

Computing the geometric measure of entanglement of multipartite pure states by means of non-negative tensors

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The geometric measure of entanglement for pure states has attracted much attention. On the other hand, the spectral theory of non-negative tensors (hypermatrices) has been developed rapidly. In this paper, we show how the spectral theory of non-negative tensors can be applied to the study of the geometric measure of entanglement for pure states. For symmetric pure multipartite qubit or qutrit states an elimination method is given. For symmetric pure multipartite qudit states, a numerical algorithm with randomization is presented. We also show that a nonsymmetric pure state can be augmented to a symmetric one whose amplitudes can be encoded in a non-negative symmetric tensor, so the geometric measure of entanglement can be calculated. Several examples, such as m GHZ states, W states, inverted W states, qudits, and nonsymmetric states, are used to demonstrate the power of the proposed methods. Given a pure state, one can always find a change of basis (a unitary transformation) so that all the probability amplitudes of the pure state are non-negative under the new basis. Therefore, the methods proposed here can be applied to a very wide class of multipartite pure states.

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I. INTRODUCTION

Quantum entanglement is regarded as one of the most essential resources in quantum information [1], and the geometric measure is one of the most important measures of quantum entanglement [2–10]. Geometric measure was proposed by Shimony [2] for bipartite systems and later generalized to multipartite systems by Wei and Goldbart [4], and has become one of the widely used entanglement measures for multiparticle cases [5–7, 11]. Among them, the study on pure symmetric states with non-negative amplitudes attracted much attention recently. Wei and Goldbart conjectured that the nearest separable state for a symmetric state can be chosen to be symmetric [[4], Sec. II A]. Independently, Wei and Severini [12] and Hayashi, Markham, Murao, Owari, and Virmani [6] proved the conjecture for the special case of symmetric states with non-negative amplitudes and showed that the corresponding nearest separable state can be chosen with non-negative amplitudes. Hübener, Kleinmann, Wei, González-Guillén, and Gühne [5] proved the conjecture completely. The computation of symmetric pure states with non-negative amplitudes was carried out by Wei and Goldbart [4] for some ground states, and systematically by Chen, Xu, and Zhu [7] for symmetric pure multipartite qubit states. For general evaluations of the geometric entanglement for symmetric pure states, please see Orús, Dusuel, and Vidal [8], Chen, Xu, and Zhu [7], and references therein.

The central problem of the computation of the geometric measure of entanglement is to find the largest entanglement eigenvalue [4, 11, 13]. Mathematically, the quantum eigenvalue problem is a generalization of the singular value problem

of a complex matrix [11, 13]. There have been several generalizations of singular values or eigenvalues of matrices to tensors (hypermatrices) recently [14–16]. These form the spectral theory of tensors [17]. In this paper we investigate the geometric measure of entanglement for pure states by means of the spectral theory of non-negative tensors. Given a pure state, one can always find a change of basis (a unitary transformation) such that all the amplitudes of the pure state are non-negative under the new basis. Therefore, without loss of generality, in this paper we focus on the geometric measure of entanglement for non-negative pure states.

To be specific, we establish a connection between the concept of Z eigenvalues of tensors [14] and the quantum eigenvalue problem. We show that the geometric measure of entanglement of a symmetric pure state with non-negative amplitudes is equal to the Z -spectral radius of the corresponding non-negative tensor (Theorem 1). Based on this connection, a method based on variable elimination [18, 19] for computing the geometric measure of entanglement for symmetric pure multipartite qubit or qutrit states with non-negative amplitudes is given. For the qubit case, it is an alternative to the method proposed in [[7], Sec. II A]; see Examples 1–3 in Sec. IV A. For the qutrit case, it is new and gives an analytical derivation of the geometric measure of entanglement for such states; see Example 4 in Sec. IV B.

For symmetric pure multipartite qudit states with non-negative amplitudes [20–22], a numerical algorithm with randomization (Algorithm 3) is presented. The method is based on the shifted higher-order power method (Algorithm 2) analyzed in [23]. We show that if the initial points are randomly chosen from the intersection of the positive orthant and the unit sphere, then with a positive probability the algorithm may find the geometric measure of entanglement for qudits. Example 5 in Sec. IV C demonstrates the proposed algorithm.

Given a nonsymmetric pure state, one can encode its amplitudes in a nonsymmetric tensor, while the latter can be

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augmented to become a symmetric one for which the geometric measure of entanglement can be computed. We illustrate this by an example in Sec. V, Example 6. Therefore, the numerical methods established above are applicable to a much larger class of pure states.

The rest of this paper is organized as follows. The definitions and some basic facts of the geometric measure of entanglement and the Z eigenvalues of tensors are presented as preliminaries in Sec. II. In Sec. III, a connection between the geometric measure of entanglement of a symmetric pure state with non-negative amplitudes and the theory of the Z -spectral radius of a non-negative tensor is established. The computational issues are discussed in Sec. IV. In Sec. V, a connection between the geometric measure of entanglement for nonsymmetric pure states and the spectral theory of non-negative multilinear forms is established. The paper is concluded with some final remarks in Sec. VI.

Notation. Denote by \mathbb{R}_+^n the non-negative orthant of \mathbb{R}^n , \mathbb{R}_{++}^n the interior of \mathbb{R}_+^n , and \mathcal{S}^{n-1} the unit sphere in \mathbb{R}^n .

II. PRELIMINARIES

In this section, some preliminary results of the geometric measure of quantum entanglement of pure states and Z eigenvalues of tensors (hypermatrices) are briefly reviewed.

