4,2} \right)^{2} - P_{12} \right|^{2} + M_{4,8}(\rho_{12}), \qquad (45)$$

where $M_{4,8}(\rho_{12})$ is a sum of three-qubit invariants. Expression for $M_{4,8}(\rho_{1j})$ is also given in subsection B 5 of appendix B. Form of each term in $M_{4,8}(\rho_{12})$ reveals that this four-qubit invariant is non-zero only on a four-qubit state. Similarly the coefficients $n_8(\rho_{13})$ and $n_8(\rho_{14})$ read as

$$n_{8}(\rho_{13}) = N_{4,8}^{(123)} + N_{4,8}^{(134)} + \frac{1}{24} \left| 3(I_{4,2})^{2} - P_{13} \right|^{2} + M_{4,8}(\rho_{13}), \qquad (46)$$

and

$$n_{8}(\rho_{14}) = N_{4,8}^{(124)} + N_{4,8}^{(134)} + \frac{1}{24} \left| 3(I_{4,2})^{2} - P_{14} \right|^{2} + M_{4,8}(\rho_{14}), \qquad (47)$$

A comparison of $n_8(\rho_{1j})$ $\{j = 2, 3, 4\}$ with the upper bound on three-tangles from Eq. (43) shows that $n_8(\rho_{1j})$ is a function of two of the three-tangles $\tau_{1|j|k}(\rho_{1jk})$ such that

$$4n_8(\rho_{1j}) = \frac{1}{4} \sum_{k=2; k \neq j}^4 \tau_{1|j|k}^2(\rho_{1jk}) + \delta_{1j}, \qquad (48)$$

where

$$\delta_{1j} \ge \frac{1}{12} \left(\tau_{1|2|3|4}^{(1)} \right)^2 + \frac{1}{8} \left(\tau_{1|2|3|4}^{(2)} \left(\rho_{1j} \right) \right)^2 + \frac{3}{32} \left(\tau_{1|2|3|4}^{(3)} \left(\rho_{1j} \right) \right)^2.$$
(49)

Here we have defined four-tangles, $\tau_{1|2|3|4}^{(2)}(\rho_{1j}) = \sqrt{32M_{4,8}(\rho_{1j})}$ and $\tau_{1|2|3|4}^{(3)}(\rho_{1j}) = \left|4(I_{4,2})^2 - \frac{4}{3}P_{1j}\right|$. The quantity δ_{1j} is a function of four-way correlations. Eq. (48) represents an interesting condition on how three-way and four-way correlations are shared by qubits. For example, if $4n_8(\rho_{12}) = \frac{1}{4}$ and $\tau_{1|2|3}^2(\rho_{123}) = 1$, then $\tau_{1|2|4}^2(\rho_{124}) = 0$ and $\delta_{12} = 0$.

VIII. CONSTRAINT ON THREE-TANGLES AND FOUR-TANGLES

We may note that the sum of degree eight coefficients constrains the amount of three-way and four-way correlations in a four-qubit state. If $N_{4,8}^{(123)}$, $N_{4,8}^{(124)}$ as well as $N_{4,8}^{(134)}$ are non-zero, then the sum $4\sum_{j=2}^{4} n_8(\rho_{1j})$ is found to satisfy the constraint

$$4\sum_{j=2}^{4} n_8\left(\rho_{1j}\right) - \frac{1}{2} \left(\tau_{1|2|3}^2\left(\rho_{123}\right) + \tau_{1|2|4}^2\left(\rho_{124}\right) + \tau_{1|3|4}^2\left(\rho_{134}\right)\right) = \sum_{j=2}^{4} \delta_{1j}$$

$$\tag{50}$$

where the residue $\sum_{i=2}^{4} \delta_{1j}$ is a function of four-way correlations characterizing the pure state $|\Psi_{1234}\rangle$ and reads as

$$\sum_{j=2}^{4} \delta_{1j} \ge \frac{1}{4} \tau_{1|2|3|4}^{(1)} + \frac{3}{32} \sum_{j=2}^{4} \left(\tau_{1|2|3|4}^{(3)} \left(\rho_{1j} \right) \right)^2 + \frac{1}{8} \sum_{j=2}^{4} \left(\tau_{1|2|3|4}^{(2)} \left(\rho_{1j} \right) \right)^2.$$
(51)

By construction $\tau_{1|2|3|4}^{(3)}(\rho_{1j})$ is non-zero if and only if the qubit pair A_1A_j in the four-qubit state is entangled to the rest of the system. It is easily verified that $|P^{A_1A_2}| = |P^{A_3A_4}|, |P^{A_1A_3}| = |P^{A_2A_4}|, \text{ and } |P^{A_1A_4}| = |P^{A_2A_3}|, \text{ as such}, \sum_{j=2}^{4} \left(\tau_{1|2|3|4}^{(3)}(\rho_{1j})\right)^2$ does not depend on the choice of focus qubit.

Four tangles $\tau_{1|2|3|4}^{(0)}$, $\tau_{1|2|3|4}^{(1)}$, $\tau_{1|2|3|4}^{(2)}$, ρ_{1j} and $\tau_{1|2|3|4}^{(3)}$, ρ_{1j} are invariant with respect to a local unitary on anyone of the four qubits. Just as a three-tangle is defined only on states with $N \ge 3$, four-tangles are defined only on states with $N \ge 4$. Here, $\tau_{1|2|3|4}^{(0)}$ is defined in terms of a degree-two invariant, while $\tau_{1|2|3|4}^{(1)}$ is a function of a single four-qubit invariant of degree eight. The genuine four-tangle $\tau_{1|2|3|4}^{(1)} > 0$ implies that each one of the qubits is entangled to the three remaining qubits due to four-way correlations. A measurement on one of the four-qubits of a pure four-qubit

state completely destroys the entanglement quantified by $\tau_{1|2|3|4}^{(1)}$. Four-tangle $\tau_{1|2|3|4}^{(1)}$ is the analog of three-tangle for three-qubit states. On a W-state of four qubits we have $\tau_{1|2|3|4}^{(1)} = 0$.

To understand the role of four-tangle, $\tau_{1|2|3|4}^{(2)}(\rho)$, we consider a simple four-qubit state on which $\tau_{1|2|3|4}^{(2)}(\rho_{12}) \neq 0$ that is

$$|\chi\rangle = a_{0000} |0000\rangle + a_{1101} |1101\rangle + a_{1110} |1110\rangle.$$
(52)

One can verify that on $|\chi\rangle$, three tangles take value $\tau_{1|2|3}(\rho_{123}) = 4 \left| (a_{0000}a_{1110})^2 \right|, \tau_{1|2|4}(\rho_{124}) = 4 \left| (a_{0000}a_{1101})^2 \right|$ and

$$\left(\tau_{1|2|3|4}^{(2)}\left(\rho_{12}\right)\right)^{2} = 4\tau_{1|2|3}\tau_{1|2|4}.$$
(53)

On the other hand $\tau_{1|2|3|4}^{(2)}(\rho_{13}) = \tau_{1|2|3|4}^{(2)}(\rho_{14}) = 0$. Four-tangle $\tau_{1|2|3|4}^{(2)}(\rho_{1j})$ is a sum of nine three-qubit invariants of degree eight. It contains contributions from products of three-tangles of underlying three-qubit subsystems.

