

A relation among tangle, 3-tangle, and von Neumann entropy of entanglement for three qubits

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In this paper, we derive a general formula of the tangle for pure states of three qubits, and present three explicit local unitary (LU) polynomial invariants. Our result goes beyond the classical work of tangle, 3-tangle and von Neumann entropy of entanglement for Acín et al.'s Schmidt decomposition (ASD) of three qubits by connecting the tangle, 3-tangle, and von Neumann entropy for ASD with Acín et al.'s LU invariants. In particular, our result reveals a general relation among tangle, 3-tangle, and von Neumann entropy, together with a relation among their averages. The relations can help us find the entangled states satisfying distinct requirements for tangle, 3-tangle, and von Neumann entropy. Moreover, we obtain all the states of three qubits of which tangles, concurrence, 3-tangle and von Neumann entropy don't vanish and these states are enduring when one of three qubits is traced out. We indicate that for the three-qubit W state, its average von Neumann entropy is maximal only within the W SLOCC class, and that under ASD the three-qubit GHZ state is the unique state of which the reduced density operator obtained by tracing any two qubits has the maximal von Neumann entropy.

INTRODUCTION

Quantum entanglement is considered as a unique quantum mechanical resource [1]. Entanglement takes an important role in quantum information and computation. Examples include quantum teleportation, quantum cryptography, quantum metrology, and quantum key distribution. Considerable efforts have been made to explore the entanglement classification via local unitary operators (LU), local operations and classical communication (LOCC), and Stochastic LOCC (SLOCC) [2]-[12]. It is known that any two states of the same LU class have the same amount of entanglement [3, 4, 11]. Under SLOCC, pure states of three qubits were partitioned into six equivalence classes: GHZ, W, A-BC, B-AC, C-AB, and A-B-C [3]. It has been established that two bipartite states are LU equivalent if and only if their Schmidt coefficients coincide [1, 12]. Acín et al. proposed the Schmidt decomposition for three qubits [8, 9]. Kraus introduced a standard form for multipartite systems and showed that two states are LU equivalent if and only if their standard forms coincide [11, 12].

Coffman et al. defined the tangle for the reduced density operator ρ_{AB} (i.e., $\text{tr}_C \rho_{ABC}$) of a three-qubit state below [13]. Let

$$\overline{\rho_{AB}} = \sigma_y \otimes \sigma_y \rho_{AB}^* \sigma_y \otimes \sigma_y, \quad (1)$$

where ρ_{AB}^* is the complex conjugate of ρ_{AB} and σ_y is the Pauli matrix. Note that $\rho_{AB} \overline{\rho_{AB}}$ has only real and non-negative eigenvalues $\eta_1^2, \eta_2^2, \eta_3^2$, and η_4^2 , where $\eta_1 \geq \eta_2 \geq \eta_3 \geq \eta_4$. Then, the entanglement

tangle of ρ_{AB} is defined as

$$\tau_{AB} = [\max\{\eta_1 - \eta_2 - \eta_3 - \eta_4, 0\}]^2. \quad (2)$$

The tangle τ_{AC} of ρ_{AC} ($= \text{tr}_B \rho_{ABC}$) and the tangle τ_{BC} of ρ_{BC} ($= \text{tr}_A \rho_{ABC}$) can be similarly defined.

The idea of taking average measure of entanglements comes from an extremely useful technique in quantum information theory, the “average subsystem approach” proposed by Page [19]. For a pure state $|\psi\rangle$ of three qubits, Dür et al. defined its average residual entanglement as $\bar{\epsilon}(\psi) = \frac{1}{3}(\epsilon(\rho_{AB}) + \epsilon(\rho_{AC}) + \epsilon(\rho_{BC}))$, where $\epsilon(\rho_{xy})$ is some entanglement measure, where notation xy means AB, AC , or BC [3]. If $\epsilon(\rho_{xy})$ is the tangle (the von Neumann entropy), then the average residual entanglement $\bar{\epsilon}(\psi)$ is the average tangle (von Neumann entropy). A state of four qubits is defined to be maximally entangled if its average bipartite entanglement (for example, the average tangle or the average entropy) with respect to all possible bi-partite cuts is maximal [18]. Significant efforts have contributed to the average tangle [3, 18, 20, 21] and von Neumann entropy, specially, the average entropy in bipartite, tripartite, and multi-partite scenarios [14–18, 20, 22], and reference [23]. Dür et al. showed that the W state of three qubits has the maximal average tangles and indicated that for the GHZ state of three qubits, the tangle vanishes [3].

Considerable efforts have also been undertaken on the study of polynomial invariants for n qubits [8, 24–27] [28]. SLOCC (LU) polynomial invariants can be used for SLOCC (LU) entanglement classification of pure states of n qubits and can also be used as entanglement measure.

In this paper, we derive a general formula of the tangle for three qubits, and obtain three LU polynomial invariants of degree 4. We calculate tangle, average tangle, 3-tangle, von Neumann entropy, and average von Neumann entropy in the framework of ASD. We derive an equation which tangle, 3-tangle, and von Neumann entropy satisfy. Via the equation, we present relations among tangles and von Neumann entropy, among tangle, 3-tangle, and von Neumann entropy, among the average tangles, the average von Neumann entropy, and 3-tangle, and among von Neumann entropy and Acín et al.'s LU invariants. The relations can help us find the entangled states satisfying distinct requirements for tangle, 3-tangle, and von Neumann entropy.

We obtain all three-qubit states whose tangle, concurrence, 3-tangle and von Neumann entropy do not vanish. Via von Neumann entropy for ASD, we indicate that the GHZ state is the unique three-qubit state under ASD that has the maximal von Neumann entropy of $\ln 2$, and the average von Neumann entropy of the W state is maximal only within the W SLOCC class.

TANGLES FOR ASD

In this section, we derive the formulas for tangles for pure states of three qubits and for the ASD, and present a relation between tangles and Acín et al.'s LU polynomial invariants.

Homogeneous polynomial of degree 4 for tangle

Let $|\psi\rangle = \sum_{i=0}^7 c_i|i\rangle$. By solving Eq. (2), we obtain τ_{AB} , τ_{AC} , and τ_{BC} as follows,

$$\tau_{AB} = \Delta - \frac{\tau_{ABC}}{2}, \quad (3)$$

$$\tau_{AC} = \Phi - \frac{\tau_{ABC}}{2}, \quad (4)$$

$$\tau_{BC} = \Psi - \frac{\tau_{ABC}}{2}, \quad (5)$$

where Δ , Φ , Ψ are defined in Eqs. (A3, A8, A12) in Appendix A. Following [31], the 3-tangle τ_{ABC} can be written as

$$\tau_{ABC} = 4|(c_0c_7 - c_2c_5 - c_1c_6 + c_3c_4)^2 - 4(c_0c_3 - c_1c_2)(c_4c_7 - c_5c_6)|. \quad (6)$$

Note that Δ , Φ , and Ψ are LU homogeneous polynomial invariants of degree 4 in the state coefficients

and their complex conjugates. Therefore, one needs only "+, -, ×" operations of the state coefficients and their complex conjugates to compute the tangles.

Williamson et al. obtained $I(\tilde{\rho}_{ab}) = \text{tr}[\rho_{ab}\tilde{\rho}_{ab}] = \tau_{ab} + \frac{1}{2}\tau_{abc}$, where $\tilde{\rho}_{ab} = \sigma_y \otimes \sigma_y \rho_{ab}^T \sigma_y \otimes \sigma_y$ [32]. Note that Coffman et al. used ρ_{ab}^* (which is the complex conjugate of ρ_{ab}) in Eq. (1) rather than ρ_{ab}^T . It is known that it is complicated to compute the reduced density operator ρ_{ab} and $\text{tr}[\rho_{ab}\tilde{\rho}_{ab}]$. Comparatively, it is easier and simpler to compute Δ than $\text{tr}[\rho_{ab}\tilde{\rho}_{ab}]$.

Tangles for ASD

Acín et al. proposed the following Schmidt decomposition for pure states of three qubits,

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\phi}|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle, \quad (7)$$

where $\lambda_i \geq 0$, $i = 0, 1, \dots, 4$, $0 \leq \phi < 2\pi$, and $\sum \lambda_i^2 = 1$ [8, 9]. Equation (7) is referred to the ASD of $|\psi\rangle$. It is known that any state of three qubits is LU equivalent to its ASD. For ASD, 3-tangle τ_{ABC} in Eq. (6) can be reduced to

$$\tau_{ABC} = 4\lambda_0^2\lambda_4^2. \quad (8)$$

τ_{AB} in Eq. (3) and τ_{AC} in Eq. (4) can be reduced similarly,

$$\tau_{AB} = 4\lambda_0^2\lambda_3^2, \quad (9)$$

$$\tau_{AC} = 4\lambda_0^2\lambda_2^2. \quad (10)$$

To reduce τ_{BC} in Eq. (5) for ASD, we write Ψ in Eq. (A12) as $\Psi = 2\Pi$, where $\Pi = [\lambda_0^2\lambda_4^2 + 2(\lambda_1\lambda_4 - \lambda_2\lambda_3)^2 + 8\lambda_1\lambda_2\lambda_3\lambda_4 \sin^2 \frac{\phi}{2}]$. Then, we have

$$\begin{aligned} \tau_{BC} &= 2(\Pi - \lambda_0^2\lambda_4^2) \\ &= 4[(\lambda_1\lambda_4 - \lambda_2\lambda_3)^2 + 4\lambda_1\lambda_2\lambda_3\lambda_4 \sin^2 \frac{\phi}{2}] \\ &= 4|\lambda_1\lambda_4 e^{i\phi} - \lambda_2\lambda_3|^2. \end{aligned} \quad (11)$$

In Table 1, we summarize the tangles τ_{AB} , τ_{AC} , τ_{BC} , and 3-tangle τ_{ABC} for ASD.