A. Geometric measure

An m -partite pure state $|\Psi\rangle$ of a composite quantum system can be regarded as a normalized element in a tensor product Hilbert space $\mathcal{H} = \bigotimes_{k=1}^m \mathcal{H}_k$, where the dimension of \mathcal{H}_k is d_k , ($k = 1, \dots, m$). A separable pure m -partite state $|\Phi\rangle \in \mathcal{H}$ can be described by a product state $|\Phi\rangle = \bigotimes_{k=1}^m |\phi^{(k)}\rangle$ with $|\phi^{(k)}\rangle \in \mathcal{H}_k$ and $\|\phi^{(k)}\| = 1$, ($k = 1, \dots, m$). A state is called *entangled* if it is not separable.

For a given m -partite pure state $|\Psi\rangle \in \mathcal{H}$, denote the maximal overlap by

$$G_\Psi \triangleq \max_{|\Phi\rangle = \bigotimes_{k=1}^m |\phi^{(k)}\rangle \in \mathcal{H}} |\langle \Psi | \Phi \rangle|. \quad (1)$$

Then the geometric measure of entanglement for $|\Psi\rangle$ is defined as

$$E_G(|\Psi\rangle) \triangleq 1 - G_\Psi.$$

Clearly, the larger the geometric measure $E_G(|\Psi\rangle)$ is, the more entangled the state $|\Psi\rangle$ is.

An alternative form of geometric measure,

$$E_G(|\Psi\rangle) = -\log_2 \max_{|\Phi\rangle = \bigotimes_{k=1}^m |\phi^{(k)}\rangle \in \mathcal{H}} |\langle \Psi | \Phi \rangle|^2,$$

has also been widely used.

It can be shown that the maximal overlap in (1) is equal to the largest *entanglement eigenvalue* λ , see e.g., [[4], Eq. (6)], satisfying

$$\begin{cases} \langle \Psi | \left(\bigotimes_{j \neq k} |\phi^{(j)}\rangle \right) = \lambda \langle \phi^{(k)} |, \\ \left(\bigotimes_{j \neq k} \langle \phi^{(j)} | \right) \Psi = \lambda |\phi^{(k)}\rangle, \\ \|\phi^{(k)}\| = 1, \quad k = 1, \dots, m. \end{cases} \quad (2)$$

A state $|\Psi\rangle \in \mathcal{H}$ is called *non-negative* if there exist orthonormal bases $\{|e_i^{(k)}\rangle\}_{i=1}^{d_k}$ for \mathcal{H}_k ($k = 1, \dots, m$) such that $a_{i_1 \dots i_m} \triangleq \langle \Psi | (|e_{i_1}^{(1)}\rangle \otimes \dots \otimes |e_{i_m}^{(m)}\rangle) \rangle \geq 0$ for all $i_j = 1, \dots, d_j$ and $j = 1, \dots, m$. Moreover it is obvious that there always exists a unitary transformation (equivalently, change of basis) that transforms a given pure state $|\Psi\rangle \in \mathcal{H}$ into a non-negative one. Thus, in this paper we focus on the geometric measure of entanglement for non-negative states.

The $d_1 \times \dots \times d_m$ multiway array consisting of the amplitudes $a_{i_1 \dots i_m}$ for the pure state $|\Psi\rangle$ is denoted by \mathcal{A}_Ψ . Clearly, when $\mathcal{H}_1 = \dots = \mathcal{H}_m$, \mathcal{A}_Ψ is symmetric if and only if $|\Psi\rangle$ is permutation symmetric. The geometric measure of symmetric states attracted much attention recently [5–8].

When $|\Psi\rangle$ is symmetric, (1) reduces to

$$G_\Psi = \max_{|\Phi\rangle = |\phi\rangle^{\otimes m} \in \mathcal{H}} |\langle \Psi | \Phi \rangle|. \quad (3)$$

That is, the nearest separable state can be a symmetric one; see, e.g., [[5], Eq. (8)] and [12].

B. Z eigenvalues of a tensor (hypermatrix)

For a real tensor (or hypermatrix) \mathcal{T} of order m and dimension n with $m, n \geq 2$, we mean a multiway array consisting of numbers $t_{i_1 \dots i_m} \in \mathbb{R}$ for all $i_j \in \{1, \dots, n\}$ and $j \in \{1, \dots, m\}$. The set of all m th order n -dimensional real tensors is denoted by $\mathbb{R}^{m, n}$. Given a vector $\mathbf{x} \in \mathbb{C}^n$, define $\mathcal{T}\mathbf{x}^{m-1}$ as an n -dimensional vector with the i th element $\sum_{i_2, \dots, i_m=1}^n t_{i i_2 \dots i_m} \mathbf{x}_{i_2} \dots \mathbf{x}_{i_m}$, $i = 1, \dots, n$. Z eigenvalues of tensors were introduced by Qi [14]. Given $\mathcal{T} \in \mathbb{R}^{m, n}$, a number $\lambda \in \mathbb{R}$ is called a Z eigenvalue of \mathcal{T} , if it, together with a nonzero vector $\mathbf{x} \in \mathbb{R}^n$, satisfies

$$\begin{cases} \mathcal{T}\mathbf{x}^{m-1} = \lambda \mathbf{x}, \\ \mathbf{x}^T \mathbf{x} = 1. \end{cases} \quad (4)$$

The vector $\mathbf{x} \in \mathbb{R}^n$ in (4) is called an associated Z eigenvector of the Z eigenvalue λ , and (λ, \mathbf{x}) is called a Z eigenpair. Obviously, $\lambda = \sum_{i_1, \dots, i_m=1}^n t_{i_1 \dots i_m} \mathbf{x}_{i_1} \dots \mathbf{x}_{i_m}$, denoted $\mathcal{T}\mathbf{x}^m$, for a Z eigenpair (λ, \mathbf{x}) of \mathcal{T} . A tensor $\mathcal{T} \in \mathbb{R}^{m, n}$ is called *non-negative*, if $t_{i_1 \dots i_m} \geq 0$ for all $i_j \in \{1, \dots, n\}$ and $j \in \{1, \dots, m\}$.