IX. CONSTRAINTS ON TANGLES OF A FOUR-QUBIT STATE

In the case of a three-qubit pure state monogamy relation is a relation between degree-four functions of state coefficients that is one-tangle $\tau_{1|23}(|\Psi_{123}\rangle)$, square of two-tangle $\tau_{1|j}^2(\rho_{1j})$ and three-tangle $\tau_{1|2|3}(|\Psi_{123}\rangle)$. Genuine four-way entanglement [27, 30], however, is quantified by a degree-eight function of state coefficients. Consequently, we have distinct sets of constraints to be satisfied by degree-four and degree-eight entanglement measures of correlations of a four-qubit state. A constraint on one-tangle and two-tangles is obtained by subtracting the sum of two tangles from Eq. (34) that is

$$S_{1} = \sum_{j=2}^{4} \left(n_{4} \left(\rho_{1j} \right) - \tau_{1|j}^{2} \left(\rho_{1j} \right) \right) - \frac{1}{2} \left(\tau_{1|2|3|4}^{(0)} \right)^{2}$$
$$= \tau_{1|234} - \sum_{j=2}^{4} \tau_{1|j}^{2} \left(\rho_{1j} \right), \tag{54}$$

where S_1 represents three- and four-way correlations.

The state ρ_{1j} $\{j = 2, 3, 4\}$ being a reduced state of ρ_{1jk} $\{k = 2, 3, 4 : k \neq j\}$ contains information about two-tangle $\tau_{1|j}(\rho_{1j})$, two of the three tangles $\tau_{1|j|k}(\rho_{1jk})$, as well as four-way correlations. If for a two-qubit marginal state ρ_{1j} $\{j = 2, 3, 4\}$ of $|\Psi_{1234}\rangle$, then the relation analogous to Eq. (12) reads as

$$n_4(\rho_{1j}) = \tau_{1|j}^2(\rho_{1j}) + \sqrt{4n_8(\rho_{1j}) + \chi^{\pm}(\rho_{1j})},$$
(55)

with $\chi^{\pm}(\rho_{1i})$ defined as in (Eqs. (13) and (14)) that is

$$\chi^{+}(\rho_{1j}) = 8\sqrt{n_{16}(\rho_{1j})} + 8\sqrt{f_{16}(\rho_{1j})} , \qquad (56)$$

and

$$\chi^{-}(\rho_{1j}) = 8\sqrt{n_{16}(\rho_{1j})} - 8\sqrt{f_{16}(\rho_{1j})} + 2n_4(\rho_{1j})|C(\rho_{1j})|^2 - |C(\rho_{1j})|^4 .$$
(57)

Recalling that for a two-qubit state $n_4(\rho_{1j}) = tr(\rho_{1j}\tilde{\rho}_{1j})$ is a calculable quantity, we obtain a set of three conditions to be satisfied by measures of two-way, three-way and four-way correlations. Substituting for coefficients $n_8(\rho_{1j})$ from Eqs. (48) into Eq. (55), we obtain the constraints:

$$\left(n_4\left(\rho_{1j}\right) - \tau_{1|j}^2\left(\rho_{1j}\right)\right)^2 - \frac{1}{4} \sum_{k=2, k\neq j}^4 \tau_{1|j|k}^2\left(\rho_{1jk}\right) = \Delta_{1j},\tag{58}$$

where $\Delta_{1j} = \delta_{1j} + \chi^{\pm}(\rho_{1j})$ and j = 2, 3, 4. Here $\delta_{1j} \ge 0$ (Eq. (49)), $n_{16}(\rho_{1j}) \ge 0$ and $f_{16}(\rho_{1j}) \ge 0$ 11) is valid. If $C(\rho_{1j}) \le 0$, then $\tau_{1|j}(\rho_{1j}) = 0$ and Eq. (58) reduces to

$$n_4^2(\rho_{1j}) - \frac{1}{4} \sum_{k=2, k \neq j}^4 \tau_{1|j|k}^2(\rho_{1jk}) = \Delta_{1j}.$$
(59)

Using Eq. (B14) and the definition of $\tau_{1|j|k}(\rho_{1jk})$ (Eq. (26)), one may verify that for $\tau_{1|j}(\rho_{1j}) = 0$, $n_4^2(\rho_{1j}) \ge \frac{1}{4} \sum_{k=2, k \neq j}^4 \tau_{1|j|k}^2(\rho_{1jk})$. As such, $\Delta_{1j} \ge 0$ is satisfied independent of the value of two-tangle. The quantity Δ_{1j} represents four-way correlations involving the qubit pair A_1A_j and the two remaining qubits of the four-qubit state. However, $\chi^-(\rho_{1j})$ may take negative values.

We notice that

$$\sum_{j=2}^{4} \left(n_4 \left(\rho_{1j} \right) - \tau_{1|j}^2 \left(\rho_{1j} \right) \right)^2 - \frac{1}{2} \left(\tau_{1|2|3}^2 \left(\rho_{123} \right) + \tau_{1|2|4}^2 \left(\rho_{124} \right) + \tau_{1|3|4}^2 \left(\rho_{134} \right) \right) = \sum_{j=2}^{4} \Delta_{1j} \tag{60}$$

where $\sum_{j=2}^{4} \Delta_{1j}$ may be taken as a degree-eight measure of residual correlations in the state $|\Psi_{1234}\rangle$. Substituting for $n_4(\rho_{1j}) - \tau_{1|j}^2(\rho_{1j})$ from Eq. (55) into Eq. (54), the constraint on one tangle may be written as

$$\tau_{1|234} + \frac{1}{2} \left(\tau_{1|2|3|4}^{(0)} \right)^2 - \sum_{j=2}^4 \tau_{1|j}^2 \left(\rho_{1j} \right) = \sum_{j=2}^4 \sqrt{\frac{1}{4} \sum_{k=2, k \neq j}^4 \tau_{1|j|k}^2 \left(\rho_{1jk} \right) + \Delta_{1j}}, \tag{61}$$

where the right hand side is a function of three-tangles of marginal three-qubit states as well as four-tangles of the pure four-qubit state. It is important to note that Eq. (61) is a relation between degree-four terms on left hand side and square root of sum of degree-eight terms on right hand side. Four-qubit states also satisfy the constraint on one-tangle reported in Eq. (47) of ref. ([13]) which involves only degree-four invariants. In that case, the contribution to one-tangle from three-qubit correlations due to the triple $A_1A_jA_k$ is found to vary between $\frac{1}{2}\tau_{1|j|k}(\rho_{1jk})$ and $\tau_{1|j|k}(\rho_{1jk})$, which is consistent with Eq. (61). Furthermore, on a state which is a product state of a three-qubit generic state with a single qubit, Eqs. (58) and (61) reduce to corresponding relations for three-qubits with the values of indices j and k restricted to 2 and 3 that is

$$n_4(\rho_{1j}) - \tau_{1|j}^2(\rho_{1j}) = \frac{1}{2} \tau_{1|2|3}(\rho_{123}); \qquad (j = 2, 3),$$
(62)

and

$$\tau_{1|234} - \sum_{j=2}^{3} \tau_{1|j}^{2} \left(\rho_{1j} \right) = \tau_{1|2|3} \left(\rho_{123} \right).$$
(63)