From Table I, it is straightforward to calculate the tangles and 3-tangle for any ASD. Because of the LU equivalence between a state and its ASD, a state and its ASD have the same tangles, 3-tangle. For example, the ASD of the W state is $(1/\sqrt{3})(|000\rangle +$

TABLE I. τ_{AB} , τ_{AC} , and τ_{BC} for ASD

$\tau_{AB} =$	$4\lambda_0^2\lambda_3^2 =$	$4J_3$
$\tau_{AC} =$	$4\lambda_0^2\lambda_2^2 =$	$4J_2$
$\tau_{BC} =$	$4 \lambda_1\lambda_4e^{i\phi} - \lambda_2\lambda_3 ^2 =$	$4J_1$
$\tau_{ABC} =$	$4\lambda_0^2\lambda_4^2 =$	$4J_4$

$|101\rangle + |110\rangle$). From Table 1, we conclude that the tangles of the W state $\tau_{AB} = \tau_{AC} = \tau_{BC} = \frac{4}{9}$, and the 3-tangle τ_{ABC} vanishes.

For ASD, Acín et al. proposed five LU invariants $J_i, i = 1, 2, 3, 4, 5$, where $J_1 = |\lambda_1\lambda_4e^{i\phi} - \lambda_2\lambda_3|^2$, and $J_i = (\lambda_0\lambda_i)^2$ for $i = 2, 3, 4$ [8, 9]. Thus, for ASD, the tangles and 3-tangle in Eqs. (9, 10, 11, 8) can be rewritten in terms of LU invariants J_i (see Table I),

$$\tau_{AB} = 4J_3, \quad (12)$$

$$\tau_{AC} = 4J_2, \quad (13)$$

$$\tau_{BC} = 4J_1, \quad (14)$$

$$\tau_{ABC} = 4J_4. \quad (15)$$

VON NEUMANN ENTROPY FOR ASD AND A RELATION BETWEEN TANGLES AND VON NEUMANN ENTROPY

von Neumann entropy for ASD

von Neumann entropy is defined as

$$S(\rho) = -\sum \eta_i \ln \eta_i, \quad (16)$$

where $\eta_i \geq 0$ are the eigenvalues of ρ , and $\sum_i \eta_i = 1$. Note that $0 \ln 0 = 0$. Via ASD, it is easy to verify that

$$S(\rho_A) = S(\rho_{BC}), \quad (17)$$

$$S(\rho_B) = S(\rho_{AC}), \quad (18)$$

$$S(\rho_C) = S(\rho_{AB}). \quad (19)$$

It is well known that the eigenvalues of ρ is just the roots of the characteristic polynomial of ρ . A tedious calculation derives the characteristic polynomials of the reduced density operators $\rho_\mu, \mu = A, B,$

C , which are $X^2 - X + \alpha_\mu$, where α_μ is just the sum of tangles and 3-tangle, ref. Table II. Thus, we establish a relation among the entanglement measures: the von Neumann entropy, tangle and 3-tangle.

From results in Table I and via ASD, a calculation yields Table II, in which abbreviation CP stands for the characteristic polynomial of the reduced density operator, ρ_μ .

TABLE II. $S(\rho_\mu)$ for ASD

μ	RDO	CP of ρ_μ	α_μ
A	ρ_A	$X^2 - X + \alpha_A$	$\alpha_A = J_2 + J_3 + J_4$ $= \frac{\tau_{AB} + \tau_{AC} + \tau_{ABC}}{4}$ $= \frac{\tau_{A(BC)}}{4}$
B	ρ_B	$X^2 - X + \alpha_B$	$\alpha_B = J_1 + J_3 + J_4$ $= \frac{\tau_{AB} + \tau_{BC} + \tau_{ABC}}{4}$ $= \frac{\tau_{B(AC)}}{4}$
C	ρ_C	$X^2 - X + \alpha_C$	$\alpha_C = J_1 + J_2 + J_4$ $= \frac{\tau_{AC} + \tau_{BC} + \tau_{ABC}}{4}$ $= \frac{\tau_{C(AB)}}{4}$

In Table II, the notation $\tau_{A(BC)}$ stands for the tangle between a qubit A and a qubit pair BC, where the qubit pair BC is considered a single object [13].

Let $\eta_\mu^{(1)}$ and $\eta_\mu^{(2)}$ be the two eigenvalues of ρ_μ . We have

$$\eta_\mu^{(1)} = \frac{1 + \sqrt{1 - 4\alpha_\mu}}{2}, \quad (20)$$

$$\eta_\mu^{(2)} = \frac{1 - \sqrt{1 - 4\alpha_\mu}}{2}. \quad (21)$$

Then, from Eq. (16), one can see that

$$S(\rho_\mu) = -(\eta_\mu^{(1)} \ln \eta_\mu^{(1)} + \eta_\mu^{(2)} \ln \eta_\mu^{(2)}), \quad (22)$$

where $\mu \in \{A, B, C\}$ and $0 \leq \alpha_\mu \leq 1/4$.

Equation (22) and Table II reveal a relation among tangles, 3-tangle and von Neumann entropy. In other words, tangles, 3-tangle, and von Neumann entropy for any pure three-qubit state must satisfy Eq. (22). See Table III for the GHZ state, the W state, as well as other states. We will explore the relation for details below.

For $\mu \in \{A, B, C\}$, the derivative of the von Neumann entropy $S(\rho_\mu)$ with respect to α_μ is given by

$$(S(\rho_\mu))'_{\alpha_\mu} = -\frac{1}{\sqrt{1-4\alpha_\mu}} \ln \frac{1-\sqrt{1-4\alpha_\mu}}{1+\sqrt{1-4\alpha_\mu}} \quad (23)$$

$(S(\rho_\mu))'_{\alpha_\mu} > 0$ when $0 < \alpha_\mu < 1/4$. Hence, $S(\rho_\mu)$ increases monotonically as α_μ increases. Recall that $0 \leq \alpha_\mu \leq 1/4$. Thus, $0 \leq S(\rho_\mu) \leq \ln 2$, and $S(\rho_\mu) = \ln 2$ iff $\alpha_\mu = 1/4$, and $S(\rho_\mu) = 0$ iff $\alpha_\mu = 0$. This means that the maximal von Neumann entropy for one particle ρ_μ is $\ln 2$.

For the GHZ state, $\alpha_\mu = \frac{1}{4}$ and $S(\rho_\mu) = \ln 2$; and for the W state, $\alpha_\mu = \frac{2}{9}$ and $S(\rho_\mu) = \frac{3 \ln 3 - 2 \ln 2}{3}$. Thus, for three qubits, the GHZ state has the maximal von Neumann entropy for any kind of the reduced density operator ρ_μ .

Relation between tangles and von Neumann entropy

Proposition 1. For any pure state of three qubits, two different types of tangles are equal iff the corresponding the von Neumann entropy are equal. That is,

- (1) $S(\rho_{AC}) = S(\rho_{BC})$ iff $\tau_{AC} = \tau_{BC}$,
- (2) $S(\rho_{AB}) = S(\rho_{BC})$ iff $\tau_{AB} = \tau_{BC}$,
- (3) $S(\rho_{AB}) = S(\rho_{AC})$ iff $\tau_{AB} = \tau_{AC}$.

Clearly, $S(\rho_{AB}) = S(\rho_{AC}) = S(\rho_{BC})$ iff $\tau_{AB} = \tau_{AC} = \tau_{BC}$ (see Table III).

Let uvw and xyz be two different three-character strings from the set $\{ABC, BAC, CAB\}$. Then, also $\tau_{u(vw)} = \tau_{x(yz)}$ iff $S(\rho_u) = S(\rho_x)$.

Proof of (1): If $\tau_{AC} = \tau_{BC}$, then from Table II, $\alpha_A = \alpha_B$, and then $S(\rho_A) = S(\rho_B)$, which leads to $S(\rho_{BC}) = S(\rho_{AC})$ from Eqs. (17–18). Conversely, if $S(\rho_{AC}) = S(\rho_{BC})$, then $S(\rho_B) = S(\rho_A)$, then $\alpha_B = \alpha_A$ because $S(\rho)$ is strictly increasing, and then $\tau_{AC} = \tau_{BC}$ from Table II. Similarly, claims (2) and (3) also hold.

Proposition 2. For any pure state of three qubits, two different types of tangles satisfy $\tau_{uv} > \tau_{xy}$ iff the corresponding the von Neumann entropy satisfy $S(\rho_{uv}) < S(\rho_{xy})$. That is,

- (1) $\tau_{AC} > \tau_{BC}$ iff $S(\rho_{AC}) < S(\rho_{BC})$,
- (2) $\tau_{AB} > \tau_{BC}$ iff $S(\rho_{AB}) < S(\rho_{BC})$,
- (3) $\tau_{AB} > \tau_{AC}$ iff $S(\rho_{AB}) < S(\rho_{AC})$.

Let uvw and xyz be two different three-character strings from the set $\{ABC, BAC, CAB\}$. Then, also $\tau_{u(vw)} > \tau_{x(yz)}$ iff $S(\rho_u) > S(\rho_x)$.