Many interesting results on Z eigenvalues of tensors were obtained recently [14, 24–26], especially, for non-negative tensors. These results give insights to the behaviors of the Z eigenvalues and powerful numerical algorithms for computing the Z -spectral radius (to be defined in the next section) of a non-negative tensor.

III. CONNECTION: SYMMETRIC CASE

In this section, we establish a connection between the geometric measure of entanglement for a symmetric pure state with non-negative amplitudes and the Z -spectral radius of a non-negative tensor. Based on this connection, the computation of the geometric measure for such states is investigated.

Let us start from an important property of symmetric states with non-negative amplitudes. Let $|\Psi\rangle \in \mathcal{H}$ be symmetric and non-negative, then it is found in [5, 6, 12] that the maximal

overlap G_Ψ can be computed by means of

$$G_\Psi = \max_{\mathbf{x} \in \mathbb{R}_+^n \cap \mathcal{S}^{n-1}} \mathcal{A}_\Psi \mathbf{x}^m. \quad (5)$$

To establish the connection, we first present some basic results of Z eigenvalues of non-negative tensors. The following concept is important for non-negative tensors. The tensor $\mathcal{T} = (t_{i_1 i_2 \dots i_m})$ is called *reducible* if there exists a nonempty proper index subset $I \subset \{1, \dots, n\}$ such that

$$t_{i_1 i_2 \dots i_m} = 0, \quad \forall i_1 \in I, \quad \forall i_2, \dots, i_m \notin I.$$

If \mathcal{T} is not reducible, then \mathcal{T} is called *irreducible*. Denote by $\mathcal{Z}(\mathcal{T})$ the set of all non-negative Z eigenvalues of tensor \mathcal{T} and $\varrho(\mathcal{T}) \triangleq \max\{|\lambda| \mid \lambda \in \mathcal{Z}(\mathcal{T})\}$ the Z -spectral radius. Some of the properties of Z eigenvalues are summarized below; more details can be found in, e.g., [24,25]. Let $\mathcal{T} \in \mathbb{R}^{m,n}$. Then

(a) if \mathcal{T} is symmetric, then it has at most $\frac{(m-1)^n - 1}{m-2}$ Z eigenvalues;

(b) if \mathcal{T} is non-negative, then there exists a non-negative Z eigenpair $(\lambda_0, \mathbf{x}^{(0)})$, i.e., $\lambda_0 \geq 0$ and $\mathbf{x}^{(0)} \in \mathbb{R}_+^n \cap \mathcal{S}^{n-1}$. If \mathcal{T} is furthermore irreducible, then $\lambda_0 > 0$ and $\mathbf{x}^{(0)} \in \mathbb{R}_{++}^n$;

(c) if \mathcal{T} is non-negative and symmetric, then $\varrho(\mathcal{T}) \in \mathcal{Z}(\mathcal{T})$ and

$$\varrho(\mathcal{T}) = \max_{\mathbf{x} \in \mathcal{S}^{n-1}} |\mathcal{T} \mathbf{x}^m| = \max_{\mathbf{x} \in \mathbb{R}_+^n \cap \mathcal{S}^{n-1}} \mathcal{T} \mathbf{x}^m. \quad (6)$$

We are now ready to establish the connection.

Theorem 1. If $|\Psi\rangle \in \mathcal{H}$ is symmetric and non-negative, then the maximal overlap for the geometric measure of entanglement for $|\Psi\rangle \in \mathcal{H}$ is equal to the Z -spectral radius of the corresponding tensor \mathcal{A}_Ψ , that is,

$$G_\Psi = \varrho(\mathcal{A}_\Psi). \quad (7)$$

Given a symmetric state $|\Psi\rangle$ with non-negative amplitudes, a symmetric non-negative tensor \mathcal{A}_Ψ can be defined accordingly. Then Theorem 1 tells us that the geometric measure equals $1 - \varrho(\mathcal{A}_\Psi)$. In terms of this important connection, in the next two sections we compute geometric measures for multipartite qubits, qutrits, and qudits.

IV. COMPUTATION

Theorem 1 above shows that the geometric measure of entanglement of symmetric pure states with non-negative amplitudes can be computed through finding the Z -spectral radii of the underlying non-negative tensors. In this subsection, based on Theorem 1, the computation of the geometric measure of entanglement of such states is discussed.

A. Multipartite qubit states

For symmetric pure multipartite qubit states with non-negative amplitudes, [[7], Sec. II A] converts the geometric measure G_Ψ into a polynomial rational fraction in one variable. By the derivatives, G_Ψ can be computed. Alternatively, according to Theorem 1, G_Ψ can be obtained by finding the Z -spectral radius of the corresponding tensor. By Algorithm 1 in the next subsection one can calculate the maximal overlap G_Ψ for an arbitrary multipartite qutrit state. Mathematically, the qubit case is a special case of the qutrit case. Therefore a simplified version of Algorithm 1 can be used to find the maximal overlap G_Ψ for the multipartite qubit case. However,

to avoid repetition the specific algorithm for the qubit case is not given here. Instead, we use the well-known GHZ, W , and inverted- W states to illustrate the effectiveness of the method.

As in [4], for $0 \leq k \leq m$ define

$$|S(m, k)\rangle := \sqrt{\frac{k!(m-k)!}{m!}} \sum_{\tau \in \mathfrak{S}_m} \left| \tau(\underbrace{0 \dots 0}_k \underbrace{1 \dots 1}_{m-k}) \right\rangle;$$

here \mathfrak{S}_m is the symmetric group on m elements.