Alternatively, after expanding the L. H. S of Eq. (61) we may rewrite the relation between tangles as

$$\tau_{1|234} - \sum_{j=2}^{4} \tau_{1|j}^{2} \left(\rho_{1j}\right) - \frac{1}{2} \sum_{j=2}^{4} \left(\sum_{k=3,k>j}^{4} \tau_{1|j|k}^{2} \left(\rho_{1jk}\right)\right)^{\frac{1}{2}} \\ = \sum_{j=2}^{4} \sqrt{\Delta_{1j}} \left(1 - f_{1j}\right) - \frac{1}{2} \left(\tau_{1|2|3|4}^{(0)}\right)^{2}, \tag{64}$$

where f_{1j} is a function of $\frac{\sqrt{\Delta_{1j}\sum_{k=3,k>j}^{4}\tau_{1|j|k}^{2}(\rho_{1jk})}}{\sqrt{\Delta_{1j}}+\sqrt{\sum_{k=3,k>j}^{4}\tau_{1|j|k}^{2}(\rho_{1jk})}}$. Therefore the L.H.S of equation Eq. (64 represents four-way

correlations. To sum up, the tangles characterizing a four-qubit state satisfy the constraints represented by Eqs. (48, 50, 58, 60, 61) and Eq. (64). In the next subsections, we consider some examples to illustrate the validity of these constraints.

X. FOUR-QUBIT GHZ STATE

Consider the maximally entangled four-qubit GHZ state

$$|GHZ\rangle = \frac{1}{\sqrt{2}} \left(|0000\rangle + |1111\rangle\right). \tag{65}$$

Coefficients in the characteristic polynomial of the matrix $\rho_{1j}\tilde{\rho}_{1j}$ are

$$n_4(\rho_{1j}) = \frac{1}{2}, \quad 4n_8(\rho_{1j}) = \frac{1}{4},$$
(66)

$$n_{16}(\rho_{1j}) = n_{12}(\rho_{1j}) = 0; \quad (j = 2, 3, 4).$$
 (67)

As such $\chi(\rho_{1j}) = 0$, $4n_8(\rho_{1j}) = \Delta_{1j}$ (Eq. (48), and $\sum_{j=2}^4 \Delta_{1j} = \frac{3}{4}$ (Eq. (50)). While all two-tangles and three-tangles are zero on this state, values of four-tangles are $\tau_{1|2|3|4}^{(0)} = \tau_{1|2|3|4}^{(1)} = \tau_{1|2|3|4}^{(2)}(\rho_{1j}) = 1$, and $\tau_{1|2|3|4}^{(3)}(\rho_{1j}) = \frac{2}{3}$. One-tangle satisfies the relation

$$\tau_{1|234} = \sum_{j=2}^{4} n_4 \left(\rho_{1j}\right) - \frac{1}{2} \left(\tau_{1|2|3|4}^{(0)}\right)^2 = 1.$$
(68)

and since $n_4(\rho_{1j}) = \sqrt{\Delta_{1j}}$, one tangle represents only four-way correlations and satisfies Eq. (61).

XI. CLUSTER STATE

Much like the $|GHZ\rangle$ state, all two-tangles and three tangles are zero on the maximally entangled cluster state

$$|\Psi_C\rangle = \frac{1}{2} (|0000\rangle + |1100\rangle + |0011\rangle - |1111\rangle),$$
 (69)

and $\tau_{1|234} = \tau_{1|2|3|4}^{(1)} = \tau_{1|2|3|4}^{(2)} (\rho_{12}) = 1$ while $\tau_{1|2|3|4}^{(3)} (\rho_{12}) = \frac{2}{3}$. But differently from $|GHZ\rangle$, $\tau_{1|2|3|4}^{(0)} = \tau_{1|2|3|4}^{(2)} (\rho_{13}) = \tau_{1|2|3|4}^{(2)} (\rho_{13}) = \tau_{1|2|3|4}^{(3)} (\rho_{13}) = \tau_{1|2|3|4}^{(3)} (\rho_{14}) = \frac{1}{3}$. Therefore $4n_8 (\rho_{1j}) = \delta_{1j}$, $n_4 (\rho_{1j}) = \sqrt{\Delta_{1j}}$, $\chi^- (\rho_{1j}) = \Delta_{1j} - \delta_{1j}$, and $\tau_{1|234} = \sum_{j=2}^{4} n_4 (\rho_{1j})$. Table I lists the coefficients $n_d (\rho_{1j})$ for d = 4, 8, 12, 16 along with δ_{1j} , and $\chi^- (\rho_{1j})$, for j = 2, 3, 4 for the state $|\Psi_C\rangle$. One can verify that four-tangles satisfy the relation (refer to Eq. (49))

$$\sum_{j=2}^{4} \delta_{1j} = \frac{1}{4} \left(\tau_{1|2|3|4}^{(1)} \right)^2 + \frac{1}{8} \left(\tau_{1|2|3|4}^{(2)} \left(\rho_{12} \right) \right)^2 + \frac{3}{32} \sum_{j=2}^{4} \left(\tau_{1|2|3|4}^{(3)} \left(\rho_{1j} \right) \right)^2.$$
(70)

TABLE I: The coefficients $n_d(\rho_{1j})$ for d = 4, 8, 12, 16 along with $\Delta_{1j}, \delta_{1j}, \chi_{1j}, P_{1j}^2$ and $\tau_{1|2|3|4}^{(2)}(\rho_{1j})$ for j = 2, 3, 4 for the state $|\Psi_C\rangle$.

State $ \Psi_C\rangle$	$n_4\left(ho_{1j} ight)$	$n_8\left(ho_{1j} ight)$	$\left n_{12}\left(ho_{1j} ight) ight $	$n_{16}\left(ho_{1j} ight)$	δ_{1j}	$\chi^{-}\left(ho_{1j} ight)$
ρ_{12}	$\frac{1}{2}$	$\frac{1}{16}$	0	0	$\frac{1}{4}$	0
ρ_{13}	$\frac{1}{4}$	$\frac{3}{128}$	$\frac{1}{1024}$	$\frac{1}{65536}$	$\frac{3}{32}$	$-\frac{1}{32}$
ρ_{14}	$\frac{1}{4}$	$\frac{3}{128}$	$\frac{1}{1024}$	$\frac{1}{65536}$	$\frac{3}{32}$	$-\frac{1}{32}$
Sum	1	$\frac{7}{64}$			$\frac{7}{16}$	$-\frac{1}{16}$

It is interesting to compare the tangles of $|\Psi_C\rangle$ with the product of two-bell states that is

$$|\Psi_P\rangle = \frac{1}{2} \left(|00\rangle + |11\rangle\right) \left(|00\rangle + |11\rangle\right). \tag{71}$$

