Separability discrimination and decomposition of quantum mixed states based on the Broyden-Fletcher-Goldfarb-Shanno algorithm

Bo Yang,[*] Ying Li,[†] and Guyan Ni[‡]

Department of Mathematics, National University of Defense Technology, Changsha, Hunan 410073, China

(Received 27 April 2023; revised 6 September 2023; accepted 23 October 2023; published 16 November 2023)

In this paper, we consider separability discrimination and decomposition problems of quantum mixed states based on the tensor optimization method. We first convert the separability determination problem of quantum mixed states to the positive Hermitian decomposition problem of Hermitian tensors. Then we study a rank-R positive Hermitian approximation model of Hermitian tensors and introduce a Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm for rank-R positive Hermitian approximation. We prove that the BFGS algorithm can be used to compute a decomposition of a mixed state if it is separable. Finally, we propose a BFGS algorithm for separability determination and decomposition of quantum mixed states. Numerical examples show the effectiveness of the algorithm.

DOI: 10.1103/PhysRevA.108.052217

I. INTRODUCTION

The concept of quantum entanglement was first introduced by Schrödinger [1], Einstein, Podolsky, and Rosen [2]. At present, quantum entanglement has played an important role in quantum information theory and in the development of the quantum technologies. Many mixed-state entanglement measures have been developed. However, so far, a directly or numerically computable measure for the entanglement of multipartite mixed states is difficult to find [3]. Hence, the question of whether a given mixed state is entangled or separable is still one of the fundamental problems in quantum information theory [4,5].

In fact, it is known to be NP hard to decide whether a given mixed state is entangled or separable [6,7]. In the past 20 years, it has aroused great interest from experts and scholars. Halder *et al.* [8] indicated that nontrivial mixtures of an arbitrary pair of an entangled state and a product state in any bipartite quantum system are always entangled. Vesperini *et al.* [3] proposed an entanglement measure of mixed states, derived from the quantum correlation measure using a regularization procedure for the density matrix. In addition, some separability discrimination methods for the quantum states also have been proposed, such as Bell's inequality, the positivity of the partial transposition of a state criterion (PPT criterion) [9,10], computable cross norm or rearrangement criterion (CCNR criterion) [11], entanglement witness [9,12], covariance matrix criterion [13], and other methods. However, these methods cannot decompose a mixed state if it is separable. For solving this problem, Li and Ni [5] proposed a semi-definite relaxation algorithm to detect the mixed state's separability and obtain its decompositions if it is separable. However, the semi-definite relaxation is hard to calculate a decomposition if the mixed state has higher order and higher dimension since the number of moments will increase sharply with the increase of its order and dimension.

Motivated by the above, we consider a numerical algorithm to detect the mixed state's separability and decompose it if it is separable. We first convert the separability determination problem of quantum mixed states to the positive Hermitian decomposition problem of Hermitian tensors. Then we study a rank-R separable approximation model of Hermitian tensors, introduce a Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm for rank-R separable approximation. Finally, we design a BFGS algorithm to determinate the separability of an m-partite quantum mixed state and decompose it if it is separable. Numerical examples show that the BFGS algorithm has good numerical performance.

The rest of the paper is structured as follows. In Sec. II, we introduce some basic concepts, including some operations of tensors, tensor representation of quantum states, and the geometric measure of quantum mixed states. In Sec. III, we establish a rank-R separable approximation optimization model of Hermitian tensors, then we deduce the gradient of the objective function $F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$. Finally, we introduce a BFGS algorithm for rank-R separable approximation. In Sec. IV, we study a numerical algorithm for separability discrimination and decomposition of quantum mixed states. Through the Algorithm 4.1, we can know whether a quantum mixed state is separable. If the quantum mixed state is a separable state, its decomposition is given. In Sec. V, we give numerical examples on the computation of separability of several quantum mixed states. Numerical examples verify the correctness of the theoretical analysis and the effectiveness of the Algorithm 4.1. A conclusion is indicated in Sec. VI.