Example 1. The m GHZ state is defined as

$$|m\text{GHZ}\rangle = [|S(m, 0)\rangle + |S(m, m)\rangle] / \sqrt{2}.$$

Under the basis $\{|0\rangle, |1\rangle\}$, we have $\mathcal{A}_{m\text{GHZ}} \in \mathbb{R}^{m,2}$ and the Z eigenpairs are

$$\left(\frac{1}{\sqrt{2}}, (1, 0)\right), \left(\frac{1}{\sqrt{2}}, (0, 1)\right), \quad \text{and} \quad \left(\frac{1}{\sqrt{2}^{m-1}}, \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)\right)$$

and five more when m is odd:

$$\left(\frac{1}{\sqrt{2}}, (-1, 0)\right), \left(\frac{1}{\sqrt{2}}, (0, -1)\right), \left(\frac{1}{\sqrt{2}^{m-1}}, \left(-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)\right), \\ \left(\frac{1}{\sqrt{2}^{m-1}}, \left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right)\right), \quad \text{and} \quad \left(\frac{1}{\sqrt{2}^{m-1}}, \left(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right)\right).$$

We have, $G(m\text{GHZ}) = \varrho(\mathcal{A}_{m\text{GHZ}}) = \frac{1}{\sqrt{2}}$ which agrees with that in [[4], Sec. II A], and it can be attained with non-negative Z eigenvectors. The corresponding nearest separable state is $|\Phi\rangle = |\phi\rangle^{\otimes m}$ with $|\phi\rangle = |0\rangle$ or $|1\rangle$.

Example 2. In this example, the W state for a three-partite qubit setting is considered. The W state is defined as

$$|W\rangle = |S(3, 2)\rangle = (|001\rangle + |010\rangle + |100\rangle) / \sqrt{3}.$$

Under the basis $\{|0\rangle, |1\rangle\}$, we have $\mathcal{A}_W \in \mathbb{R}^{3,2}$ and the Z eigenpairs are

$$(0, (0, 1)), \left(\frac{2}{3}, \left(\sqrt{\frac{2}{3}}, \sqrt{\frac{1}{3}}\right)\right), \left(\frac{2}{3}, \left(-\sqrt{\frac{2}{3}}, \sqrt{\frac{1}{3}}\right)\right), \\ \left(-\frac{2}{3}, \left(\sqrt{\frac{2}{3}}, -\sqrt{\frac{1}{3}}\right)\right), \quad \text{and} \quad \left(-\frac{2}{3}, \left(-\sqrt{\frac{2}{3}}, -\sqrt{\frac{1}{3}}\right)\right).$$

Again, $G(\mathcal{A}_W) = \varrho(\mathcal{A}_W) = \frac{2}{3}$ which agrees with that in [[4], Sec. II A]. The corresponding nearest separable state can be obtained by a non-negative Z eigenvector, that is $|\Phi\rangle = |\phi\rangle^{\otimes 3}$ with $|\phi\rangle = \sqrt{\frac{2}{3}}|0\rangle + \sqrt{\frac{1}{3}}|1\rangle$.

Example 3. In this example, the inverted- W state for a three-partite qubit setting is considered. It is defined as

$$|\tilde{W}\rangle = |S(3, 1)\rangle = (|110\rangle + |101\rangle + |011\rangle) / \sqrt{3}.$$

Similarly, we have $\mathcal{A}_{\tilde{W}} \in \mathbb{R}^{3,2}$. After switching \mathbf{x}_1 and \mathbf{x}_2 , the Z -eigenvalue equations (4) of \tilde{W} become that for W . Consequently, $G(\tilde{W}) = \varrho(\mathcal{A}_{\tilde{W}}) = \frac{2}{3}$ by Example 2 with the corresponding nearest separable state being $|\Phi\rangle = |\phi\rangle^{\otimes 3}$ with $|\phi\rangle = \sqrt{\frac{1}{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle$.

B. Multipartite qutrit states

We consider multipartite qutrit states in this part. The separability and measure of qutrit entanglement were discussed by Caves and Milburn [20], and Hassan and Joag [22].

Let $\mathcal{H}_1 = \dots = \mathcal{H}_m$ with $d_1 = \dots = d_m = 3$. Denote $\mathcal{H} := \bigotimes_{k=1}^m \mathcal{H}_k$. Given a symmetric pure state $|\Psi\rangle \in \mathcal{H}$, if $|\Psi\rangle$ is non-negative, i.e., there exists a basis $\{|e_i\rangle\}_{i=1}^3$ such that the tensor \mathcal{A}_Ψ is non-negative, then by Theorem 1, G_Ψ is equal to the Z -spectral radius of the tensor \mathcal{A}_Ψ .