A simple calculation shows that $\tau_{1|234} = 1$, $\tau_{1|2}^2(\rho_{12}) = 1$, $(C_{12} = 1)$, $\tau_{1|3}^2(\rho_{12}) = \tau_{1|4}^2(\rho_{12}) = 0$, $(C_{13} = C_{14} = -\frac{1}{2})$, $\tau_{1|2|3|4}^{(0)}(|\Psi_P\rangle) = 1$ while Four tangles $\tau_{1|2|3|4}^{(1)}(|\Psi_P\rangle) = \tau_{1|2|3|4}^{(2)}(\rho_{1j}) = 0$. It turns out that $n_8(\rho_{1j}) = \frac{3}{2^7}$, $n_{12}(\rho_{1j}) = \frac{1}{2^{10}}$, $n_{16}(\rho_{1j}) = \frac{1}{2^{16}}$ and $f_{16}(\rho) = \frac{1}{2^{12}}$ for j = 3 and 4. Consequently, $n_4(1j) = C_{1j}^2$ indicating that the state does not have three or four-qubit correlations. Recalling that

$$\sum_{j=2}^{4} n_4 \left(1j\right) = \tau_{1|2}^2 \left(\rho_{12}\right) + \sum_{j=3}^{4} C_{1j}^2, \tag{72}$$

and one tangle satisfies the relation corresponding to Eq. (61), we obtain

$$\sum_{j=3}^{4} C_{1j}^2 = \frac{1}{2} \left(\tau_{1|2|3|4}^{(0)} \left(|\Psi_P\rangle \right) \right)^2, \tag{73}$$

clarifying that $\tau_{1|2|3|4}^{(0)}(|\Psi_P\rangle)$ does not quantify four-way correlations.

XII. STATES $L_{a,ia,(ia)_2}$

A natural extension of CKW inequality to four-qubit states may be written as

$$\tau_{1|234} \ge \sum_{j=2}^{4} \tau_{1|j}^{2} \left(\rho_{1j}\right) + \sum_{\substack{(j,k)=2\\k>j}}^{4} \tau_{1|j|k} \left(\rho_{1jk}\right).$$

$$\tag{74}$$

Regula et al. [9] have shown that a subset of four-qubit pure states violates the inequality of Eq. (74). Based on numerical evidence, the authors of [9] conjecture that four-qubit tangles satisfy a modified monogamy inequality, which for four-qubits with A_1 as focus qubit, (Eq. (9) in ref. [9]) reads as

$$\tau_{1|234} \left(|\Psi_{1234} \rangle \right) \ge \left[\tau_{1|2} \left(\rho_{12} \right) \right]^2 + \left[\tau_{1|3} \left(\rho_{13} \right) \right]^2 + \left[\tau_{1|4} \left(\rho_{14} \right) \right]^2 \\ + \left[\tau_{1|2|3} \left(\rho_{123} \right) \right]^{\frac{3}{2}} + \left[\tau_{1|2|4} \left(\rho_{124} \right) \right]^{\frac{3}{2}} + \left[\tau_{1|3|4} \left(\rho_{134} \right) \right]^{\frac{3}{2}}.$$
(75)

Here three tangles are raised to the power $\frac{3}{2}$, so that the "residual four tangle" may not become negative. Consider the product of a three qubit entangled state with the fourth qubit in state $|0\rangle$, that is

$$|\Psi_s\rangle = a_{0000} |0000\rangle + a_{1110} |1110\rangle, \qquad (76)$$

for which $\tau_{1|234}(|\Psi_{1234}\rangle) = \tau_{1|2|3}(\rho_{123}) = 4 |a_{0000}a_{1110}|^2$. The inequality of Eq. (75) implies that the state $|\Psi_s\rangle$ has a "residual four tangle" given by $\tau_{1|234}(|\Psi_{1234}\rangle) - [\tau_{1|2|3}(\rho_{123})]^{\frac{3}{2}}$, which is not true. On the other hand Eq. (61) yields $\tau_{1|234} = \tau_{1|2|3}(\rho_{123})$ on the state $|\Psi_s\rangle$, as expected.

It was also pointed out by Regula et al. [9] that states with particularly large violations of the inequality represented by Eq. (74) can be constructed by starting with the state L_{abc_2} of ref. [26] with b = c and additionally imposing b = c = ia with parameter $a \ge 0$, that is

$$L_{a,ia.(ia)_{2}} = a\left(\frac{1+i}{2}\right)(|0000\rangle + |1111\rangle) + a\left(\frac{1-i}{2}\right)(|0011\rangle + |1100\rangle) + ia(|0101\rangle + |1010\rangle) + |0110\rangle.$$
(77)

For these states, one tangle $\tau_{1|234} = \frac{8a^2 + 16a^4}{(4a^2 + 1)^2}$ satisfies Eq. (34). All three tangles have the same value that is $\tau_{1|2|3} = \tau_{1|3|4} = \tau_{1|2|4} = \frac{8a^3}{(4a^2 + 1)^2}$, genuine four-tangle $\tau_{1|2|3|4}^{(1)} = 0$ and $\left(\tau_{1|2|3|4}^{(0)}\right)^2 = \frac{4a^4}{(4a^2 + 1)^2}$. One can verify that (Eq. (48))

$$4n_8\left(\rho_{12}\right) = \frac{1}{4}\tau_{1|2|3}^2 + \frac{1}{4}\tau_{1|2|4}^2 + \frac{1}{8}\left(\tau_{1|2|3|4}^{(2)}\left(\rho_{12}\right)\right)^2,$$

where $\tau_{1|2|3|4}^{(2)}(\rho_{12}) = \frac{8\sqrt{3}a^4}{(4a^2+1)^2}$ and $\tau_{1|2|3|4}^{(3)}(\rho_{12}) = 0$. However $\tau_{1|2|3|4}^{(3)}(\rho_{13}) = \tau_{1|2|3|4}^{(3)}(\rho_{14}) = \frac{4\sqrt{5}a^4}{(4a^2+1)^2}$, while the value of four-tangle $\tau_{1|2|3|4}^{(2)}(\rho_{13}) = \tau_{1|2|3|4}^{(2)}(\rho_{13}) = \tau_{1|2|3|4}^{(2)}(\rho_{13}) = \tau_{1|2|3|4}^{(2)}(\rho_{14}) = \frac{4a^3\sqrt{6a^2+10}}{(4a^2+1)^2}$ consistent with $4n_8(\rho_{13}) = 4n_8(\rho_{14})$. By using the values of $n_4(\rho_{1j})$ calculated from reduced two-qubit states,

$$n_4(\rho_{12}) = \frac{4(a^4 + a^2)}{(4a^2 + 1)^2}; n_4(\rho_{13}) = n_4(\rho_{14}) = \frac{(2a^2 + 7a^4)}{(4a^2 + 1)^2},$$

net four-way correlations can be calculated from the constraint (Eq. (60)),

$$\sum_{j=2}^{4} \left(n_4 \left(\rho_{1j} \right) - \tau_{1|j}^2 \left(\rho_{1j} \right) \right)^2 - \frac{1}{2} \left(\tau_{1|2|3}^2 + \tau_{1|2|4}^2 + \tau_{1|3|4}^2 \right) = \sum_{j=2}^{4} \Delta_{1j}.$$



FIG. 1: Plot of one-tangle $\tau_{1|234}$ (black solid line), $S_1 = \tau_{1|234} - \sum_{j=2}^4 \tau_{1|j}^2 (\rho_{1j})$ (Red dash), an estimate of residual correlations $S = S_1 - \left[\frac{1}{2} \left(\tau_{1|2|3}^2 + \tau_{1|2|4}^2 + \tau_{1|3|4}^2\right)\right]^{\frac{1}{2}}$ (Dark Green Dash Dot), and partial four-way correlations $R = \sum_{j=2}^4 \delta_{1j}$ (blue dot-dot), versus state parameter *a* for the states $L_{a,ia.(ia)_2}$.