Notations. $\mathbb{R}$ and $\mathbb{C}$ denote the real field and complex field, respectively. An uppercase letter in calligraphic font denotes a tensor, e.g., $\mathcal{T}$. An uppercase letter represents a matrix, e.g., U. A boldface lowercase letter represents a vector, e.g., $\mathbf{v}$. A

[*]boyangemail@163.com

[†]Corresponding author: liying801@163.com

[‡]guyan-ni@nudt.edu.cn

lowercase letter represents a scalar, e.g., x. $(U)_{ij}$ denotes the element with row index i and column index j in a matrix U, [also $(\mathbf{v})_i$ and $(\mathcal{T})_{i_1 i_2 \dots i_N} = \mathcal{T}_{i_1 i_2 \dots i_N}$]. Let $m > 0$ be an integer, denote $[m] := \{1, 2, \dots, m\}$ as an integer set. For vectors, $\| \cdot \|$ refers to the two-norm. For tensors and matrices, $\| \cdot \|_F$ refers to the Frobenius norm. $\prod_{i=1}^{n} \|a_i\| = \|a_1\| \|a_2\| \cdots \|a_n\|$ represents a continuous multiplication. $(\cdot)^*$ denotes its conjugation. $(\cdot)^\dagger$ denotes its conjugate transposition.

II. PRELIMINARIES

A. Tensor and matrix operations

An mth-order complex tensor denoted by $\mathcal{A} = (\mathcal{A}_{i_1 \dots i_m}) \in \mathbb{C}^{n_1 \times \cdots \times n_m}$ is a multiarray consisting of numbers $\mathcal{A}_{i_1 \dots i_m} \in \mathbb{C}$ for all $i_k \in [n_k]$ and $k \in [m]$. If tensors $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \cdots \times I_m}$ and $\mathcal{B} \in \mathbb{C}^{J_1 \times J_2 \times \cdots \times J_m}$, then the tensor product of tensors $\mathcal{A}$ and $\mathcal{B}$ is defined as

$$\mathcal{A} \circ \mathcal{B} := \left(\mathcal{A}_{i_1 \dots i_m} \mathcal{B}_{j_1 \dots j_m}\right) \in \mathbb{C}^{I_1 \times \cdots \times I_m \times J_1 \times \cdots \times J_m}.$$

If tensors $\mathcal{A},\ \mathcal{B} \in \mathbb{C}^{n_1 \times \cdots \times n_m}$, then their inner product, denoted as $\langle \mathcal{A}, \mathcal{B} \rangle$ or $\mathcal{A} \cdot \mathcal{B}$, is defined as

$$\langle \mathcal{A}, \mathcal{B} \rangle := \sum_{i_1, i_2, \dots, i_m = 1}^{n_1, n_2, \cdots, n_m} \mathcal{A}^*_{i_1 i_2 \dots i_m} \mathcal{B}_{i_1 i_2 \dots i_m},$$

where $\mathcal{A}^*_{i_1 i_2 \dots i_m}$ represents the complex conjugate of $\mathcal{A}_{i_1 i_2 \dots i_m}$. The Frobenius norm of a tensor $\mathcal{A}$ is

$$||\mathcal{A}||_F := \sqrt{\langle \mathcal{A}, \mathcal{A} \rangle}.$$

Definition 2.1 [14]. A $2m$th-order tensor $\mathcal{H} = (\mathcal{H}_{i_1 \dots i_m j_1 \dots j_m}) \in \mathbb{C}^{n_1 \times \cdots \times n_m \times n_1 \times \cdots \times n_m}$ is called a Hermitian tensor if

$$\mathcal{H}_{i_1 \dots i_m j_1 \dots j_m} = \mathcal{H}^*_{j_1 \dots j_m i_1 \dots i_m},$$