Example 4. In this example, a general GHZ state [[22], Eq. (9)] for a three-partite qutrit setting is considered. It is defined as

$$|\Psi\rangle = \alpha|111\rangle + \beta|222\rangle + \gamma|333\rangle, \quad \alpha^2 + \beta^2 + \gamma^2 = 1.$$

Here $\{|1\rangle, |2\rangle, |3\rangle\}$ is the basis for each qutrit. We see that $\mathcal{A}_\Psi \in \mathbb{R}^{3,3}$ is non-negative and symmetric when $\alpha, \beta, \gamma \geq 0$. In this situation, the Z -eigenvalue equations (8) become

$$\alpha \mathbf{x}_1^2 = \lambda \mathbf{x}_1, \quad \beta \mathbf{x}_2^2 = \lambda \mathbf{x}_2, \quad \gamma \mathbf{x}_3^2 = \lambda \mathbf{x}_3,$$

$$\text{and } \mathbf{x}_1^2 + \mathbf{x}_2^2 + \mathbf{x}_3^2 = 1.$$

When $\alpha\beta\gamma = 0$, the Z spectra can be computed through Theorem 1 in [18]. We mainly consider the nondegenerate case when $\alpha\beta\gamma > 0$. By Algorithm 1, we can compute all the non-negative Z eigenpairs as

$$(\alpha, (1, 0, 0)), (\beta, (0, 1, 0)), (\gamma, (0, 0, 1));$$

$$\left(\frac{\alpha\beta}{\sqrt{\alpha^2 + \beta^2}}, \left(\frac{\beta}{\sqrt{\alpha^2 + \beta^2}}, \frac{\alpha}{\sqrt{\alpha^2 + \beta^2}}, 0 \right) \right),$$

$$\left(\frac{\alpha\gamma}{\sqrt{\alpha^2 + \gamma^2}}, \left(\frac{\gamma}{\sqrt{\alpha^2 + \gamma^2}}, 0, \frac{\alpha}{\sqrt{\alpha^2 + \gamma^2}} \right) \right),$$

$$\left(\frac{\beta\gamma}{\sqrt{\beta^2 + \gamma^2}}, \left(0, \frac{\gamma}{\sqrt{\beta^2 + \gamma^2}}, \frac{\beta}{\sqrt{\beta^2 + \gamma^2}} \right) \right),$$

$$\left(\frac{\alpha\beta\gamma}{\tau}, \left(\frac{\beta\gamma}{\tau}, \frac{\alpha\gamma}{\tau}, \frac{\alpha\beta}{\tau} \right) \right)$$

with $\tau := \sqrt{\alpha^2\beta^2 + \beta^2\gamma^2 + \alpha^2\gamma^2}$.

We see that $G_\Psi = \varrho(\mathcal{A}_\Psi) = \max\{\alpha, \beta, \gamma\}$. The corresponding nearest separable state is $|\Phi\rangle = |\phi\rangle^{\otimes 3}$ with $|\phi\rangle := |1\rangle$ when $G_\Psi = \alpha$, $|2\rangle$ when $G_\Psi = \beta$, and $|3\rangle$ when $G_\Psi = \gamma$.

C. Multipartite qudit states

In this subsection we study how to compute the geometric measure of entanglement of a given symmetric multipartite qudit ($n > 3$) $|\Psi\rangle$ with non-negative amplitudes. Denote the corresponding tensor by \mathcal{A}_Ψ .

The following shifted higher-order power method is proposed in [23] and further studied in [28].

Algorithm 2 (shifted higher-order power method (SHOPM) for symmetric tensors $\mathcal{A} \in \mathbb{R}^{m,n}$).

Step 0. Initialization: choose $\mathbf{x}^{(0)} \in \mathbb{R}_{++}^n \cap \mathcal{S}^{n-1}$ and $\alpha > 0$. Set $k := 0$ and $\lambda_0 := \mathcal{A}(\mathbf{x}^{(0)})^m$.

Step 1. Compute

$$\hat{\mathbf{x}}^{(k+1)} := \mathcal{A}(\mathbf{x}^{(k)})^{m-1} + \alpha \mathbf{x}^{(k)},$$

$$\mathbf{x}^{(k+1)} := \frac{\hat{\mathbf{x}}^{(k+1)}}{\|\hat{\mathbf{x}}^{(k+1)}\|},$$

$$\lambda_{k+1} := \mathcal{A}(\mathbf{x}^{(k+1)})^m.$$

Step 2. If $\mathcal{A}(\mathbf{x}^{(k+1)})^{m-1} = \lambda_{k+1} \mathbf{x}^{(k+1)}$, stop. Otherwise, set $k := k + 1$, go to Step 1.

Let $\mathcal{A} \in \mathbb{R}^{m,n}$ be non-negative and symmetric. Let $\alpha > (m-1)\varrho(\mathcal{A})$. Then by [[23], Theorem 4.4], the properties of symmetric non-negative tensors outlined in Section III, and [5], it can be shown that the iterates $(\lambda_k, \mathbf{x}^{(k)})$ generated by Algorithm 2 have the following properties.

(a) The sequence $\{\lambda_k\}$ is nondecreasing and converges to a Z eigenvalue $\lambda_* \geq 0$.

(b) The sequence $\{\mathbf{x}^{(k)}\}$ converges a Z eigenvector of \mathcal{A} associated with λ_* .

Algorithm 2 enables us to find Z eigenpairs of a non-negative irreducible symmetric tensor \mathcal{A} . The next algorithm helps us to find the Z -spectral radius.

Algorithm 3 (an algorithm for the Z -spectral radius of a non-negative irreducible symmetric tensor \mathcal{A}).

Step 0. Let $k := 0$ and compute the Z eigenvalue λ_0 of \mathcal{A} through Algorithm 2. Set $\mathcal{A} := \frac{\mathcal{A}}{\lambda_0}$.

Step 1. Choose N initial points in $\mathbb{R}_{++}^n \cap \mathcal{S}^{n-1}$. For the i th initial point, compute the Z eigenvalue μ_i of \mathcal{A} through Algorithm 2. Let $\mu := \max_{1 \leq i \leq N} \mu_i$.

Step 2. If $\mu = 1$, denote $\lambda := \prod_{0 \leq j \leq k} \lambda_j$, and terminate the algorithm. Otherwise, set $\lambda_{k+1} := \mu, \mathcal{A} := \frac{\mathcal{A}}{\lambda_{k+1}}$, and $k := k + 1$; go to Step 1.