Proof of (1): If $\tau_{AC} > \tau_{BC}$, then $\alpha_A > \alpha_B$ from Table II, and then $S(\rho_A) > S(\rho_B)$, i.e. $S(\rho_{BC}) > S(\rho_{AC})$, because $S(\rho)$ is strictly increasing. Conversely, if $S(\rho_{AC}) < S(\rho_{BC})$, i.e. $S(\rho_B) < S(\rho_A)$, then $\alpha_B < \alpha_A$ because $S(\rho)$ is strictly increasing, and then $\tau_{AC} > \tau_{BC}$. Similarly, claims (2) and (3) also hold.

Next, we study the relation between the difference of two tangles and the difference of the corresponding von Neumann entropy s . Using the differential Mean Value theorem, we have

$$S(\rho_A) - S(\rho_B) = (S(\rho_\mu))'_{\alpha_\mu}(\xi_1)(\alpha_A - \alpha_B) \quad (24)$$

$$S(\rho_A) - S(\rho_C) = (S(\rho_\mu))'_{\alpha_\mu}(\xi_2)(\alpha_A - \alpha_C) \quad (25)$$

$$S(\rho_B) - S(\rho_C) = (S(\rho_\mu))'_{\alpha_\mu}(\xi_3)(\alpha_B - \alpha_C) \quad (26)$$

From Eq. (23), we have $(S(\rho_\mu))'_{\alpha_\mu}(\xi_i) > 0$, $i = 1, 2, 3$. Clearly, we can also use Eqs. (24, 25, 26) to prove Propositions 1 and 2. We next calculate $(S(\rho_\mu))'_{\alpha_\mu}$ using the second order Taylor expansion of $\ln(1 \pm x)$,

$$\begin{aligned} (S(\rho_\mu))'_{\alpha_\mu} &= -\frac{1}{\sqrt{1-4\alpha_\mu}} [\ln(1 - \sqrt{1-4\alpha_\mu}) - \ln(1 + \sqrt{1-4\alpha_\mu})] \\ &\approx -\frac{1}{\sqrt{1-4\alpha_\mu}} \times \\ &\quad [(-\sqrt{1-4\alpha_\mu} - \frac{1-4\alpha_\mu}{2}) - (\sqrt{1-4\alpha_\mu} - \frac{1-4\alpha_\mu}{2})] \\ &= 2. \end{aligned}$$

Therefore, $(S(\rho_\mu))'_{\alpha_\mu}(\xi_i) \approx 2$. Via Eqs. (24, 25, 26) we arrive at the following Proposition.

Proposition 3. For any pure state of three qubits, the difference of two tangles is approximately twice as large as the difference of the corresponding von Neumann entropy. We further explain this in details below.

Let different uvw and xyz belong to $\{ABC, BAC, CAB\}$. Then,

$$\tau_{u(vw)} - \tau_{x(yz)} = \tau_{yz} - \tau_{vw} \approx 2[S(\rho_{vw}) - S(\rho_{yz})].$$

That is,

$$\begin{aligned} \tau_{A(BC)} - \tau_{B(AC)} &= \tau_{AC} - \tau_{BC} \approx 2[S(\rho_{BC}) - S(\rho_{AC})], \\ \tau_{A(BC)} - \tau_{C(AB)} &= \tau_{AB} - \tau_{BC} \approx 2[S(\rho_{BC}) - S(\rho_{AB})], \\ \tau_{B(AC)} - \tau_{C(AB)} &= \tau_{AB} - \tau_{AC} \approx 2[S(\rho_{AC}) - S(\rho_{AB})]. \end{aligned}$$

Relation between the von Neumann entropy and Acín et al.'s LU invariants

It is well known that LU invariants are considered as entanglement measure [8, 9, 25]. So far, no one discusses the relations between LU invariants (as measures) and other entanglement measures. Here, we establish the relation between von Neumann entropy and LU invariants (as entanglement measure) J_i , $i = 1, 2, 3, 4$. From Eq. (22) and Table II, we can write the von Neumann entropy with Acín et al.'s LU invariants J_i , $i = 1, 2, 3, 4$. Thus, we have the following immediate results.

(1). For any pure state of three qubits, two different types of Acín et al.'s LU invariants are equal *iff* the corresponding the von Neumann entropy are equal. That is, $S(\rho_A) = S(\rho_B)$ *iff* $J_2 = J_1$; $S(\rho_A) = S(\rho_C)$ *iff* $J_3 = J_1$; $S(\rho_B) = S(\rho_C)$ *iff* $J_3 = J_2$.

(2). $S(\rho_A) > S(\rho_B)$ *iff* $J_2 > J_1$; $S(\rho_A) > S(\rho_C)$ *iff* $J_3 > J_1$; $S(\rho_B) > S(\rho_C)$ *iff* $J_3 > J_2$.

Via Eqs. (24, 25, 26) and $(S(\rho_\mu))'_{\alpha_\mu}(\xi_i) \approx 2$, then we obtain the following.

(3). For any pure state of three qubits, the difference of two von Neumann entropy is approximately twice as large as the difference of the corresponding Acín et al.'s LU invariants.

$$S(\rho_A) - S(\rho_B) \approx 2(J_2 - J_1) \quad (27)$$

$$S(\rho_A) - S(\rho_C) \approx 2(J_3 - J_1) \quad (28)$$

$$S(\rho_B) - S(\rho_C) \approx 2(J_3 - J_2) \quad (29)$$

RELATION AMONG TANGLE, 3-TANGLE, AND VON NEUMANN ENTROPY

Equation (22) can be reduced to

$$S(\rho_\mu) = -[\eta_\mu^{(1)} \ln(1 + \sqrt{1 - 4\alpha_\mu}) + \eta_\mu^{(2)} \ln(1 - \sqrt{1 - 4\alpha_\mu}) - \ln 2]. \quad (30)$$

Then by the second order Taylor expansion of $\ln(1 \pm x)$, we approximate $S(\rho_\mu)$ as follows,

$$\begin{aligned} S(\rho_\mu) &\approx -[\eta_\mu^{(1)}(\sqrt{1 - 4\alpha_\mu} - \frac{1 - 4\alpha_\mu}{2}) \\ &\quad + \eta_\mu^{(2)}(-\sqrt{1 - 4\alpha_\mu} - \frac{1 - 4\alpha_\mu}{2}) - \ln 2] \\ &= \ln 2 - \frac{1}{2} + 2\alpha_\mu, \end{aligned} \quad (31)$$

where $\mu \in \{A, B, C\}$. From Eq. (31), we obtain the following relation among tangle, 3-tangle, and the

von Neumann entropy :

$$\begin{aligned} 2S(\rho_A) &\approx 2\ln 2 - 1 + \tau_{A(BC)} \\ &= 2\ln 2 - 1 + \tau_{AB} + \tau_{AC} + \tau_{ABC}, \\ 2S(\rho_B) &\approx 2\ln 2 - 1 + \tau_{B(AC)} \\ &= 2\ln 2 - 1 + \tau_{AB} + \tau_{BC} + \tau_{ABC}, \\ 2S(\rho_C) &\approx 2\ln 2 - 1 + \tau_{C(AB)} \\ &= 2\ln 2 - 1 + \tau_{AC} + \tau_{BC} + \tau_{ABC}. \end{aligned}$$

The states in Table III satisfy the above relations. The above relations can help us find the states which satisfy special requirements for tangle, 3-tangle, and von Neumann entropy, or the states of which tangle, 3-tangle, and von Neumann entropy are as big as possible. For example, for the state $|\kappa\rangle$ in Table III, $S(\rho_A) = 0.687$, $\tau_{AB} = \tau_{AC} = 4/9$, and $\tau_{ABC} = 8/81$.

Next, we demonstrate how to use the above relation to explore properties of tangle, 3-tangle, and von Neumann entropy. Let $S(\rho_A) = \ln 2$ (maximum). Then, tangles τ_{AB} and τ_{AC} , and 3-tangle τ_{ABC} must satisfy the following.

$$\tau_{AB} + \tau_{AC} + \tau_{ABC} \approx 1. \quad (32)$$

For example, if $\tau_{ABC} = 1$, then τ_{AB} and τ_{AC} vanish; if $\tau_{ABC} = 1/2$, then $\tau_{AB} + \tau_{AC} = 1/2$.

RELATION AMONG THE AVERAGE TANGLE, THE AVERAGE VON NEUMANN ENTROPY, AND 3-TANGLE

Lots of efforts have contributed to investigate the the average tangle [3, 18] and the average von Neumann entropy [23]. So far, no one discusses the relation among them. In this subsection, we establish the relation.

Definition for the average tangle

Let $A(\psi)$ be the average tangles for the state $|\psi\rangle$. Then,

$$A(\psi) = \frac{\tau_{AB} + \tau_{AC} + \tau_{BC}}{3}. \quad (33)$$

We explain how to calculate the average tangle A. First, take partial traces over qubit A (resp. B and C) to get the reduced density operators ρ_{BC} (resp. ρ_{AC} , and ρ_{AB}), then by the definition of the tangle in Eq. (2) calculate the tangle τ_{AB} (resp.

τ_{AC} , and τ_{BC}) for the reduced density operator ρ_{AB} (resp. ρ_{AC} , and ρ_{BC}). Finally make the average of the tangles τ_{AB} , τ_{AC} , and τ_{BC} to get the average tangle A .

One can see that $A = 0$ for the GHZ state and $A = 4/9$ for the W state. It is known that the W state has the maximal average tangles $A = 4/9$ [3]. Thus, $0 \leq A \leq 4/9$.