for all $i_k, j_k \in [n_k]$, $k \in [m]$. The space of all Hermitian tensors is denoted by $\mathbb{H}[n_1, \dots, n_m]$. A Hermitian tensor $\mathcal{H}$ is called a symmetric Hermitian tensor if $n_1 = \cdots = n_m$ and its entries $\mathcal{H}_{i_1 \dots i_m j_1 \dots j_m}$ are invariant under any permutation operator P of $\{1, \dots, m\}$, i.e.,

$$\mathcal{H}_{i_1 \dots i_m j_1 \dots j_m} = \mathcal{H}_{P[i_1 \dots i_m] P[j_1 \dots j_m]},$$

where $P[i_1 \dots i_m]$ denotes $[i_{P(1)}, \dots, i_{P(m)}]$. The space of all symmetric Hermitian tensors is denoted by $s\mathbb{H}[n_1, \dots, n_m]$.

Definition 2.2 [14]. Let $\mathcal{H} \in \mathbb{H}[n_1, \dots, n_m]$ be a Hermitian tensor. If it can be written as

$$\mathcal{H} = \sum_{i=1}^{R} \lambda_i \, \mathbf{v}_i^{(1)} \circ \cdots \circ \mathbf{v}_i^{(m)} \circ \mathbf{v}_i^{(1)*} \circ \cdots \circ \mathbf{v}_i^{(m)*}, \qquad (1)$$

where $\lambda_i \in \mathbb{R}$, $\mathbf{v}_i^{(k)} \in \mathbb{C}^{n_k}$, $\|\mathbf{v}_i^{(k)}\| = 1$, and $k \in [m]$, then Eq. (1) is called a Hermitian decomposition of $\mathcal{H}$. If $\lambda_i \geqslant 0$ for all $i \in [R]$, then Eq. (1) is called a positive Hermitian decomposition of $\mathcal{H}$ and $\mathcal{H}$ is called positive Hermitian decomposable or separable.

The set of all positive Hermitian decomposable Hermitian tensors in Hilbert space $\mathbb{H}[n_1, \dots, n_m]$ is denoted by $\mathrm{phd}(\mathbb{H})$. The Hermitian rank of a Hermitian tensor $\mathcal{H} \in \mathbb{H}[n_1, \dots, n_m]$ is the smallest number of R in Eq. (1), denoted by $\mathrm{rank}_{\mathbb{H}} \mathcal{H}$.

Definition 2.3 [14]. The matrix trace of Hermitian tensor $\mathcal{H} \in \mathbb{H}[n_1, \cdots, n_m]$ is defined as

$$\mathrm{Tr}_M(\mathcal{H}) := \sum_{i_1, \cdots, i_m = 1}^{n_1, \dots, n_m} \mathcal{H}_{i_1 \dots i_m i_1 \dots i_m}.$$

If matrices $A \in \mathbb{C}^{I \times K}$ and $B \in \mathbb{C}^{J \times K}$, then the Khatri-Rao product of A and B, denoted by $A \odot B$, is defined as

$$A \odot B := \begin{bmatrix} a_{11}\mathbf{b}_1 & a_{12}\mathbf{b}_2 & \cdots & a_{1K}\mathbf{b}_K \\ a_{21}\mathbf{b}_1 & a_{22}\mathbf{b}_2 & \cdots & a_{2K}\mathbf{b}_K \\ \vdots & \vdots & \ddots & \vdots \\ a_{I1}\mathbf{b}_1 & a_{I2}\mathbf{b}_2 & \cdots & a_{IK}\mathbf{b}_K \end{bmatrix} \in \mathbb{C}^{IJ \times K},$$

where $\mathbf{b}_j \in \mathbb{C}^{n_j}$ and $j \in [K]$.