By Algorithm 3, if the number of the initial size N is very big, then with big probability the Z -spectral radius can be found, hence the maximal overlap can be obtained with big probability. More details of the convergence analysis of Algorithm 3 is given in the Appendix.

Example 5. Given a multipartite qudit state $|\Psi\rangle$ of the form

$$|\Psi\rangle = \frac{1}{\sqrt{4}} \sum_{i=0}^3 |i\rangle \otimes \cdots \otimes |i\rangle. \quad (11)$$

Employing Algorithm 3 we get the numerical value 0.5. So the maximal overlap $G_\Psi \geq 0.5$. Interestingly, for this example, by solving the system of Z -eigenvalue equations (4) directly one may get

$$0.5x_1^3 = \lambda x_1, \quad 0.5x_2^3 = \lambda x_2, \quad 0.5x_3^3 = \lambda x_3, \quad 0.5x_4^3 = \lambda x_4.$$

Because $\|x\| = 1$, there is at least one x_i such that $0 < i \leq 1$. Then $\lambda = 0.5x_i^2$, that is $\lambda \leq 0.5$. Therefore $G_\Psi = 0.5$ attained at Z eigenvectors $(1, 0, 0, 0)$, $(0, 1, 0, 0)$, $(0, 0, 1, 0)$, or $(0, 0, 0, 1)$.

V. CONNECTION: NONSYMMETRIC CASE

In this section, we extend the results in the last section to *nonsymmetric* pure states with non-negative amplitudes. To this end, we need the spectral theory for real tensors; see e.g., [15,28,29]. We first present several properties of non-negative real tensors.

Let $\mathcal{A} = (a_{i_1 \dots i_m})$ be a $d_1 \times \dots \times d_m$ real tensor (hypermatrix). $\sigma \in \mathbb{R}$ is called a *singular value* of \mathcal{A} , if it, together with $\mathbf{x}^{(1)} \in \mathbb{R}^{d_1} \cap \mathcal{S}^{d_1-1}, \dots, \mathbf{x}^{(m)} \in \mathbb{R}^{d_m} \cap \mathcal{S}^{d_m-1}$, satisfies

$$\sum_{1 \leq i_j \leq d_j, j \neq k} a_{i_1 \dots i_m} \mathbf{x}_{i_1}^{(1)} \cdots \mathbf{x}_{i_{j-1}}^{(j-1)} \mathbf{x}_{i_{j+1}}^{(j+1)} \cdots \mathbf{x}_{i_m}^{(m)} = \sigma \mathbf{x}_{i_k}^{(k)}, \quad (12)$$

$\forall i_k = 1, \dots, d_k, \forall k = 1, \dots, m$. The vector $\mathbf{x}^{(k)}$ is called the mode- k singular vector associated with the singular value σ [15,28]. Denote the largest singular value of \mathcal{A} by $\sigma(\mathcal{A})$. Then,

$$\sigma(\mathcal{A}) = \max_{\mathbf{x}^{(1)} \in \mathcal{S}^{d_1-1}, \dots, \mathbf{x}^{(m)} \in \mathcal{S}^{d_m-1}} \mathcal{A} \mathbf{x}^{(1)} \cdots \mathbf{x}^{(m)}. \quad (13)$$

Moreover, if \mathcal{A} is non-negative, then the mode- k singular vectors $\mathbf{x}^{(k)}$ associated with $\sigma(\mathcal{A})$ can be chosen to be non-negative [15,28].

Next we connect the geometric measure of entanglement of a nonsymmetric non-negative pure state $|\Phi\rangle$ to the largest singular value of a nonsymmetric non-negative tensor \mathcal{A} . If $|\Psi\rangle \in \mathcal{H}$ is non-negative with the underlying orthonormal bases $\{|e_i^{(k)}\rangle\}_{i=1}^{d_k}$ for $k = 1, \dots, m$, then $|\Phi\rangle = \bigotimes_{k=1}^m |\phi^{(k)}\rangle$ in (1) can be chosen with $\langle e_i^{(k)} | \phi^{(k)} \rangle \geq 0$ for all $i = 1, \dots, d_k$ and $k = 1, \dots, m$. Consequently,

$$G_\Psi = \max_{\mathbf{x}^{(1)} \in \mathbb{R}_+^{d_1} \cap \mathcal{S}^{d_1-1}, \dots, \mathbf{x}^{(m)} \in \mathbb{R}_+^{d_m} \cap \mathcal{S}^{d_m-1}} \mathcal{A}_\Psi \mathbf{x}^{(1)} \cdots \mathbf{x}^{(m)}.$$

On the basis of the above analysis, the following result provides the connection between the geometric measure of nonsymmetric pure states with non-negative amplitudes and the spectral theory of nonsymmetric non-negative tensors.

Theorem 3. If $|\Psi\rangle \in \mathcal{H}$ is non-negative, then

$$G_\Psi = \sigma(\mathcal{A}_\Psi).$$

The remaining problem is how to compute the largest singular value of a nonsymmetric non-negative tensor? To this end, symmetric embedding introduced in [28] is needed. Let $\mathcal{A} = (a_{i_1 \dots i_m})$ be a $d_1 \times \cdots \times d_m$ real tensor and $\mathcal{S}_\mathcal{A}$ be the symmetric embedding of tensor \mathcal{A} [[28], Sec. 2.2]. $\mathcal{S}_\mathcal{A}$ is an m th order $N = \sum_{k=1}^m d_k$ -dimensional symmetric tensor. For example, given a matrix $A \in \mathbb{R}^{n_1 \times n_2}$,

$$\mathcal{S}_A := \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix} \in \mathbb{R}^{(n_1+n_2) \times (n_1+n_2)}$$

is its symmetric embedding.