Definition for the average von Neumann entropy

Let $m(\psi)$ be the average of the von Neumann entropy of all the reduced density operators for the state $|\psi\rangle$. Then,

$$m(\psi) = \frac{S(\rho_A) + S(\rho_B) + S(\rho_C)}{3}. \quad (34)$$

We explain how to calculate the average von Neumann entropy m . First, take partial traces over qubits A and B (resp. A and C, and B and C) to get the reduced density operators ρ_C (resp. ρ_B , and ρ_A), then calculate the von Neumann entropy $S(\rho_A)$ (resp. $S(\rho_B)$, and $S(\rho_C)$) of ρ_A (resp. ρ_B , and ρ_C) by the definition in Eq. (16). Finally, make the average of $S(\rho_A)$, $S(\rho_B)$, and $S(\rho_C)$ to get the average von Neumann entropy m .

It is easy to see that the GHZ state has the maximal average von Neumann entropy of $\ln 2$, while the W state has the average von Neumann entropy of $\frac{3 \ln 3 - 2 \ln 2}{3}$. Thus, $0 \leq m \leq \ln 2$.

Relation among the average tangle, the average von Neumann entropy, and 3-tangle

So far, no one explains why the GHZ state has the maximal 3-tangle but vanishing tangle and conversely, and why the W state has the maximal average tangle but vanishing 3-tangle. We will answer why the states GHZ and W have the opposite properties.

Using Eq. (31), the average von Neumann entropy and the average tangle satisfy the following equation for any pure state of three qubits.

$$m - A - \frac{\tau_{ABC}}{2} \approx \ln 2 - \frac{1}{2}, \quad (35)$$

where $0 \leq m \leq \ln 2$ and $0 \leq A \leq 4/9$.

Eq. (35) reveals a relation among the average von Neumann entropy m , the average tangle A , and the

3-tangle τ_{ABC} . Clearly, $m = \ln 2$, $A = 4/9$, $\tau_{ABC} = 1$ don't satisfy Eq. (35). It means that for any state, the average von Neumann entropy, the average tangle, and 3-tangle cannot reach the maximum simultaneously. Below, we will investigate when m (resp. A and τ_{ABC}) reaches the maximum, what happen to other two measures.

Equation (35) implies that the value of $(m - A)$, i.e. the difference between the average von Neumann entropy and the average tangle, increases linearly with the 3-tangle τ_{ABC} . For the GHZ SLOCC class, $0 < \tau_{ABC} \leq 1$ and almost $\ln 2 - 1/2 < m - A \leq \ln 2$. While for other SLOCC classes, $\tau_{ABC} = 0$ and $(m - A) \approx \ln 2 - 1/2$. Thus, we obtain almost $\ln 2 - 1/2 \leq (m - A) \leq \ln 2$ for any state of three qubits.

The relation can help find the states which satisfy different requirements for the average von Neumann entropy and the average tangle and 3-tangle.

Clearly, the requirements for the average tangle, the average von Neumann entropy, and 3-tangle must satisfy Eq. (35). For example, $|G\rangle$ in Table III has $A = 1/4$, $m = 0.56$, and $\tau_{ABC} = 1/4$.

It is known that the GHZ state has vanishing tangle. This means that for the GHZ state, if one of three qubits is traced out, the corresponding reduced density operator becomes separable. In other words, the entanglement properties of the GHZ state are fragile under particle losses [3]. One can use Eq. (35) to find the states of which the average von Neumann entropy, the average tangle, and 3-tangle are big enough. Clearly, the states are genuine entangled ones even losing one particle.

The relation helps understand properties of the average tangle, 3-tangle, and the average von Neumann entropy

We next explore when a state has the maximal average von Neumann entropy, then what Eq. (35) can tell us about the average tangle and the 3-tangle for this state.

Let $m = \ln 2$ (for example, for the GHZ state). Then, Eq. (35) becomes

$$A + \frac{\tau_{ABC}}{2} \approx \frac{1}{2}. \quad (36)$$

Clearly, if $A = 0$ then $\tau_{ABC} \approx 1$, and vice versa. Eq. (36) tells us if a state has the maximal average von Neumann entropy, then the average tangle and the 3-tangle must satisfy Eq. (36).

For example, Eq. (36) tells us there are the states with $m = \ln 2$, $\tau_{ABC} \approx 1/2$, and $A \approx 1/4$. One can see that these states belong to GHZ SLOCC class, but different from the states GHZ state. The three entanglement measures: tangle, 3-tangle, and von Neumann entropy tell us that the states are genuine entangled state even though one of three qubits is traced over and have the maximal average von Neumann entropy.

We next explore when a state has the maximal 3-tangle, then what Eq. (35) can tell us about the average von Neumann entropy and the average tangle for this state.

Let $\tau_{ABC} = 1$ (for example, for the GHZ state). For the case, Eq. (35) becomes

$$m - \ln 2 \approx A. \quad (37)$$

It is easy to see that $m = \ln 2$ and $A = 0$ is the unique solution of Eq. (37) because if $m < \ln 2$ then $A < 0$.

This explains when a state has the maximal 3-tangle, then the state must have the maximal average von Neumann entropy and vanishing the average tangle, i.e. $\tau_{\mu\nu} = 0$, where $\mu\nu = \{AB, AC, BC\}$. This is why the GHZ state has the maximal 3-tangle and the maximal average von Neumann entropy but vanishing tangle $\tau_{\mu\nu}$, where $\mu\nu = \{AB, AC, BC\}$.

We next explore when a state has the maximal average tangles of $4/9$, then what Eq. (35) can tell us about the average von Neumann entropy and the 3-tangle for this state.

Let $A = 4/9$ (for example, for the W state). Via Eq. (35), one can know that $\max \tau_{ABC} \approx 1/9$ when $m = \ln 2$ and $\min m \approx \ln 2 - 1/18 \approx 0.63759$ when $\tau_{ABC} = 0$. It means the average von Neumann entropy almost is maximal.

This explains when a state has the maximal average tangle of $4/9$, then the state has almost vanishing 3-tangle and the almost maximal average von Neumann entropy. This is why the W state has the maximal average tangles but vanishing 3-tangle.

TANGLES AND VON NEUMANN ENTROPY FOR GHZ SLOCC CLASS

It is well known that an ASD state belongs to the GHZ SLOCC class iff $\lambda_0\lambda_4 \neq 0$ [29, 30]. So, in this section we assume $\lambda_0\lambda_4 \neq 0$. We first discuss the properties of tangle. It is known that if $\tau_{\mu\nu}$, vanishes, then $\rho_{\mu\nu}$ is separable, where $\mu\nu \in \{AB, AC, BC\}$. From Table I, one can see that the tangles for the GHZ SLOCC class have the following properties.

Property (1). $0 \leq \tau_{AB}, \tau_{AC}, \tau_{BC} < 1$.

Property (2).

(2.1). $\tau_{AB} = 0$ iff $\lambda_3 = 0$.

(2.2). $\tau_{AC} = 0$ iff $\lambda_2 = 0$.

(2.3). $\tau_{BC} = 0$ iff $\lambda_1\lambda_4 = \lambda_2\lambda_3 \neq 0$ and $\phi = 0$ or $\lambda_1 = 0$ and $\lambda_2\lambda_3 = 0$.

Property (3). When only one of τ_{AB} , τ_{AC} , and τ_{BC} vanishes,

(3.1). $\tau_{AB} = 0$ and $\tau_{AC}\tau_{BC} \neq 0$ iff $\lambda_3 = 0$ and $\lambda_1\lambda_2 \neq 0$.

(3.2). $\tau_{AC} = 0$ and $\tau_{AB}\tau_{BC} \neq 0$ iff $\lambda_2 = 0$ and $\lambda_1\lambda_3 \neq 0$.

(3.3). $\tau_{BC} = 0$ and $\tau_{AB}\tau_{AC} \neq 0$ iff $\lambda_1\lambda_4 = \lambda_2\lambda_3 \neq 0$ and $\phi = 0$.

Proof of (3.3): Clearly, $\tau_{AB}\tau_{AC} \neq 0$ iff $\lambda_2\lambda_3 \neq 0$.

If $\tau_{BC} = 0$, then from Table I, $\lambda_1\lambda_4 e^{i\phi} - \lambda_2\lambda_3 = 0$, i.e. $\lambda_1\lambda_4 = \lambda_2\lambda_3 \neq 0$ and $\phi = 0$. Conversely, if $\lambda_1\lambda_4 = \lambda_2\lambda_3 \neq 0$ and $\phi = 0$, then $\tau_{AB}\tau_{AC} \neq 0$ and $\tau_{BC} = 0$.

Property (4). When only two of τ_{AB} , τ_{AC} , and τ_{BC} vanish,

(4.1). $\tau_{AB} = \tau_{AC} = 0$ and $\tau_{BC} \neq 0$ iff $\lambda_2 = \lambda_3 = 0$ and $\lambda_1 \neq 0$.

(4.2). $\tau_{AB} = \tau_{BC} = 0$ and $\tau_{AC} \neq 0$ iff $\lambda_1 = \lambda_3 = 0$ and $\lambda_2 \neq 0$.

(4.3). $\tau_{AC} = \tau_{BC} = 0$ and $\tau_{AB} \neq 0$ iff $\lambda_1 = \lambda_2 = 0$ and $\lambda_3 \neq 0$.

Property (5). When all τ_{AB} , τ_{AC} , and τ_{BC} vanish,

$\tau_{AB} = \tau_{AC} = \tau_{BC} = 0$ iff $\lambda_1 = \lambda_2 = \lambda_3 = 0$, i.e. the state is of the form $\lambda_0|000\rangle + \lambda_4|111\rangle$. For instance, the GHZ state.