The mode-k matricization of tensor $\mathcal{A} \in \mathbb{C}^{n_1 \times n_2 \times \cdots \times n_m}$ is denoted by $A_{(k)}$ with size $n_k \times (\prod_{i=1}^{m} n_i / n_k)$ and arranges the tensor $\mathcal{A}$ into a matrix such that tensor element $\mathcal{A}_{i_1 i_2 \dots i_m}$ is equal to matrix element $(A_{(k)})_{i_k j}$, where

$$j = 1 + \sum_{l=1, l \neq k}^{m} \left[(i_l - 1) \prod_{p=1, p \neq k}^{l-1} n_p \right].$$

B. Tensor representation of quantum states

Here, we introduce the tensor representation of quantum pure states and quantum mixed states. For more details, please refer to Refs. [5,14–17]. An m-partite pure state $|\psi\rangle$ of a composite quantum system can be regarded as a normalized complex tensor in the space $\mathbb{C}^{n_1 \times \cdots \times n_m}$. The pure state $|\psi\rangle$ is written by

$$|\psi\rangle = \sum_{i_1, \dots, i_m = 1}^{n_1, \dots, n_m} \mathcal{X}_{i_1 \dots i_m} \big| e_{i_1}^{(1)} \dots e_{i_m}^{(m)} \big\rangle,$$

where $\mathcal{X}_{i_1 \dots i_m} \in \mathbb{C}$ such that $\langle \psi | \psi \rangle = 1$, $\{|e_{i_k}^{(k)}\rangle : i_k = 1, 2, \dots, n_k\}$ is an orthonormal basis of $\mathbb{C}^{n_k}$ [17]. Hence, an m-partite pure state uniquely corresponds to a complex tensor $\mathcal{X}_\psi = (\mathcal{X}_{i_1 \dots i_m})$ under a given orthonormal basis with $\|\mathcal{X}_\psi\|_F = 1$ [15].

For instance, a three-partite pure state $|W\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$. Assume that $\mathcal{X}_W$ is the corresponding tensor of $|W\rangle$. Then it is a third-order two-dimensional symmetric tensor and its nonzero elements are $(\mathcal{X}_W)_{112} = (\mathcal{X}_W)_{121} = (\mathcal{X}_W)_{211} = \frac{1}{\sqrt{3}}$.

Definition 2.4. If an m-partite pure state $|\psi\rangle \in \mathbb{C}^{n_1 \times \cdots \times n_m}$ can be expressed as

$$|\psi\rangle = \circ_{k=1}^{m} |\phi^{(k)}\rangle := |\phi^{(1)} \phi^{(2)} \cdots \phi^{(m)}\rangle,$$

where $|\phi^{(k)}\rangle \in \mathbb{C}^{n_k}$, then $|\psi\rangle$ is called a separable state. Otherwise, it is called an entangled state.

For example, a two-partite pure state $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |01\rangle) = |\phi^{(1)}\rangle \circ |\phi^{(2)}\rangle = |\phi^{(1)} \phi^{2}\rangle$, where $|\phi^{(1)}\rangle = |0\rangle$ and $|\phi^{(2)}\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Hence $|\psi\rangle$ is a separable pure state. Let $\mathbf{u}^{(1)} = (1, 0)^\top$, $\mathbf{u}^{(2)} = (1/\sqrt{2}, 1/\sqrt{2})^\top$. Then $\mathcal{X}_\psi = \mathbf{u}^{(1)} \circ \mathbf{u}^{(2)}$, which means that the corresponding tensor $\mathcal{X}_\psi$ is a rank-1 tensor.

For an m-partite mixed state, its density matrix ρ is always written as

$$\rho = \sum_{i=1}^{s} \lambda_i |\psi_i\rangle\langle\psi_i|,$$

where $\sum_{i=1}^{s} \lambda_i = 1, \lambda_i \geqslant 0, |\psi_i\rangle$ is an m-partite pure state and $\langle\psi_i|$ is the complex conjugate transposition of $|\psi_i\rangle$.