We have the following result:

Theorem 4. Let $\mathcal{A} = (a_{i_1 \dots i_m})$ be a $d_1 \times \cdots \times d_m$ real tensor. Then, σ is a nonzero singular value of \mathcal{A} if and only if $\frac{m!}{\sqrt{m^m}} \sigma$ is a nonzero Z eigenvalue of $\mathcal{S}_\mathcal{A}$.

The proof of Theorem 4 is outlined as follows. The ‘‘only if’’ part follows from [[28], Theorem 4.7]. We show the ‘‘if’’ part in the following. Now, suppose that $\mathbf{y} := (\mathbf{y}^{(1)T}, \dots, \mathbf{y}^{(m)T})^T \in \mathbb{R}^N \cap \mathcal{S}^{N-1}$ with $\mathbf{y}^{(k)} \in \mathbb{R}^{d_k}$ for each k is a Z eigenvector of $\mathcal{S}_\mathcal{A}$ corresponding to Z eigenvalue $\lambda \neq 0$. Suppose, without loss of generality, that $\mathbf{y}^{(1)} \neq \mathbf{0}$. By the definition of $\mathcal{S}_\mathcal{A}$, we have

$$\begin{aligned} \lambda (\mathbf{y}^{(1)})^T \mathbf{y}^{(1)} &= \sum_{i_1=1}^{d_1} \mathbf{y}_{i_1}^{(1)} \left[\sum_{i_2, \dots, i_m=1}^N (\mathcal{S}_\mathcal{A})_{i_1 i_2 \dots i_m} \mathbf{y}_{i_2} \cdots \mathbf{y}_{i_m} \right] \\ &= (m-1)! \mathcal{A} \mathbf{y}^{(1)} \cdots \mathbf{y}^{(m)} \\ &= \sum_{i_k=1}^{d_k} \mathbf{y}_{i_k}^{(k)} \left[\sum_{1 \leq i_j \leq N, j \neq k} (\mathcal{S}_\mathcal{A})_{i_1 i_2 \dots i_m} \mathbf{y}_{i_1} \cdots \mathbf{y}_{i_m} \right] \\ &= \lambda (\mathbf{y}^{(k)})^T \mathbf{y}^{(k)} \end{aligned}$$

for all $k = 2, \dots, m$. Consequently, $(\mathbf{y}^{(k)})^T \mathbf{y}^{(k)} = \frac{1}{m}$ for all $k = 1, \dots, m$. Moreover,

$$\begin{aligned} &\sum_{i_2, \dots, i_m=1}^N (\mathcal{S}_\mathcal{A})_{i_1 i_2 \dots i_m} \mathbf{y}_{i_2} \cdots \mathbf{y}_{i_m} \\ &= (m-1)! \sum_{i_2=1}^{d_2} \cdots \sum_{i_m=1}^{d_m} a_{i_1 i_2 \dots i_m} \mathbf{y}_{i_2}^{(2)} \cdots \mathbf{y}_{i_m}^{(m)} \\ &= \lambda \mathbf{y}_{i_1}^{(1)}, \quad \forall i_1 = 1, \dots, d_1. \end{aligned}$$

Let $\mathbf{x}^{(k)} := \sqrt{m} \mathbf{y}^{(k)}$ for all $k = 1, \dots, m$. We then have

$$\begin{aligned} (m-1)! \frac{1}{\sqrt{m^{m-1}}} \sum_{i_2=1}^{d_2} \cdots \sum_{i_m=1}^{d_m} a_{i_1 i_2 \dots i_m} \mathbf{x}_{i_2}^{(2)} \cdots \mathbf{x}_{i_m}^{(m)} \\ = \lambda \frac{1}{\sqrt{m}} \mathbf{x}_{i_1}^{(1)}, \quad \forall i_1 = 1, \dots, d_1. \end{aligned}$$

Similarly, we have

$$\begin{aligned} (m-1)! \frac{1}{\sqrt{m^{m-1}}} \sum_{1 \leq i_j \leq d_j, j \neq k} a_{i_1 \dots i_m} \mathbf{x}_{i_1}^{(1)} \cdots \mathbf{x}_{i_m}^{(m)} \\ = \lambda \frac{1}{\sqrt{m}} \mathbf{x}_{i_k}^{(k)}, \quad \forall i_k = 1, \dots, d_k, \quad \forall k = 2, \dots, m. \end{aligned}$$

This, together with (12), implies that $\frac{\sqrt{m^m}}{m!} \lambda$ is a nonzero singular value of \mathcal{A} . The proof is complete.

Let $\mathcal{A} = (a_{i_1 \dots i_m})$ be a $d_1 \times \cdots \times d_m$ real tensor. By Theorem 4, it has at most $\frac{(m-1)^{N-1}}{m-2}$ nonzero singular values, here $N = \sum_{k=1}^m d_k$. Moreover, if $|\Psi\rangle \in \mathcal{H}$ is non-negative, then

$$G_\Psi = \sigma(\mathcal{A}_\Psi) = \frac{\sqrt{m^m}}{m!} \varrho(\mathcal{S}_{\mathcal{A}_\Psi}).$$

So, the calculation of the geometric measure of entanglement for nonsymmetric pure states with non-negative amplitudes can be accomplished by converting it to the symmetric case. Consequently, the numerical methods in the previous section are applicable.