Figure (1) displays one-tangle $\tau_{1|234}$, the sum of three-way and four-way correlations $S_1 = \tau_{1|234} - \sum_{j=2}^4 \tau_{1|j}^2 (\rho_{1j})$ (Eq. (54)), estimated four-way correlations $S = S_1 - \left[\frac{1}{2}\left(\tau_{1|2|3}^2 + \tau_{1|2|4}^2 + \tau_{1|3|4}^2\right)\right]^{\frac{1}{2}}$, and partial residual four-way correlations quantified by $R = \left[\sum_{j=2}^4 \delta_{1j}\right]^{\frac{1}{2}}$, versus state parameter *a* for the states $L_{a,ia.(ia)_2}$. We notice that $S \ge 0$ and $R \ge 0$ for all the values of *a*, as expected.

XIII. CLASSIFICATION OF FOUR-QUBIT STATES

Three-qubit states have been shown to belong to six equivalent classes under stochastic local operations and classical communication (SLOCC) In [20]. However, N > 3, there are infinite SLOCC classes [33], as such it is highly desirable to partition the infinite classes into a finite number of families. [26], Verstraete et al. have shown that there are nine families in four-qubit entanglement. Residue δ_{1j} is greater or equal to weighted sum of four tangles. These tangles are natural labels for fully entangled four-qubit states. Besides that, three tangles, and two-tangles of sub-systems are helpful to understand the extent to which the states can be manipulated by local operations. In a recent articles [34] a classification of four-qubit states based on graph states is given. The underlying spirit of this classification is similar to ours, however our classification has the advantage that the entanglement quantifiers obey the monogamy constraints listed in Eqs. (48,50,58,60,61,64).

We notice that the four qubit states may be grouped together in finite number of entanglement types by using a set of unitary invariant functions of state coefficients to label the states. The set contains - two-tangles to quantify the entanglement of two qubit sub-systems, $\tau_{i|j|k}$ to quantify entanglement of sub-systems due to three-way correlations, and $\tau_{1|2|3|4}^{(1)}$, $\tau_{1|2|3|4}^{(2)}$, (ρ_{1j}) , and $\tau_{1|2|3|4}^{(3)}$, (ρ_{1j}) , (j = 2 - 4) to quantify entanglement due to four-way correlations. Besides that we can also use the unitary invariant coefficients n_{12} , (ρ_{1j}) and n_{16} , (ρ_{1j}) , j = 2, 3, 4, to distinguish between different entanglement types. On the basis of these invariants, four-qubit entangled states lie in the following groups:

Group I - Two-qubit and three qubit subsystems are entangled. Some or all of the four-tangles are non-zero.

Group II - Three qubit subsystems are entangled. Some or all of the four-tangles are non-zero.

Group III - Two-qubit subsystems are entangled. Some or all of the four-tangles are non-zero.

$Class \Rightarrow$	L_{abc_2}	Laba	L_{a_A}	$L_{0_{7\oplus 1}}$	$L_{05\oplus 3}$	$L_{a_2b_2}$	G_{abcd}	$L_{a_20_{3\oplus 1}}$
Tangle \Downarrow				-101	-000			~2·501
$\tau_{1 2 3 4}^{(2)}(\rho_{1j})$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$
$ au_{1 2 3 4}^{(1)}$	$\neq 0$	0	0	0	0	$\neq 0$	$\neq 0$	$\neq 0$
$\tau^{(3)}_{1 2 3 4}(\rho_{13})$	$\neq 0$	$\neq 0$	0	0	0	$\neq 0$	$\neq 0$	$\neq 0$
$\tau_{1 2 3 4}^{(3)}\left(\rho_{12}\right),\tau_{1 2 3 4}^{(3)}\left(\rho_{14}\right)$	$\neq 0$	$\neq 0$	$\neq 0$	0	0	$\neq 0$	$\neq 0$	$\neq 0$
$\tau_{1 3 4}$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	0	0	0	0
$\tau_{1 2 3}$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	0	0	0
$\tau_{1 2 4}$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	0	0
$ \tau_{1 2}^2$	$\neq 0$	$\neq 0$	$\neq 0$	0	0	$\neq 0$	$\neq 0$	$\neq 0$
$\tau_{1 3}^2$	$\neq 0$	$\neq 0$	$\neq 0$	0	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$
$ \tau_{1 2}^2$	$\neq 0$	$\neq 0$	$\neq 0$	0	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$
$n_{16}(\rho_{12})$	$\neq 0$	$\neq 0$	$\neq 0$	0	0	$\neq 0$	$\neq 0$	0
$n_{16}(ho_{13})$	$\neq 0$	$\neq 0$	0	0	0	$\neq 0$	$\neq 0$	0
$n_{16}(\rho_{14})$	$\neq 0$	$\neq 0$	$\neq 0$	0	0	$\neq 0$	$\neq 0$	0

TABLE II: Entanglement measures for four-qubit entangled states. Class refers to group of states [26] which gives rise to tangles when qubit A_1 is the focus qubit. Qubit A_1 is separable in class $L_{0_{3+\overline{1}}0_{3+\overline{1}}}$.

Group IV - Two-qubit subsystems are entangled. All of the four-tangles are zero. Four-way entanglement arises due to pair-wise entanglement.

The states in the nine classes of four-qubit states [26] fit in Groups I, II and III. Table II is a list of tangles useful to label eight classes of four-qubit entangled states [26]. The parameters characterizing the states are taken to have distinct values. With the exception of $L_{0_{3+\bar{1}}0_{3+\bar{1}}}$ states, the four-tangle $\tau_{1|2|3|4}^{(2)}(\rho_{1j}) \neq 0$ on nine classes of states listed in ref. [26]. Class L_{abc_2} contains states on which all four tangles, three tangles, and two-tangles are non-zero. States in classes L_{ab_3} , L_{a_4} , $L_{0_{7\oplus 1}}$, and $L_{0_{5\oplus 3}}$ have $\tau_{1|2|3|4}^{(1)}(\rho_{1j}) = 0$. State $L_{0_{5\oplus 3}}$ is special in that the four-tangle $\tau_{1|2|3|4}^{(2)}(\rho_{1j})$ is product of three tangles. For states in G_{abcd} and $L_{a_20_{3\oplus 1}}$, three-qubit subsystems have zero three tangles. An example of states in Group IV is maximally entangled W-state,

$$\left|\widetilde{W}\right\rangle = \frac{1}{2} \left(\left|0000\right\rangle + \left|1100\right\rangle + \left|1010\right\rangle + \left|1001\right\rangle\right).$$

All four-tangles and three-tangles are zero on state $|\widetilde{W}\rangle$, and four-way entanglement is due to two-way correlations. The state $L_{0_{3+\overline{1}}0_{3+\overline{1}}}$ does not have four-qubit entanglement.