Under an orthonormal basis of $\mathbb{C}^{n_k}$ for $k = 1, 2, \dots, m$, assume that $\mathcal{X}_i$ is the corresponding complex tensor of $|\psi_i\rangle$ for $i = 1, 2, \dots, s$. Then the density matrix ρ of the mixed state corresponds to the following Hermitian tensor:

$$\mathcal{H}_\rho := \sum_{i=1}^{s} \lambda_i \mathcal{X}_i \circ \mathcal{X}_i^*.$$

Hence, an m-partite mixed state uniquely corresponds to a Hermitian tensor $\mathcal{H}_\rho \in \mathbb{H}[n_1, \dots, n_m]$ under a given orthonormal basis.

For example, if a two-partite mixed state's density matrix $\rho = \frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|01\rangle\langle 01|$, then $\mathcal{H}_\rho$ is a fourth-order two-dimensional Hermitian tensor and its nonzero elements are $(\mathcal{H}_\rho)_{1111} = (\mathcal{H}_\rho)_{1212} = \frac{1}{2}$.

Definition 2.5 [17]. An m-partite quantum mixed state is called separable if its density matrix ρ can be written as

$$\rho = \sum_{i=1}^{R} p_i \big|\phi_i^{(1)} \cdots \phi_i^{(m)}\big\rangle\big\langle\phi_i^{(1)} \cdots \phi_i^{(m)}\big|,$$

where $p_i \geqslant 0$, $\sum_{i=1}^{R} p_i = 1$, $|\phi_i^{(k)}\rangle \in \mathbb{C}^{n_k}$, $i \in [R]$, and $k \in [m]$. The set of all separable mixed states in Hilbert space $\mathbb{H}[n_1, \dots, n_m]$ is denoted by $Separ(\mathbb{H})$.

Similarly, if $\mathcal{H}_\rho$ is the corresponding Hermitian tensor of ρ, then we have that

$$\mathcal{H}_\rho = \sum_{i=1}^{R} p_i \, \mathbf{v}_i^{(1)} \circ \cdots \circ \mathbf{v}_i^{(m)} \circ \mathbf{v}_i^{(1)*} \circ \cdots \circ \mathbf{v}_i^{(m)*},$$

where $p_i \geqslant 0$, $\sum_{i=1}^{R} p_i = 1$, $\mathbf{v}_i^{(k)} \in \mathbb{C}^{n_k}$, $\|\mathbf{v}_i^{(k)}\| = 1$, $i \in [R]$, and $k \in [m]$. Hence, the mixed state ρ is separable if and only if its corresponding Hermitian tensor $\mathcal{H}_\rho$ is separable.

C. Geometric measure of quantum mixed states

For a quantum mixed state ρ, $E(\rho)$ denotes the distance between the state and the nearest separable mixed state, called the geometric measure of the quantum mixed states ρ.

Definition 2.6. Assume that ρ is quantum mixed state. Its geometric measure $E(\rho)$ is defined by

$$E(\rho) := \min_{\rho_{\text{sep}} \in \text{Separ}(\mathbb{H})} \|\rho - \rho_{\text{sep}}\|_F.$$

Assume that a Hermitian tensor $\mathcal{H}_\rho$ corresponds to the state ρ. Then the geometric measure $E(\rho)$ can be written as the following tensor optimization problem:

$$E(\rho) = \min_{\bar{\mathcal{H}} \in \text{Separ}(\mathbb{H})} ||\mathcal{H}_\rho - \bar{\mathcal{H}}||_F.$$

Denote $R_{\max} := \max_{\bar{\mathcal{H}} \in \text{Separ}(\mathbb{H})} rank_{\mathbb{H}} \bar{\mathcal{H}}$. For every $\bar{\mathcal{H}} \in \text{Separ}(\mathbb{H})$, it can be written as

$$\bar{\mathcal{H}} = \sum_{i=1}^{R_{\max}} p_i \mathbf{v}_i^{(1)} \circ \cdots \circ \mathbf{v}_i^{(m)} \circ \mathbf{v}_i^{(1)*} \circ \cdots \circ \mathbf{v}_i^{(m)*},$$

with $p_i \geqslant 0, \mathbf{v}_i^{(k)} \in \mathbb{C}^{n_k}, \|\mathbf{v}_i^{(k)}\| = 1, k \in [m], i \in [R_{\max}]$.