Example 6. The nonsymmetric state

$$|\Psi\rangle = \sqrt{\frac{1}{3}} |001\rangle + \sqrt{\frac{2}{3}} |100\rangle$$

has an associated tensor \mathcal{A}_Ψ who has two nonzero entries: $a_{1,1,2} = \sqrt{\frac{1}{3}}$ and $a_{2,1,1} = \sqrt{\frac{2}{3}}$. We have

$$G_\Psi = \sigma(\mathcal{A}_\Psi) = \frac{\sqrt{m^m}}{m!} \varrho(\mathcal{S}_{\mathcal{A}_\Psi}) = \frac{\sqrt{3^3}}{3!} \times 0.9423 = 0.8165,$$

with the corresponding separable state

$$|\Phi\rangle = |1\rangle \otimes |0\rangle \otimes |0\rangle.$$

Clearly, this nearest product state is not symmetric.

VI. CONCLUSION

We have established a connection between the geometric measure of entanglement for pure states and the spectral theory of non-negative tensors. Especially, we have shown that the geometric measure of entanglement of a symmetric pure state with non-negative amplitudes can be expressed in terms of the Z -spectral radius of the corresponding non-negative symmetric tensor, and the geometric measure of entanglement of a nonsymmetric pure state with non-negative amplitudes is equal to the largest singular value of the underlying non-negative tensor. By means of symmetric embedding, the nonsymmetric case can be converted to the symmetric case. Several algorithms have been proposed. Examples have been used to illustrate the effectiveness of the proposed methods.

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APPENDIX: ON THE CONVERGENCE OF ALGORITHM 3

To establish the convergence of Algorithm 3 we prove the following lemma first.

Lemma 1. Let $\mathcal{A} \in \mathbb{R}^{m,n}$ be non-negative, irreducible, and symmetric. For $\varrho(\mathcal{A})$, if \mathbf{x}^* is a corresponding Z eigenvector, then there exists $\epsilon > 0$ such that for any $\mathbf{x}^{(0)} \in \mathbb{R}_{++}^n \cap \{\mathbf{x} \in \mathcal{S}^{n-1} \mid \|\mathbf{x} - \mathbf{x}^*\| \leq \epsilon\}$, the sequence $\{\lambda_k\}$ generated by Algorithm 3 with $\alpha > (m-1)\varrho(\mathcal{A})$ converges to $\varrho(\mathcal{A})$.

Proof. Recall that $\mathcal{Z}(\mathcal{A})$ is the set of all non-negative Z eigenvalues of tensor \mathcal{A} . If $\mathcal{Z}(\mathcal{A})$ is the singleton $\{\varrho(\mathcal{A})\}$, then the result follows immediately from Algorithm 2 with arbitrary $\epsilon > 0$. Now, suppose that the cardinality of $\mathcal{Z}(\mathcal{A})$ is larger than 1. Denote by $\lambda_2(\mathcal{A}) := \max\{\lambda \mid \lambda \in \mathcal{Z}(\mathcal{A}) \setminus \{\varrho(\mathcal{A})\}\}$, and $\kappa := \frac{\varrho(\mathcal{A}) - \lambda_2(\mathcal{A})}{2}$. By Algorithm 2, we see that the open set $\{\beta \in \mathbb{R} \mid |\beta - \varrho(\mathcal{A})| < \kappa\}$ is disjoint with the union of the finitely many open sets $\{\beta \in \mathbb{R} \mid |\beta - \lambda| < \kappa\}$ for $\lambda \in$

$\mathcal{Z}(\mathcal{A}) \setminus \{\varrho(\mathcal{A})\}$. Since $\lambda_0 := \mathcal{A}(\mathbf{x}^{(0)})^m$ and $\varrho(\mathcal{A}) := \mathcal{A}(\mathbf{x}^*)^m$, we can choose $\epsilon > 0$ such that $|\lambda_0 - \varrho(\mathcal{A})| < \kappa$ for any $\mathbf{x}^{(0)} \in \mathbb{R}_{++}^n \cap \{\mathbf{x} \in \mathcal{S}^{n-1} \mid \|\mathbf{x} - \mathbf{x}^*\| \leq \epsilon\}$. Consequently, this, together with Eq. (6), implies that $\varrho(\mathcal{A}) - \kappa < \lambda_0 \leq \varrho(\mathcal{A})$. By Algorithm 2, $\{\lambda_k\}$ is nondecreasing and converges to a Z eigenvalue λ_* of \mathcal{A} . As we can see, the only possibility is that $\lambda_* = \varrho(\mathcal{A})$. The proof is complete.

If the N initial points in Algorithm 3 are chosen such that there is at least one point in the set $\{\mathbf{x} \in \mathbb{R}_{++}^n \cap \mathcal{S}^{n-1} \mid \|\mathbf{x} - \mathbf{x}^*\| \leq \epsilon\}$ with ϵ being determined by Lemma 1, then we say such a set of initial points satisfies the so-called absolutely convergent condition (ACC for short). We have the following result.

Theorem 5. Let $\mathcal{A} \in \mathbb{R}^{m,n}$ be non-negative, irreducible, and symmetric. For $\alpha > (m-1)\varrho(\mathcal{A})$, if the set of N initial points satisfy the ACC assumption, then Algorithm 3 is terminated with $k=1$ and $\lambda = \varrho(\mathcal{A})$. In general, the sequence $\{\lambda_k\}$ converges to a positive Z eigenvalue of \mathcal{A} .

Proof. The results follow from Algorithm 2, Lemma 1, and the above ACC assumption.

So, if we uniformly randomly choose initial points in $\mathbb{R}_{++}^n \cap \mathcal{S}^{n-1}$, then with positive probability Algorithm 3 finds the Z -spectral radius. By Theorem 5 and the ACC assumption, we see that the probability that Algorithm 3 converges to the Z -spectral radius under the uniformly random framework is determined by ϵ in Lemma 1.

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