Property (6). When none of the tangles vanishes, $\tau_{AB}\tau_{AC}\tau_{BC} > 0$ iff (i). $\lambda_2\lambda_3 \neq 0$ and $\lambda_1 = 0$, or

(ii). $\lambda_1\lambda_2\lambda_3(\lambda_1\lambda_4 - \lambda_2\lambda_3) \neq 0$ and $\phi = 0$, or (iii). $\lambda_1\lambda_2\lambda_3 \neq 0$ and $\phi \neq 0$.

The GHZ state is the unique one under ASD which has the maximal von Neumann entropy .

In Appendix B, we show that for any ASD state of three qubits, if $S(\rho_\mu) = \ln 2$, then the state must be GHZ. It means that the GHZ state is the unique state of three qubits under ASD such that $S(\rho_\mu)$ achieves the maximal value. Thus, for any state of GHZ LU class, $S(\rho_\mu) = \ln 2$, where $\mu \in \{A, B, C\}$.

TANGLE AND VON NEUMANN ENTROPY FOR W SLOCC CLASS

Each state of the W SLOCC class is of the following form [29, 30],

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\phi}|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle, \quad (38)$$

where $\lambda_0\lambda_2\lambda_3 \neq 0$ and $\lambda_4 = 0$.

Tangle for the W SLOCC class

From Table I, we obtain tangles for the W SLOCC class,

$$\begin{aligned} \tau_{AB} &= 4\lambda_0^2\lambda_3^2, \\ \tau_{AC} &= 4\lambda_0^2\lambda_2^2, \\ \tau_{BC} &= 4\lambda_2^2\lambda_3^2, \\ \tau_{ABC} &= 0. \end{aligned}$$

Clearly, $0 < \tau_{AB}, \tau_{AC}, \tau_{BC} < 1$.

The W state is the unique state of the W SLOCC class under ASD whose average von Neumann entropy is the maximal within the W SLOCC class.

Next, we show that the average von Neumann entropy of the W state is maximal only within the W SLOCC class. From Table II, for W SLOCC class, one can see that

$$\alpha_A = \lambda_0^2(\lambda_2^2 + \lambda_3^2), \quad (39)$$

$$\alpha_B = \lambda_3^2(\lambda_0^2 + \lambda_2^2), \quad (40)$$

$$\alpha_C = \lambda_2^2(\lambda_0^2 + \lambda_3^2). \quad (41)$$

Let $\mu\nu\nu$ be a string from the set $\{ABC, BAC, CAB\}$. When $\alpha_\mu = 1/4$, $S(\rho_\mu) = \ln 2$, $S(\rho_\nu) < \ln 2$ and $S(\rho_\nu) < \ln 2$. It means that the von Neumann entropy of the W state is not maximal even within the W SLOCC class. We next show that the average von Neumann entropy of the W state is maximal within the W SLOCC class.

In Appendix C, we derive the extrema of m with the constraint $\sum_{i=0}^3 \lambda_i^2 = 1$. A straightforward and tedious calculation yields that m has the extrema $\frac{3\ln 3 - 2\ln 2}{3}$ at $\lambda_1 = 0$ and $\lambda_0 = \lambda_2 = \lambda_3 = 1/\sqrt{3}$, which is just the ASD of the W state, and the extrema is the maximum. Therefore, the W state is the unique state under ASD of which the average von Neumann entropy of all kinds of the reduced density operators is maximal within the W SLOCC class, although the W state does not have the maximal average of the von Neumann entropy for all states of three qubits.

THE STATES FOR WHICH THE TANGLE, CONCURRENCE, 3-TANGLE AND VON NEUMANN ENTROPY DON'T VANISH

It is known that τ_{ABC} vanishes for the SLOCC classes W, A-BC, B-AC, C-AB, and A-B-C and the tangles $\tau_{AB} \geq 0$, $\tau_{AC} \geq 0$, and $\tau_{BC} \geq 0$ for the GHZ SLOCC class. Next, we present all the states for which the tangles, concurrence, 3-tangle and von Neumann entropy do not vanish. We know these states can only come from the GHZ SLOCC class. For these states, when one of three qubits is traced out, their reduced density operators are entangled while the reduced density operator of the GHZ state is separable. It seems that the states are more entangled than the GHZ state under tangle and the W state under 3-tangle, respectively. Note that the tangle is the square of the concurrence. Therefore, if a tangle does not vanish, the concurrence does not either, and hence, we do not need to discuss the concurrence separately.

Therefore, if a state satisfies $\tau_{AB}\tau_{AC}\tau_{BC} \neq 0$, $S(\rho_A)S(\rho_B)S(\rho_C) \neq 0$, and $\tau_{ABC} \neq 0$, then the state belongs to the GHZ SLOCC class and it falls in one of the three cases: (i). $\lambda_2\lambda_3 \neq 0$ and $\lambda_1 = 0$, i.e., the state is

$$|\varpi_1\rangle = \lambda_0|000\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle, \quad (42)$$

or (ii). $\lambda_1\lambda_2\lambda_3(\lambda_1\lambda_4 - \lambda_2\lambda_3) \neq 0$ and $\phi = 0$, i.e., the

state is

$$|\varpi_2\rangle = \lambda_0|000\rangle + \lambda_1|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle, \quad (43)$$

where $\lambda_1\lambda_4 \neq \lambda_2\lambda_3$, or (iii). $\lambda_1\lambda_2\lambda_3 \neq 0$ and $\phi \neq 0$, i.e., the state is

$$|\varpi_3\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\phi}|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle. \quad (44)$$

Thus, all states with non-vanishing tangles, 3-tangle, and von Neumann entropy can be written in the form of $|\varpi_1\rangle$, $|\varpi_2\rangle$ or $|\varpi_3\rangle$ with suitable λ 's. For example, the following states in the form of $|\varpi_1\rangle$.

$$|\kappa\rangle = \frac{2}{3}|000\rangle + \frac{1}{2}|101\rangle + \frac{1}{2}|110\rangle + \frac{\sqrt{2}}{6}|111\rangle, \quad (45)$$

$$|G\rangle = \frac{1}{2}(|000\rangle + |101\rangle + |110\rangle + |111\rangle), \quad (46)$$

$$|\vartheta\rangle = \frac{\sqrt{5}}{10}(3|000\rangle + |101\rangle + |110\rangle + 3|111\rangle). \quad (47)$$

See Table III for details. Furthermore, there exist other interesting states approximating the tangle and 3-tangle of the W state and the GHZ state.

(a). Let $\lambda_2 = \lambda_3 = \lambda_0$ in $|\varpi_1\rangle$, we obtain a new state

$$|\omega\rangle = \lambda_0|000\rangle + \lambda_0|101\rangle + \lambda_0|110\rangle + \lambda_4|111\rangle.$$

The tangles are

$$\tau_{AB} = \tau_{AC} = \tau_{BC} = A = 4\lambda_0^4 = \frac{4}{9}(1 - \lambda_4^2)^2. \quad (48)$$

From Eq. (48), we know that when λ_4 is small enough, then the tangles, the average tangle, 3-tangle, and von Neumann entropy of $|\omega\rangle$ are almost equal to those of the W state.

(b). Let $\lambda_4 = \lambda_0$, and let $\lambda_3 = \lambda_2$, we obtain a new state

$$|\varkappa\rangle = \lambda_0|000\rangle + \lambda_2|101\rangle + \lambda_2|110\rangle + \lambda_0|111\rangle.$$

The tangles and 3-tangle are given by

$$\tau_{AB} = \tau_{AC} = 4\lambda_0^2\lambda_2^2, \tau_{BC} = 4\lambda_2^4, \tau_{ABC} = 4\lambda_0^4. \quad (49)$$

For $|\varkappa\rangle$, we have $\lim_{\lambda_2 \rightarrow 0} S(\rho_\mu) = \ln 2$, where $\mu \in \{A, B, C\}$, $\lim_{\lambda_2 \rightarrow 0} \tau_{ABC} = 1$, and $\lim_{\lambda_2 \rightarrow 0} \tau_{\mu\nu} = 0$, where $\mu\nu \in \{AB, AC, BC\}$. Thus, when λ_2 is small enough, then the tangles, the average tangle, 3-tangle, and von Neumann entropy of $|\varkappa\rangle$ are almost

equal to those of the GHZ state. See $|\vartheta\rangle$ in Table III.

Next, we demonstrate that tangles τ_{AB} , τ_{AC} , and τ_{BC} with $\tau_{AB}\tau_{AC}\tau_{BC} \neq 0$ determine a unique state of the form of $|\varpi_1\rangle$. In other words, the LU invariants $\{J_i|i = 1, 2, 3\}$ with $J_1J_2J_3 \neq 0$ can determine a unique state of the form of $|\varpi_1\rangle$.