XIV. ENTANGLEMENT TRANSFER TO ENVIRONMENT

If one of the two entangled qubits, interacts successively with environment qubits resulting in an increase in residual correlations, then the entanglement of the pair tends to zero. Here we present a toy model that uses CNOT Gate to generate additional correlations between qubit one and the environment represented by a product state of additional qubits. For simplicity a single parameter model with two qubits, initially in pure state $|\Psi_{12}\rangle = \frac{1}{\sqrt{x}} (|00\rangle + \sqrt{x-1} |11\rangle)$, is considered. Environment qubits are in a product state $\prod_{j} |\phi_{j}\rangle$ where $|\phi_{j}\rangle = \frac{1}{\sqrt{x}} (|0\rangle + \sqrt{x-1} |1\rangle)$, as such the

initial state of the system

$$\left|\Psi_{12}\right\rangle\left|E\right\rangle = \frac{1}{\sqrt{x}}\left(\left|00\right\rangle + \sqrt{x-1}\left|11\right\rangle\right)\left|\phi_{3}\right\rangle\left|\phi_{4}\right\rangle\ldots\left|\phi_{N}\right\rangle\right\rangle$$

is an entangled state with one tangle $\tau_{1|2E} = \tau_{1|2}^2$ given by

$$\tau_{1|2}^{2} = \frac{4(x-1)}{x^{2}} = n_{4}(\rho_{12}); \quad n_{8}(\rho_{12}) = 0; x \neq 0, 1.$$



FIG. 2: Circuit model for entanglement transfer

A CNOT gate on qubit pair A_1A_3 generates three-way correlations with a decrease in two-tangle, while the value of one-tangle is not changed. After this step the system is in state $|\Psi_{123}\rangle|E_{N-1}\rangle$ and $\tau_{1|2}^2 = \left(\frac{4(x-1)}{x^2}\right)^2$. Next step is applying a CNOT to qubit pair A_1A_4 with A_4 as target qubit. Successive applications of CNOT, always with qubit A_1 as control qubit and one of the environment qubits as target qubit, do not change $\tau_{1|2E}$, but generate correlations distributed over a larger number of qubits. One can verify that after M applications of CNOT (M varies from 1 to N-2), two tangles of the state satisfy

$$\tau_{1|2}^{2}(\rho_{12}) = \left(\frac{4(x-1)}{x^{2}}\right)^{M+1}; \quad \tau_{1|j}^{2}(\rho_{1j}) = 0 \text{ for } j = 3 \text{ to N}.$$

whereas residual correlations are given by

$$\tau_{1|2E} - \tau_{1|2}^2 \left(\rho_{12} \right) = \frac{4 \left(x - 1 \right)}{x^2} - \left(\frac{4 \left(x - 1 \right)}{x^2} \right)^{M+1}.$$

Fig. (3) displays $\tau_{1|2E}$, $\tau_{1|2}^2(\rho_{12})$ and residual correlations Δ for M = 1 and M = 8 as a function of variable x. One may notice that for x = 2, no entanglement transfer to additional qubits occurs. After eight steps most of the two-way correlations have leaked to environment for x = 6. Notably, interaction with a single qubit (M = 1) which generates only three-way correlations, results in $\tau_{1|2}^2(\rho_{12}) = \Delta$ for $x_1 = 1.1716$ and $x_2 = 6.8284$.

XV. CONCLUDING REMARKS

Two-tangle (refs. [15, 16]) of a two-qubit mixed state ρ is a known function of eigenvalues of non Hermitian matrix $\rho\tilde{\rho}$ where $\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y)$. As shown in ref. [7] if the state ρ is known to be part of an *N*-qubit system in a pure state then the non-Hermitian matrix $\rho\tilde{\rho}$ can be used to extract information about the correlations of the pair of qubits with (N-2) qubits in the state $|\Psi_N\rangle$. In this article it is shown that if a two-qubit state is a marginal state of a four-qubit pure state then the residual correlations are quantified by well defined unitary invariant functions of state coefficients.



FIG. 3: Plot of one-tangle $\tau_{1|234}$ (black solid line), $\tau_{1|2}^2$ (red dash), Residual correlations Δ (blue dots) for M = 8 and $\tau_{1|2}^2$ (wine dash dot), Residual correlations Δ (navy blue dash dot dot) for M = 1.

Our main result is the set of constraints on one-tangle of a focus qubit, two-tangles, three-tangles and four-way correlations, obtained by expressing the coefficients in the characteristic polynomial of $\rho\tilde{\rho}$ in terms of state coefficients of a four-qubit pure state. The tangles characterizing a four-qubit state satisfy the constraints represented by Eqs. (48, 50, 58, 60, 61) and Eq. (64). The residual four-qubit correlations obtained by subtracting two-tangles and three-tangles as in Eqs. (58) represent contributions from all possible four-qubit entanglement modes. One tangle of a four-qubit pure state satisfies the constraints given by Eqs. (61) and (64) independent of the class to which a given four-qubit state belongs. In particular, these constraints are satisfied by the set of states $L_{a,ia.(ia)_2}$ of ref. [26] that violate the entanglement monogamy relation obtained by generalizing the CKW inequality. The difference between one tangle and contributions from two-tangles and three-tangles in Eq. (64) represents the residual correlations beyond three-way correlations present in a 4-qubit pure state.

Four tangles $\tau_{1|2|3|4}^{(0)}$, $\tau_{1|2|3|4}^{(1)}$, $\tau_{1|2|3|4}^{(2)}$, (ρ_{1j}) and $\tau_{1|2|3|4}^{(3)}$, (ρ_{1j}) , (j = 2 - 4), may be used to identify and label entangled states that are equivalent under local unitary transformations. Local unitary equivalence is an important marker to group together states with similar properties. Using the elements of the set containing two-tangles, three-tangles and four-tangles to label four-qubit states the states in nine classes of four-qubit states [26], and W state are grouped together in four-groups as shown in Table II. Using a simple circuit model, monogamy of entanglement is also shown to result in loss of entanglement of a pair of qubits when one of the qubits interacts successively with environment qubits.

This work reveals constraints on the sharing of entanglement at multiple levels and offers insight into quantification of those features of quantum correlations, which only emerge beyond the bipartite scenario. It will be interesting to investigate the interplay between the entanglement trade-off and frustration phenomena in complex quantum systems [35]. Our approach also paves the way to understanding scaling of entanglement distribution as qubits are added to obtain larger multiqubit quantum systems.