Hence, the computation problem of $E(\rho)$ can be converted to a rank-$R_{\max}$ approximation problem of Hermitian tensors. Furthermore, the state ρ is separable if and only if $E(\rho) = 0$. So, we discuss a rank-R separable approximation optimization problem of Hermitian tensors in the next section.

III. RANK-*R* SEPARABLE APPROXIMATION OF HERMITIAN TENSORS

Given a positive integer R and a Hermitian tensor $\mathcal{H} \in \mathbb{H}[n_1, \dots, n_m]$, the rank-$R$ separable approximation problem of $\mathcal{H}$ is the following optimization problem:

$$\min_{\hat{\mathcal{H}} \in \text{phd}(\mathbb{H})} ||\mathcal{H} - \hat{\mathcal{H}}||_F^2. \tag{2}$$

For every $\hat{\mathcal{H}} \in \text{phd}(\mathbb{H})$, the tensor can be expressed as

$$\hat{\mathcal{H}} = \sum_{i=1}^{R} \lambda_i \, \mathbf{v}_i^{(1)} \circ \cdots \circ \mathbf{v}_i^{(m)} \circ \mathbf{v}_i^{(1)*} \circ \cdots \circ \mathbf{v}_i^{(m)*}, \tag{3}$$

where $\lambda_i \geqslant 0, \mathbf{v}_i^{(k)} \in \mathbb{C}^{n_k}, \|\mathbf{v}_i^{(k)}\| = 1, i \in [R], k \in [m]$.

Since $\lambda_i \geqslant 0$ for all $i \in [R]$, we rewrite the tensor $\hat{\mathcal{H}}$ as

$$\hat{\mathcal{H}} = \sum_{i=1}^{R} \mathbf{u}_i^{(1)} \circ \cdots \circ \mathbf{u}_i^{(m)} \circ \mathbf{u}_i^{(1)*} \circ \cdots \circ \mathbf{u}_i^{(m)*},$$

where $\mathbf{u}_i^{(k)} = \sqrt[2m]{\lambda_i} \mathbf{v}_i^{(k)}, \mathbf{u}_i^{(k)} \in \mathbb{C}^{n_k}, i \in [R], k \in [m]$.

The constrained optimization problem (2) becomes the following unconstrained optimization problem:

$$\min_{\mathbf{u}_i^{(1)}, \cdots, \mathbf{u}_i^{(m)}} \left\| \mathcal{H} - \sum_{i=1}^{R} \mathbf{u}_i^{(1)} \circ \cdots \circ \mathbf{u}_i^{(m)} \circ \mathbf{u}_i^{(1)*} \circ \cdots \circ \mathbf{u}_i^{(m)*} \right\|_F^2. \tag{4}$$

Let $U_k = (\mathbf{u}_1^{(k)}, \mathbf{u}_2^{(k)}, \dots, \mathbf{u}_R^{(k)})$ be a complex matrix, where $\mathbf{u}_i^{(k)} \in \mathbb{C}^{n_k}$, $i \in [R]$, $k \in [m]$. $U_1, \dots, U_m$ are called factor matrices of Hermitian tensor $\hat{\mathcal{H}}$. $\hat{\mathcal{H}}$ can be expressed as $\hat{\mathcal{H}} := [\![U_1, \dots, U_m, U_1^*, \dots, U_m^*]\!]$.

In addition, denote

$$F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*) := ||\mathcal{H} - \hat{\mathcal{H}}||_F^2. \tag{5}$$

Then the optimization problem (4) can be concisely expressed as

$$\min_{\hat{\mathcal{H}}} F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*). \tag{6}$$

In the next subsection, we deduce the gradient of the objective function.