Suppose the tangles $\tau_{AB} = 4\lambda_0^2\lambda_3^2 = p^4$, $\tau_{AC} = 4\lambda_0^2\lambda_2^2 = q^4$, and $\tau_{BC} = 4\lambda_2^2\lambda_3^2 = r^4$, where $pqr \neq 0$. It is known that $p^4 + q^4 + r^4 < 4/3$ from the CKW inequality $\tau_{AB} + \tau_{AC} + \tau_{BC} < 4/3$ (see Appendix B and also [3]). The unique state corresponding to the tangles is

$$\frac{1}{\sqrt{2}} \frac{pq}{r} |000\rangle + \frac{1}{\sqrt{2}} \frac{qr}{p} |101\rangle + \frac{1}{\sqrt{2}} \frac{pr}{q} |110\rangle + \lambda_4 |111\rangle,$$

$$\text{where } \lambda_4^2 = 1 - \frac{1}{2}((\frac{pq}{r})^2 + (\frac{qr}{p})^2 + (\frac{pr}{q})^2).$$

On the other hand, the five LU invariants $\{J_i|i = 1, \dots, 5\}$ cannot uniquely determine a state of three qubits. For instance, for $|\varpi_1\rangle$, from that $\lambda_0^2 + \sum_{i=2}^4 \lambda_i^2 = 1$ we can derive $J_4 = \sqrt{J_2J_3/J_1} - (J_2J_3/J_1 + J_2 + J_3)$. That is, J_4 is a function of J_1 , J_2 , and J_3 , which explains why $\{J_i|i = 1, \dots, 5\}$ cannot determine a unique state of three qubits [9].

TABLE III. Tangle, 3-tangle and von Neumann entropy for some states ($\delta = \frac{3\ln 3 - 2\ln 2}{3} = 0.63651$)

State	τ_{AB}	τ_{AC}	τ_{BC}	$S(\rho_A)$	$S(\rho_B)$	$S(\rho_C)$	τ_{ABC}
GHZ	0	0	0	$\ln 2$	$\ln 2$	$\ln 2$	1
W	$\frac{4}{9}$	$\frac{4}{9}$	$\frac{4}{9}$	δ	δ	δ	0
$ G\rangle$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.56	0.56	0.56	$\frac{1}{4}$
$ \kappa\rangle$	$\frac{4}{9}$	$\frac{4}{9}$	$\frac{1}{4}$	0.687	0.587	0.587	$\frac{8}{81}$
$ \vartheta\rangle$	$\frac{9}{100}$	$\frac{9}{100}$	$\frac{1}{100}$	0.688	0.647	0.647	$\frac{81}{100}$

CKW INEQUALITIES FOR GHZ SLOCC CLASS

For GHZ SLOCC class, $\lambda_0\lambda_4 \neq 0$, we have the following CKW inequalities. The arguments for CKW inequalities are summarized in Appendix D.

1. If $\lambda_1 = \lambda_2 = \lambda_3 = 0$, then $\tau_{AB} + \tau_{AC} + \tau_{BC} = 0$. This is the generated GHZ state $p|000\rangle + q|111\rangle$.
2. If $\lambda_1 = \lambda_2 = 0$, and $\lambda_3 \neq 0$, then $\tau_{AB} + \tau_{AC} + \tau_{BC} < 1$.
3. If $\lambda_1 = \lambda_3 = 0$, and $\lambda_2 \neq 0$, then $\tau_{AB} + \tau_{AC} + \tau_{BC} < 1$.
4. If $\lambda_2 = \lambda_3 = 0$, and $\lambda_1 \neq 0$, then $\tau_{AB} + \tau_{AC} + \tau_{BC} < 1$.
5. If $\lambda_1 = 0$, and $\lambda_2\lambda_3 \neq 0$, then $\tau_{AB} + \tau_{AC} + \tau_{BC} < \frac{4}{3}$.
6. If $\lambda_2 = 0$, and $\lambda_1\lambda_3 \neq 0$, then $\tau_{AB} + \tau_{AC} + \tau_{BC} \leq \frac{1}{2}$.
7. If $\lambda_3 = 0$, and $\lambda_1\lambda_2 \neq 0$, then $\tau_{AB} + \tau_{AC} + \tau_{BC} \leq \frac{1}{2}$.
8. If $\lambda_1\lambda_2\lambda_3 \neq 0$, then $\tau_{AB} + \tau_{AC} + \tau_{BC} \leq 1$.

SUMMARY

In this paper, we have given a general formula of the tangles for pure states of three qubits, which are LU polynomial invariants of degree 4. We derived tangles and von Neumann entropy for ASD, and presented a relation among tangles, 3-tangle, and von Neumann entropy, as well as a relation among the average tangle, the average von Neumann entropy, and 3-tangle.

Via the von Neumann entropy for ASD, we indicated that the GHZ state is the unique state of three qubits under ASD that has the maximal von Neumann entropy for all kinds of the reduced density operators, while the average von Neumann entropy of the W state is maximal only within the W SLOCC class.

It is known that the tangles of the GHZ state and the 3-tangle of the W state would vanish. We obtained all states of three qubits with non-vanishing

tangle, concurrence, 3-tangle and von Neumann entropy. For example, $|\vartheta\rangle$ is such a state. It means that when one of the three qubits is traced out, the remaining state from $|\vartheta\rangle$ is still entangled, while the remaining state of the GHZ state becomes separable. From Table III, it is shown that $S(\rho_\mu)$ of $|\vartheta\rangle$ is bigger than that of the W state, where $\mu \in \{A, B, C\}$. Therefore, state $|\vartheta\rangle$ seems to be more entangled than the GHZ state under tangle and more tangled than the W state under von Neumann entropy and 3-tangle.

APPENDIX A. CALCULATION OF TANGLES.

(A) Calculating τ_{AB}

From the definition of τ_{AB} in Eq. (2), we obtain the characteristic polynomial (CP) of $\rho_{AB}\overline{\rho_{AB}}$ as follows,

$$(X^2 - \Delta X + \Theta^2)X^2, \quad (\text{A1})$$

where

$$\begin{aligned} \Theta = & |(c_0c_7 - c_2c_5)^2 + (c_1c_6 - c_3c_4)^2 \\ & - 2(c_0c_7 + c_2c_5)(c_1c_6 + c_3c_4) \\ & + 4c_0c_3c_5c_6 + 4c_1c_2c_4c_7|, \end{aligned} \quad (\text{A2})$$

$$\begin{aligned} \Delta = & 2(|c_0|^2 + |c_1|^2)(|c_6|^2 + |c_7|^2) \\ & + 2(|c_2|^2 + |c_3|^2)(|c_4|^2 + |c_5|^2) \\ & + 2|c_0c_6^* + c_1c_7^*|^2 + 2|c_2c_4^* + c_3c_5^*|^2 \\ & - 4 * re((c_0c_2^* + c_1c_3^*)(c_6c_4^* + c_7c_5^*)) \\ & - 4 * re((c_0c_4^* + c_1c_5^*)(c_6c_2^* + c_7c_3^*)), \end{aligned} \quad (\text{A3})$$

and $re(c)$ indicates the real part of a complex number c . Moreover, one can find

$$4\Theta = \tau_{ABC}. \quad (\text{A4})$$

Hence, the eigenvalues of $\rho_{AB}\overline{\rho_{AB}}$ are 0, 0, and $\frac{\Delta \pm \sqrt{\Delta^2 - 4\Theta^2}}{2}$. It is known that $\rho_{AB}\overline{\rho_{AB}}$ has only real and non-negative eigenvalues [13]. Then, by the definition of τ_{AB} in Eq. (2), we obtain

$$\begin{aligned} \tau_{AB} = & \left(\sqrt{\frac{\Delta + \sqrt{\Delta^2 - 4\Theta^2}}{2}} - \sqrt{\frac{\Delta - \sqrt{\Delta^2 - 4\Theta^2}}{2}} \right)^2 \\ = & \Delta - 2\Theta \\ = & \Delta - \frac{\tau_{ABC}}{2}. \end{aligned} \quad (\text{A5})$$

(B) Calculating τ_{AC}

Similarly, we can obtain the CP of $\rho_{AC}\overline{\rho_{AC}}$ as follows,

$$X^2(X^2 - \Phi X + \Upsilon^2), \quad (\text{A6})$$

where

$$\Upsilon = \Theta, \quad (\text{A7})$$

$$\begin{aligned} \Phi = & 2 \left(|c_0|^2 + |c_2|^2 \right) \left(|c_5|^2 + |c_7|^2 \right) \\ & + 2 \left(|c_1|^2 + |c_3|^2 \right) \left(|c_4|^2 + |c_6|^2 \right) \\ & + 2 |c_0 c_5^* + c_2 c_7^*|^2 + 2 |c_1 c_4^* + c_3 c_6^*|^2 \\ & - 4 * re((c_0 c_1^* + c_2 c_3^*)(c_5 c_4^* + c_7 c_6^*)) \\ & - 4 * re((c_0 c_4^* + c_2 c_6^*)(c_5 c_1^* + c_7 c_3^*)). \end{aligned} \quad (\text{A8})$$

Then, we obtain

$$\tau_{AC} = \Phi - 2\Upsilon = \Phi - \frac{\tau_{ABC}}{2}. \quad (\text{A9})$$

(C) Calculating τ_{BC}

Similarly, the characteristic polynomial of $\rho_{BC}\overline{\rho_{BC}}$ is given by

$$X^2(X^2 - \Psi X + F^2), \quad (\text{A10})$$

where

$$F = \Theta, \quad (\text{A11})$$

$$\begin{aligned} \Psi = & 2 \left(|c_0|^2 + |c_4|^2 \right) \left(|c_3|^2 + |c_7|^2 \right) \\ & + 2 \left(|c_1|^2 + |c_5|^2 \right) \left(|c_2|^2 + |c_6|^2 \right) \\ & + 2 |c_0 c_3^* + c_4 c_7^*|^2 + 2 |c_1 c_2^* + c_5 c_6^*|^2 \\ & - 4 * re((c_0 c_1^* + c_4 c_5^*)(c_3 c_2^* + c_7 c_6^*)) \\ & - 4 * re((c_0 c_2^* + c_4 c_6^*)(c_3 c_1^* + c_7 c_5^*)). \end{aligned} \quad (\text{A12})$$