Appendix A: Derivation of Eq. (10)

To obtain Eq. (10) we use the expressions for the coefficients $n_d(\rho)$ (d = 4, 8, 12, 16) in terms of eigenvalues of matrix $(\rho\tilde{\rho})$, Eqs. (7), (8) and (9) along with the condition $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ and $C(\rho) = \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}$, that is

$$n_{4}(\rho) - |C(\rho)|^{2} = (\lambda_{1} + \lambda_{2} + \lambda_{3} + \lambda_{4}) - (\sqrt{\lambda_{1}} - \sqrt{\lambda_{2}} - \sqrt{\lambda_{3}} - \sqrt{\lambda_{4}})^{2}$$

$$= 2\sqrt{\left(\frac{\sqrt{\lambda_{1}}(\sqrt{\lambda_{2}} + \sqrt{\lambda_{3}} + \sqrt{\lambda_{4}})}{-(\sqrt{\lambda_{2}}\sqrt{\lambda_{3}} + \sqrt{\lambda_{2}}\sqrt{\lambda_{4}} + \sqrt{\lambda_{3}}\sqrt{\lambda_{4}})}\right)^{2}}$$

$$= 2\sqrt{n_{8}(\rho) + 2\sqrt{n_{16}(\rho)} + 2C(\rho)\left(\frac{\sqrt{\lambda_{1}}\sqrt{\lambda_{2}}\sqrt{\lambda_{3}} + \sqrt{\lambda_{1}}\sqrt{\lambda_{2}}\sqrt{\lambda_{4}}}{+\sqrt{\lambda_{1}}\sqrt{\lambda_{3}}\sqrt{\lambda_{4}} - \sqrt{\lambda_{2}}\sqrt{\lambda_{3}}\sqrt{\lambda_{4}}}\right)}$$
(A1)

Furthermore, we can rewrite the expression given above as

$$n_{4}(\rho) = |C(\rho)|^{2} + 2\sqrt{\frac{n_{8}(\rho) + 2\sqrt{n_{16}(\rho)}}{\sqrt{n_{12}(\rho) + \sqrt{n_{16}(\rho)}\left(n_{4}(\rho) - |C(\rho)|^{2}\right)}}}.$$
(A2)

Substituting $C(\rho) = \pm |C(\rho)|$ in Eq. (A2), the coefficient $n_4(\rho)$ satisfies the relation

$$n_4(\rho) = |C(\rho)|^2 + 2\sqrt{n_8(\rho) + 2\sqrt{n_{16}(\rho)} \pm 2\sqrt{f_{16}(\rho)}},$$
(A3)

where

$$f_{16}(\rho) = |C(\rho)|^2 \left(n_{12}(\rho) + \sqrt{n_{16}(\rho)} \left(n_4(\rho) - |C(\rho)|^2 \right) \right).$$
(A4)

Appendix B: Expressions for $n_4(\rho_{1j})$, $n_8(\rho_{1j})$, $\{I_{A_4}^{4-m,m}: m = 0, 4\}$, $N_{4,8}^{(1jk)}$ and P_{1j} in terms of two-qubit unitary invariants

1. Notation

In this subsection we set up the notation used to express the relevant three and four-qubit invariants in terms of two-qubit unitary invariants. In section (V) a general four-qubit pure state was written as

$$|\Psi_{1234}\rangle = \sum_{i_1, i_2, i_3} \left(a_{i_1 i_2 i_3 0} \left| i_1 i_2 i_3 0 \right\rangle + a_{i_1 i_2 i_3 1} \left| i_1 i_2 i_3 1 \right\rangle \right), \quad (i_m = 0, 1),$$
(B1)

and the determinants of negativity fonts of the state defined as $D^{00}_{(A_3)_{i_3}(A_4)_{i_4}} = a_{00i_3i_4}a_{11i_3i_4} - a_{10i_3i_4}a_{01i_3i_4}$ (two-way), $D^{00}_{(A_2)_{i_2}(A_4)_{i_4}} = a_{00i_3i_4}a_{1i_2i_1} - a_{1i_2i_30}a_{0i_2i_1}$ (two-way), $D^{00}_{(A_2)_{i_2}(A_3)_{i_3}} = a_{0i_2i_30}a_{1i_2i_31} - a_{1i_2i_30}a_{0i_2i_31}$ (two-way), $D^{00i_4}_{(A_4)_{i_4}} = a_{00i_3i_4}a_{11i_3\oplus 1,i_4} - a_{10i_3i_4}a_{01,i_3\oplus 1,i_4}$ (three-way), $D^{00i_4}_{(A_3)_{i_3}} = a_{00i_3i_4}a_{11i_3,i_4\oplus 1} - a_{10i_3i_4}a_{01i_3,i_4\oplus 1}$ (three-way), $D^{00i_4}_{(A_2)_{i_2}} = a_{0i_20i_4}a_{1i_21i_4\oplus 1} - a_{1i_20i_4}a_{0i_21i_4\oplus 1}$ (three-way), and $D^{00i_3i_4} = a_{00i_3i_4}a_{11,i_3\oplus 1,i_4\oplus 1} - a_{10i_3i_4}a_{01,i_3\oplus 1,i_4\oplus 1}$ (fourway). The notation for two-qubit unitary invariants for qubit pairs A_1A_2 , A_1A_3 , and A_1A_4 follows. The set of invariants with respect to unitary transformations on qubits A_1 and A_2 are given by

$$E_2 = D_{(A_3)_0(A_4)_0}^{00}, D_2 = D_{(A_3)_1(A_4)_1}^{00}, C_2 = D_{(A_3)_1(A_4)_0}^{00}, B_2 = D_{(A_3)_0(A_4)_1}^{00}, B_3 = D_{(A_3)_0(A_4)_1}^{00}, B_4 = D_{(A_3)_0(A_4)_1}^{00}$$

$$F_2 = D_{(A_4)_0}^{000} + D_{(A_4)_0}^{001}, L_2 = D_{(A_4)_1}^{000} + D_{(A_4)_1}^{001},$$
(B3)

$$G_2 = D_{(A_3)_0}^{000} + D_{(A_3)_0}^{001}, K_2 = D_{(A_3)_1}^{000} + D_{(A_3)_1}^{001},$$
(B4)

$$H_{02} = D^{0000} + D^{0011}, H_{12} = D^{0001} + D^{0010}.$$
 (B5)

Two-qubit invariants with respect to unitaries on qubits A_1 and A_3 are denoted by

$$E_3 = D^{00}_{(A_2)_0(A_4)_0}, D_3 = D^{00}_{(A_2)_1(A_4)_1}, C_3 = D^{00}_{(A_2)_1(A_4)_0}, B_3 = D^{00}_{(A_2)_0(A_4)_1},$$
(B6)

$$F_3 = D_{(A_4)_0}^{000} - D_{(A_4)_0}^{001}, L_3 = D_{(A_4)_1}^{000} - D_{(A_4)_1}^{001},$$
(B7)

$$G_3 = D_{(A_2)_0}^{000} + D_{(A_2)_0}^{001}, K_3 = D_{(A_2)_1}^{000} + D_{(A_4)_1}^{001},$$
(B8)

$$H_{03} = D^{0000} - D^{0010}, H_{13} = D^{0001} - D^{0011}.$$
 (B9)

Invariants with respect to unitaries on qubits \mathbf{A}_1 and \mathbf{A}_4 read as

$$E_4 = D^{00}_{(A_2)_0(A_3)_0}, D_4 = D^{00}_{(A_2)_1(A_3)_1}, C_4 = D^{00}_{(A_2)_1(A_3)_0}, B_4 = D^{00}_{(A_2)_0(A_3)_1},$$
(B10)

$$F_4 = D_{(A_3)_0}^{000} - D_{(A_3)_0}^{001}, L_4 = D_{(A_3)_1}^{000} - D_{(A_3)_1}^{001},$$
(B11)

$$G_4 = D_{(A_2)_0}^{000} - D_{(A_2)_0}^{001}, K_4 = D_{(A_2)_1}^{000} - D_{(A_4)_1}^{001},$$
(B12)

$$H_{04} = D^{0000} - D^{0001}, H_{14} = D^{0010} - D^{0011},$$
(B13)

2. The coefficients $n_4(\rho_{1j})$ and $n_8(\rho_{1j})$

The coefficient $n_4(\rho_{1j}) = tr(\rho_{1j}\widetilde{\rho_{1j}})$ is found to have the form

$$n_4(\rho_{1j}) = 4\left(|E_j|^2 + |B_j|^2 + |C_j|^2 + |D_j|^2\right) + 2\left(|G_j|^2 + |K_j|^2\right) + 2\left(|F_j|^2 + |L_j|^2\right) + |H_{0j} + H_{1j}|^2 + |H_{0j} - H_{1j}|^2.$$
(B14)

Maximum value of $n_4(\rho_{1j})$ is one.