A. Gradient calculation of $F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$

Here, the function $F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$ is defined as in Eq. (5), where $\hat{\mathcal{H}} = [\![U_1, \dots, U_m, U_1^*, \dots, U_m^*]\!]$. Obviously,

$F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$ is continuous and differentiable. Specifically, for every $k \in [m]$, fix $\{U_1, \ldots, U_{k-1}, U_{k+1}, \ldots, U_m\}$, we regard $F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$ as a function of U_k and U_k^*. Then, its fastest growth direction, defined as the gradient of $F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$, denoted by G_k, is

$$G_k := \nabla_{U_k^*} F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*) = \frac{\partial F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)}{\partial U_k^*}.$$

Theorem 3.1 [18]. Let $\mathcal{H} \in \mathbb{H}[n_1, \ldots, n_m]$ be a Hermitian tensor, R be a positive integer, $U_k \in \mathbb{C}^{n_k \times r}$ for all $k \in [m]$ be factor matrices of Hermitian tensor $\hat{\mathcal{H}}$, and $\hat{\mathcal{H}} = [\![U_1, \ldots, U_m, U_1^*, \ldots, U_m^*]\!]$. Then, for each $k \in [m]$, the partial derivative of $F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$ defined in Eq. (5) with respect to U_k^* is

$$\begin{aligned}\frac{\partial F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)}{\partial U_k^*} = &-2(\mathcal{H}_{(k+m)} - \hat{\mathcal{H}}_{(k+m)})^* \, (U_m^* \odot \cdots \\ &\odot U_{k+1}^* \odot U_{k-1}^* \odot \cdots \odot U_1^* \odot U_m \\ &\odot \cdots \odot U_1),\end{aligned} \tag{7}$$

where $\hat{\mathcal{H}}_{(k+m)}$ represents the mode-$(k+m)$ unfolding matrix of tensor $\hat{\mathcal{H}}$.

The proof of Theorem 3.1 is shown in Appendix A. Hence, we obtain the gradient of the objective function $F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$, denoted by G, as follows:

$$G := \nabla F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*) = [G_1, G_2, \ldots, G_m]^\top.$$

B. BFGS algorithm for rank-R separable approximation

In this subsection, we deduce the BFGS method combined with the Wolfe line search for solving the optimization problem (6). For every $k \in [m]$, we also denote $F_{\mathcal{H}}(U_k, U_k^*) := F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$ as a function of U_k and U_k^*. For more details, please refer to Ref. [18]. We choose the initial point U^1 and $\mathcal{B}^1$ first, i.e., $U^1 = \{U_1^1, U_2^1, \ldots, U_m^1\}$, $\mathcal{B}^1 = \{\mathcal{B}_1^1, \mathcal{B}_2^1, \ldots, \mathcal{B}_m^1\}$.

In iteration t, for every $k \in [m]$, the search direction of the algorithm, denoted as D_k^t, is computed by

$$\mathcal{B}_k^t \cdot D_k^t = -G_k^t,$$

where

$$G_k^t = \frac{\partial F_{\mathcal{H}}(U_k^t, U_k^{t*})}{\partial U_k^*},$$

$$(\mathcal{B}_k^t \cdot D_k^t)_{i_1 i_2} = \sum_{j_1, j_2 = 1}^{n_k} (\mathcal{B}_k^t)_{i_1 i_2 j_1 j_2} (D_k^t)_{j_1 j_2}.$$