Then, we obtain

$$\tau_{BC} = \Psi - 2F = \Psi - \frac{\tau_{ABC}}{2}. \quad (\text{A13})$$

(D) By solving CKW equations [13]

$$\tau_{AB} + \tau_{AC} + \tau_{ABC} = \tau_{A(BC)}, \quad (\text{A14})$$

$$\tau_{AB} + \tau_{BC} + \tau_{ABC} = \tau_{B(AC)}, \quad (\text{A15})$$

$$\tau_{AC} + \tau_{BC} + \tau_{ABC} = \tau_{C(AB)}, \quad (\text{A16})$$

where $\tau_{A(BC)} = 4 \det \rho_A$, $\tau_{B(AC)} = 4 \det \rho_B$, and $\tau_{C(AB)} = 4 \det \rho_C$, we obtain

$$\tau_{AB} = \frac{\tau_{A(BC)} + \tau_{B(AC)} - \tau_{C(AB)} - \tau_{ABC}}{2}, \quad (\text{A17})$$

$$\tau_{AC} = \frac{\tau_{A(BC)} - \tau_{B(AC)} + \tau_{C(AB)} - \tau_{ABC}}{2}, \quad (\text{A18})$$

$$\tau_{BC} = \frac{-\tau_{A(BC)} + \tau_{B(AC)} + \tau_{C(AB)} - \tau_{ABC}}{2}. \quad (\text{A19})$$

When the 3-tangle τ_{ABC} is zero, we obtain the following,

$$\Delta = \frac{\tau_{A(BC)} + \tau_{B(AC)} - \tau_{C(AB)}}{2}, \quad (\text{A20})$$

$$\Phi = \frac{\tau_{A(BC)} - \tau_{B(AC)} + \tau_{C(AB)}}{2}, \quad (\text{A21})$$

$$\Psi = \frac{-\tau_{A(BC)} + \tau_{B(AC)} + \tau_{C(AB)}}{2}. \quad (\text{A22})$$

Obviously, Δ , Φ , Ψ are simple polynomial of degree 4 although it is hard to compute $\det \rho_A$, $\det \rho_B$, and $\det \rho_C$.

APPENDIX B THE GHZ STATE IS UNIQUE STATE OF THREE QUBITS WHICH HAS MAXIMALLY VON NEUMANN ENTROPY

Claim: If a state of three qubits possesses the maximal von Neumann entropy, $S(\rho_\mu) = \ln 2$, where $\mu \in \{A, B, C\}$, then the state must be GHZ.

Proof: Clearly, $S(\rho_\mu)$ increases strictly monotonically as α_μ increases. Therefore, $S(\rho_\mu) = \ln 2$ iff $\alpha_\mu = 1/4$. Thus, we have the following equations

$$\alpha_A = J_2 + J_3 + J_4 = 1/4, \quad (\text{B1})$$

$$\alpha_B = J_1 + J_3 + J_4 = 1/4, \quad (\text{B2})$$

$$\alpha_C = J_1 + J_2 + J_4 = 1/4, \quad (\text{B3})$$

and we obtain

$$J_1 = J_2 = J_3. \quad (\text{B4})$$

Using Tables I and II, equation (B1) leads to

$$\lambda_0^4 - \lambda_0^2(1 - \lambda_1^2) + 1/4 = 0. \quad (\text{B5})$$

From (B5), we have a solution

$$\lambda_1 = 0, \quad (\text{B6})$$

$$\lambda_0 = 1/\sqrt{2}, \quad (\text{B7})$$

$$\lambda_2^2 + \lambda_3^2 + \lambda_4^2 = 1/2. \quad (\text{B8})$$

Using $J_2 = J_3$ in Eq. (B4), we have

$$\lambda_2 = \lambda_3. \quad (\text{B9})$$

From that $J_1 = J_2$ in Eq. (B4), we obtain

$$\lambda_2 \lambda_3 = \lambda_0 \lambda_2. \quad (\text{B10})$$

There are two scenarios for λ_2 : $\lambda_2 \neq 0$ and $\lambda_2 = 0$. The first scenario is impossible since if $\lambda_2 \neq 0$, then from Eqs. (B7, B9, B10), we obtain

$$\lambda_0 = \lambda_2 = \lambda_3 = 1/\sqrt{2}. \quad (\text{B11})$$

From Eq. (B8), we know clearly that Eq. (B11) cannot hold. Therefore, λ_2 must be zero.

With $\lambda_2 = 0$, from Eqs. (B8, B9) we obtain

$$\lambda_2 = \lambda_3 = 0, \quad (\text{B12})$$

$$\lambda_4 = 1/\sqrt{2}. \quad (\text{B13})$$

The state satisfying Eqs. (B6, B7, B12, B13) is just GHZ.

APPENDIX C THE EXTREMA FOR W SLOCC CLASS

We next find an extrema of m with the constraint of $\sum_{i=0}^3 \lambda_i^2 = 1$ for the W SLOCC class. For states of W SLOCC class, $\alpha_A = \lambda_0^2(\lambda_2^2 + \lambda_3^2)$, $\alpha_B = \lambda_3^2(\lambda_0^2 + \lambda_2^2)$, and $\alpha_C = \lambda_2^2(\lambda_0^2 + \lambda_3^2)$

We define

$$F = \frac{1}{3}(S(\rho_A) + S(\rho_B) + S(\rho_C)) + \ell \left(\sum_{i=0}^3 \lambda_i^2 - 1 \right), \quad (\text{C1})$$

where ℓ is the Lagrange multiplier. In light of the constrained extreme theorem, we need to solve the equations $\frac{\partial F}{\partial \lambda_i} = 0$, for $i = 0, 1, 2, 3$, and $\frac{\partial F}{\partial \ell} = 0$ to find the extrema. From $\frac{\partial F}{\partial \lambda_1} = 2\ell\lambda_1 = 0$, we obtain $\lambda_1 = 0$. Then, F is reduced to

$$F = \frac{1}{3}(S(\rho_A) + S(\rho_B) + S(\rho_C)) + \ell(\lambda_0^2 + \lambda_2^2 + \lambda_3^2 - 1). \quad (\text{C2})$$

From $\frac{\partial F}{\partial \ell} = 0$ we obtain

$$\lambda_0^2 + \lambda_2^2 + \lambda_3^2 = 1. \quad (\text{C3})$$

From Eq. (C2), we obtain

$$\frac{\partial F}{\partial \lambda_0} = \frac{1}{3} \left[\frac{\partial S(\rho_A)}{\partial \lambda_0} + \frac{\partial S(\rho_B)}{\partial \lambda_0} + \frac{\partial S(\rho_C)}{\partial \lambda_0} \right] + 2\ell\lambda_0, \quad (\text{C4})$$

where

$$\frac{\partial S(\rho_\mu)}{\partial \lambda_0} = \frac{dS(\rho_\mu)}{d\alpha_\mu} \frac{\partial \alpha_\mu}{\partial \lambda_0}, \mu \in \{A, B, C\}. \quad (\text{C5})$$

The derivative of $S(\rho_A)$ is

$$\frac{dS(\rho_A)}{d\alpha_A} = - \left[\frac{d\eta_A^{(1)}}{d\alpha_A} (1 + \ln \eta_A^{(1)}) + \frac{d\eta_A^{(2)}}{d\alpha_A} (1 + \ln \eta_A^{(2)}) \right], \quad (\text{C6})$$

where

$$\frac{d\eta_A^{(1)}}{d\alpha_A} = -\frac{1}{\sqrt{1-4\alpha_A}}, \quad \frac{d\eta_A^{(2)}}{d\alpha_A} = \frac{1}{\sqrt{1-4\alpha_A}}. \quad (\text{C7})$$

Thus,

$$\begin{aligned} \frac{dS(\rho_A)}{d\alpha_A} &= - \left[-\frac{1 + \ln \eta_A^{(1)}}{\sqrt{1-4\alpha_A}} + \frac{1 + \ln \eta_A^{(2)}}{\sqrt{1-4\alpha_A}} \right] \\ &= -\frac{1}{\sqrt{1-4\alpha_A}} \ln \frac{\eta_A^{(2)}}{\eta_A^{(1)}}. \end{aligned} \quad (\text{C8})$$

Similarly, we obtain

$$\frac{dS(\rho_B)}{d\alpha_B} = -\frac{1}{\sqrt{1-4\alpha_B}} \ln \frac{\eta_B^{(2)}}{\eta_B^{(1)}}, \quad (\text{C9})$$

$$\frac{dS(\rho_C)}{d\alpha_C} = -\frac{1}{\sqrt{1-4\alpha_C}} \ln \frac{\eta_C^{(2)}}{\eta_C^{(1)}}. \quad (\text{C10})$$

From Eqs. (C5, C8, C9, C10), we obtain

$$\frac{\partial S(\rho_A)}{\partial \lambda_0} = -\frac{2\lambda_0(\lambda_2^2 + \lambda_3^2)}{\sqrt{1-4\alpha_A}} \ln \frac{\eta_A^{(2)}}{\eta_A^{(1)}}, \quad (\text{C11})$$

$$\frac{\partial S(\rho_B)}{\partial \lambda_0} = -\frac{2\lambda_0\lambda_3^2}{\sqrt{1-4\alpha_B}} \ln \frac{\eta_B^{(2)}}{\eta_B^{(1)}}, \quad (\text{C12})$$

$$\frac{\partial S(\rho_C)}{\partial \lambda_0} = -\frac{2\lambda_0\lambda_2^2}{\sqrt{1-4\alpha_C}} \ln \frac{\eta_C^{(2)}}{\eta_C^{(1)}}. \quad (\text{C13})$$