The degree eight coefficient $n_8(\rho_{1j}) = \frac{1}{2} \left(tr(\rho_{1j}\widetilde{\rho_{1j}}) \right)^2 - \frac{1}{2} tr\left(\left(\rho_{1j}\widetilde{\rho_{1j}}\right)^2 \right)$, which is a function of three-qubit invariants reads as

$$n_{8}(\rho_{1j}) = |G_{j}^{2} - 4E_{j}B_{j}|^{2} + |K_{j}^{2} - 4C_{j}D_{j}|^{2} + |F_{j}^{2} - 4E_{j}C_{j}|^{2} + |L_{j}^{2} - 4B_{j}D_{j}|^{2} + |H_{0j}^{2} - 4E_{j}D_{j}|^{2} + |H_{1j}^{2} - 4B_{j}C_{j}|^{2} + 2|G_{j}K_{j} - F_{j}L_{j}|^{2} + 2|H_{0j}H_{1j} - G_{j}K_{j}|^{2} + 2|(H_{0j}H_{1j} - F_{j}L_{j})|^{2} + 2|F_{j}G_{j} - 2E_{j}H_{1j}|^{2} + 2|F_{j}K_{j} - 2C_{j}H_{0j}|^{2} + 2|G_{j}L_{j} - 2B_{j}H_{0j}|^{2} + 2|K_{j}L_{j} - 2H_{1j}D_{j}|^{2} + 2|H_{0j}F_{j} - 2E_{j}K_{j}|^{2} + 2|H_{0j}G_{j} - 2E_{j}L_{j}|^{2} + 2|H_{0j}K_{j} - 2F_{j}D_{j}|^{2} + 2|H_{0j}L_{j} - 2G_{j}D_{j}|^{2} + 2|H_{1j}F_{j} - 2C_{j}G_{j}|^{2} + 2|H_{1j}K_{j} - 2C_{j}L_{j}|^{2} + 2|H_{1j}G_{j} - 2B_{j}F_{j}|^{2} + 2|H_{1j}L_{j} - 2B_{j}K_{j}|^{2}$$
(B15)

One can verify that $0 \leq 16n_8 (\rho_{1j}) \leq 1$.

3. Degree four three-qubit invariants $\left\{I_{A_4}^{4-m,m}:m=0,4\right\}$

Degree four three-qubit invariants of a four-qubit state relevant to constructing the upper bound on $\tau_{1|2|3}(\rho_{123})$ in terms of two-qubit invariants for the pair A_1A_2 are listed below:

$$I_{A_4}^{4,0} = F_2^2 - 4E_2C_2; I_{A_4}^{0,4} = L_2^2 - 4B_2D_2,$$
(B16)

$$I_{A_4}^{3,1} = \frac{1}{2} F_2 \left(H_{02} + H_{12} \right) - \left(E_2 K_2 + C_2 G_2 \right), \tag{B17}$$

$$I_{A_4}^{1,3} = \frac{1}{2} L_2 \left(H_{02} + H_{12} \right) - \left(B_2 K_2 + D_2 G_2 \right), \tag{B18}$$

and

$$I_{A_4}^{2,2} = \frac{1}{6} \left(H_{02} + H_{12} \right)^2 - \frac{2}{3} G_2 K_2 + \frac{1}{3} F_2 L_2 - \frac{2}{3} \left(E_2 D_2 + B_2 C_2 \right).$$
(B19)

4. Degree eight invariants $N_{4,8}^{\left(123\right)},N_{4,8}^{\left(134\right)}$ and $N_{4,8}^{\left(143\right)}$

In order to write down the coefficients $n_8(\rho_{1j}), \{j = 2 - 4\}$, we need the form of $N_{4,8}^{(123)}, N_{4,8}^{(134)}$ and $N_{4,8}^{(143)}$. The coefficients $N_{4,8}^{(123)}$ and $N_{4,8}^{(143)}$ are obtained by substituting, respectively, j = 2 and 4 in the following equation:

$$N_{4,8}^{(1j3)} = \left| \left(F_j^2 - 4E_j C_j \right) \right|^2 + \left| \left(H_{0j} + H_{1j} \right) F_j - 2E_j K_j - 2C_j G_j \right|^2 + \frac{1}{6} \left| \left(H_{0j} + H_{1j} \right)^2 - 4G_j K_j + 2F_j L_j - 4B_j C_j - 4E_j D_j \right|^2 + \left| \left(H_{0j} + H_{1j} \right) L_j - 2G_j D_j - 2B_j K_j \right|^2 + \left| L_j^2 - 4B_j D_j \right|^2,$$
(B20)

whereas $N_{4,8}^{(124)}$ is given by

$$N_{4,8}^{(124)} = \left| \left(G_3^2 - 4E_3 B_3 \right) \right|^2 + \left| \left(H_{03} + H_{13} \right) G_3 - 2E_3 L_3 - 2B_3 F_3 \right|^2 + \frac{1}{6} \left| \left(H_{03} + H_{13} \right)^2 + 2G_3 K_3 - 4F_3 L_3 - 4E_3 D_3 - 4B_3 C_3 \right|^2 + \left| \left(H_{03} + H_{13} \right) K_3 - 2F_3 D_3 - 2C_3 L_3 \right|^2 + \left| \left(K_3^2 - 4C_3 D_3 \right) \right|^2.$$
(B21)

5. Invariants P_{1j} and $M_{4,8}(\rho_{1j})$

Invariants P_{1j} are degree four functions of determinants of negativity fonts and read as

$$P_{1j} = (H_{0j} + H_{1j})^2 - 4F_jL_j - 4G_jK_j + 8E_jD_j + 8B_jC_j.$$
(B22)

Term $M_{4,8}(\rho_{1j})$ is a sum of three-qubit invariants, that is

$$M_{4,8}(\rho_{1j}) = 2 |F_j G_j - 2E_j H_{1j}|^2 + |((H_{1j} - H_{0j}) G_j + 2E_j L_j - 2B_j F_j)|^2 + 2 |G_j L_j - 2B_j H_{0j}|^2 + |((H_{1j} - H_{0j}) F_j + 2E_j K_j - 2C_j G_j)|^2 + \frac{1}{2} |H_{1j}^2 - H_{0j}^2 + 4E_j D_j - 4B_j C_j|^2 + |((H_{1j} - H_{0j}) L_j + 2G_j D_j - 2B_j K_j)|^2 + 2 |F_j K_j - 2C_j H_{0j}|^2 + |(H_{1j} - H_{0j}) K_j + 2F_j D_j - 2C_j L_j|^2 + 2 |K_j L_j - 2D_j H_{1j}|^2.$$
(B23)

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