From Eqs. (C4, C11, C12, C13) and $\frac{\partial F}{\partial \lambda_0} = 0$, we obtain

$$\begin{aligned} \ell &= \frac{1}{3} \left(\frac{\lambda_2^2 + \lambda_3^2}{\sqrt{1-4\alpha_A}} \ln \frac{\eta_A^{(2)}}{\eta_A^{(1)}} \right. \\ &\quad + \frac{\lambda_3^2}{\sqrt{1-4\alpha_B}} \ln \frac{\eta_B^{(2)}}{\eta_B^{(1)}} \\ &\quad \left. + \frac{\lambda_2^2}{\sqrt{1-4\alpha_C}} \ln \frac{\eta_C^{(2)}}{\eta_C^{(1)}} \right). \end{aligned} \quad (\text{C14})$$

Similarly, we consider

$$\frac{\partial F}{\partial \lambda_2} = \frac{1}{3} \left(\frac{\partial S(\rho_A)}{\partial \lambda_2} + \frac{\partial S(\rho_B)}{\partial \lambda_2} + \frac{\partial S(\rho_C)}{\partial \lambda_2} \right) + 2\ell\lambda_2. \quad (\text{C15})$$

Clearly,

$$\frac{\partial S(\rho_\mu)}{\partial \lambda_2} = \frac{dS(\rho_\mu)}{d\alpha_\mu} \frac{\partial \alpha_\mu}{\partial \lambda_2}, \mu \in \{A, B, C\}. \quad (\text{C16})$$

From Eqs. (C8, C9, C10, C15, C16) and $\frac{\partial F}{\partial \lambda_2} = 0$, we obtain

$$\begin{aligned} \ell = \frac{1}{3} & \left(\frac{\lambda_0^2}{\sqrt{1-4\alpha_A}} \ln \frac{\eta_A^{(2)}}{\eta_A^{(1)}} \right. \\ & + \frac{\lambda_3^2}{\sqrt{1-4\alpha_B}} \ln \frac{\eta_B^{(2)}}{\eta_B^{(1)}} \\ & \left. + \frac{\lambda_0^2 + \lambda_3^2}{\sqrt{1-4\alpha_C}} \ln \frac{\eta_C^{(2)}}{\eta_C^{(1)}} \right). \end{aligned} \quad (\text{C17})$$

Similarly, from $\frac{\partial F}{\partial \lambda_3} = 0$ we obtain

$$\begin{aligned} \ell = \frac{1}{3} & \left(\frac{\lambda_0^2}{\sqrt{1-4\alpha_A}} \ln \frac{\eta_A^{(2)}}{\eta_A^{(1)}} \right. \\ & + \frac{\lambda_0^2 + \lambda_2^2}{\sqrt{1-4\alpha_B}} \ln \frac{\eta_B^{(2)}}{\eta_B^{(1)}} \\ & \left. + \frac{\lambda_2^2}{\sqrt{1-4\alpha_C}} \ln \frac{\eta_C^{(2)}}{\eta_C^{(1)}} \right). \end{aligned} \quad (\text{C18})$$

From Eqs. (C3, C14, C17), we obtain

$$\frac{1-2\lambda_0^2}{\sqrt{1-4\alpha_A}} \ln \frac{\eta_A^{(2)}}{\eta_A^{(1)}} = \frac{1-2\lambda_2^2}{\sqrt{1-4\alpha_C}} \ln \frac{\eta_C^{(2)}}{\eta_C^{(1)}}. \quad (\text{C19})$$

From Eqs. (C3, C14, C18), we obtain

$$\frac{1-2\lambda_0^2}{\sqrt{1-4\alpha_A}} \ln \frac{\eta_A^{(2)}}{\eta_A^{(1)}} = \frac{1-2\lambda_3^2}{\sqrt{1-4\alpha_B}} \ln \frac{\eta_B^{(2)}}{\eta_B^{(1)}}. \quad (\text{C20})$$

From Eqs. (C3, C17, C18), we obtain

$$\frac{1-2\lambda_3^2}{\sqrt{1-4\alpha_B}} \ln \frac{\eta_B^{(2)}}{\eta_B^{(1)}} = \frac{1-2\lambda_2^2}{\sqrt{1-4\alpha_C}} \ln \frac{\eta_C^{(2)}}{\eta_C^{(1)}}. \quad (\text{C21})$$

When $\lambda_0 = \lambda_2 = \lambda_3$, Eqs. (C19, C20, C21) hold. Via Eq. (C3), one can see that $\lambda_0 = \lambda_2 = \lambda_3 = 1/\sqrt{3}$ is an extrema of m with the constraint $\sum_{i=0}^3 \lambda_i^2 = 1$.

APPENDIX D. CKW INEQUALITIES FOR GHZ SLOCC CLASS.

Note that for the GHZ SLOCC class, $\lambda_0 \lambda_4 \neq 0$. There is also an additional constraint $\sum_{i=0}^4 \lambda_i^2 = 1$.

(A) When $\lambda_1 = \lambda_3 = 0$ and $\lambda_2 \neq 0$, we have

$$A = \frac{4}{3}(\lambda_0^2 \lambda_2^2).$$

Clearly,

$$A = \frac{4}{3}(\lambda_0^2 \lambda_2^2) \leq \frac{4}{3} \left(\frac{\lambda_0^2 + \lambda_2^2}{2} \right)^2 = \frac{1}{3} (1 - \lambda_4^2)^2 < \frac{1}{3}$$

Similarly, we can obtain $A < \frac{1}{3}$ for the case with $\lambda_1 = \lambda_2 = 0, \lambda_3 \neq 0$ and the case with $\lambda_2 = \lambda_3 = 0, \lambda_1 \neq 0$.

(B) When $\lambda_1 \lambda_3 \neq 0$ and $\lambda_2 = 0$, A is reduced to

$$A = \frac{4}{3}(\lambda_0^2 \lambda_3^2 + \lambda_1^2 \lambda_4^2).$$

In light of constrained extreme theorem, we consider the following function

$$U = \frac{4}{3}(\lambda_0^2 \lambda_3^2 + \lambda_1^2 \lambda_4^2) + q(\lambda_0^2 + \lambda_1^2 + \lambda_3^2 + \lambda_4^2 - 1).$$

From $\frac{\partial U}{\partial \lambda_i} = 0$, obtain only one extreme $\lambda_0 = \lambda_1 = \lambda_3 = \lambda_4 = \frac{1}{2}$, i.e. $\frac{1}{2}(|000\rangle + |100\rangle + |110\rangle + |111\rangle)$, at which $\max A = \frac{1}{6}$.

(C) When $\lambda_1 \lambda_2 \neq 0$ and $\lambda_3 = 0$, A is reduced to

$$A = \frac{4}{3}(\lambda_0^2 \lambda_2^2 + \lambda_1^2 \lambda_4^2).$$

The discussion is similar to (B), there is only one extreme $\lambda_0 = \lambda_1 = \lambda_2 = \lambda_4 = \frac{1}{2}$, i.e. $\frac{1}{2}(|000\rangle + |100\rangle + |101\rangle + |111\rangle)$, $\max A = \frac{1}{6}$.

(D) When $\lambda_1 = 0$ and $\lambda_2 \lambda_3 \neq 0$, then

$$A = \frac{4}{3}(\lambda_0^2 \lambda_3^2 + \lambda_2^2 \lambda_4^2 + \lambda_2^2 \lambda_3^2).$$

The constraint is

$$\lambda_0^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 = 1,$$

where λ_4 is considered as a parameter. In light of constrained extreme theorem, for a fixed λ_4 , when $\lambda_0 = \lambda_2 = \lambda_3$, i.e., $\lambda_0|000\rangle + \lambda_0|101\rangle + \lambda_0|110\rangle +$

$\lambda_4|111\rangle$, then A has the maximum $A = 4\lambda_0^4 = \frac{4}{9}(1 - \lambda_4^2)^2 < \frac{4}{9}$.

(E) When $\lambda_1\lambda_2\lambda_3 \neq 0$, let

$$f = \frac{4}{3}(\lambda_0^2\lambda_3^2 + \lambda_0^2\lambda_2^2 + (\lambda_1\lambda_4 + \lambda_2\lambda_3)^2).$$

Clearly, $A \leq f$. We next calculate the maximum value of f . The constraint reads $\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 = 1$. In light of the constrained extreme theorem, we consider the function

$$F = f + g(\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 - 1).$$

From $\frac{\partial F}{\partial \lambda_i} = 0$, $i = 0, 1, 2, 3, 4$, we obtain $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4$ and $\lambda_0 = 0$. Thus, f has the maximum value $\frac{1}{3}$. However, we require that λ_0 do not vanish. From $\sum_{i=0}^4 \lambda_i^2 = 1$, we get $\lambda_0^2 + 4\lambda_4^2 = 1$. Thus, when $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4$, $A = \frac{4}{3}((2\lambda_4^2))(1 - 2\lambda_4^2) < 1/3$. Clearly, $\lim_{\lambda_0 \rightarrow 0} A = \frac{1}{3}$. For example, when $\lambda_0^2 = \frac{1}{100}$, then $A = \frac{3333}{10000} \approx \frac{1}{3}$.

Data Availability Statement: The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Conflicts of interest/Competing interests: The authors have no conflicts of interest to declare that are relevant to the content of this article.

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