We denote by $D^t = (D_1^t, D_2^t, \ldots, D_m^t)$, $U^t = (U_1^t, U_2^t, \ldots, U_m^t)$. The iteration step α^t of line search algorithm satisfies the Wolfe condition, i.e.,

$$\begin{aligned}&F_{\mathcal{H}}(U^t + \alpha^t D^t, U^{t*} + \alpha^t D^{t*}) \leqslant F_{\mathcal{H}}(U^t, U^{t*}) + \eta \alpha^t \langle G^t, D^t \rangle, \\ &\langle \nabla F_{\mathcal{H}}(U^t + \alpha^t D^t, U^{t*} + \alpha^t D^{t*}), D^t \rangle \geqslant \sigma \langle G^t, D^t \rangle,\end{aligned} \tag{8}$$

where $0 < \eta < 0.5$, $\eta < \sigma < 1$. η and σ are the parameters of the line search algorithm. Then the next iteration is computed by $U^{t+1} = U^t + \alpha^t D^t$. Let $S_k^t = U_k^{t+1} - U_k^t$ and $Y_k^t = G_k^{t+1} - G_k^t$ with $S^t = \{S_k^t | k = 1, \ldots, m\}$ and $Y^t = \{Y_k^t | k = 1, \ldots, m\}$.

The updated formula of $\mathcal{B}_k^t$ is

$$\mathcal{B}_k^{t+1} = \mathcal{B}_k^t - \frac{(\mathcal{B}_k^t S_k^t) \circ [\mathcal{B}_k^t (S_k^t)^\dagger]}{\langle \mathcal{B}_k^t S_k^t, S_k^t \rangle} + \frac{Y_k^t \circ (Y_k^t)^\dagger}{\langle Y_k^t, S_k^t \rangle}, \tag{9}$$

where $k \in [m]$. $\mathcal{B}^t = \{\mathcal{B}_k^t | k = 1, \ldots, m\}$ is an approximation of a Hessian.

Then we have the BFGS algorithm for rank-R separable approximation of Hermitian tensor is shown in Algorithm 3.1.

Algorithm 3.1. (The BFGS algorithm for rank-R separable approximation).

Input: A Hermitian tensor $\mathcal{H}$ and a positive number R. Select parameters $\eta \in (0, 0.5)$, $\sigma \in (\eta, 1)$, $t = 1$, the initial factor matrice $U^1 = \{U_1^1, U_2^1, \ldots, U_m^1\}$, the tolerance error $\epsilon > 0$, the initial fourth-order unit Hermitian tensor $\mathcal{B}^1 = \{\mathbb{I}_1^1, \mathbb{I}_2^1, \ldots, \mathbb{I}_m^1\}$.

Output: A couple of factor matrices $U = \{U_1, U_2, \ldots, U_m\}$ of a rank-R separable approximation of $\mathcal{H}$.

Step 1: Based on $\mathcal{H}$ and $U^t = \{U_1^t, U_2^t, \ldots, U_m^t\}$, we calculate $G^t = \nabla F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)$ from Eq. (7).

Step 2: If $\|G^t\|_F \leqslant \epsilon$, then go to Step 6. Otherwise, go to the next step.

Step 3: Solving equations $\mathcal{B}^t D^t = -G^t$, the search direction D^t is obtained.

Step 4: Compute the iteration step α^t according to Wolfe conditions (8).

Step 5: Let $U^{t+1} = U^t + \alpha^t D^t$. Update variable $\mathcal{B}^{t+1}$, $\mathcal{B}^{t+1} = \{\mathcal{B}_k^{t+1} | k = 1, \ldots, m\}$ is determined by formula (9). Let $t = t + 1$, then go to Step 1.

Step 6: Return $U = U^t$.

IV. SEPARABILITY CRITERION AND DECOMPOSITION OF QUANTUM MIXED STATES

In this section, we will use Algorithm 3.1 to study the separability criterion and decomposition of quantum mixed states. We know that, under a given standard orthogonal base, a quantum mixed state ρ corresponds to a Hermitian tensor $\mathcal{H}_\rho$. Hence, we use Algorithm 3.1 to solve a separable approximation of $\mathcal{H}_\rho$. If we find a suitable $R (1 \leqslant R \leqslant R_{\max})$ to make the residual error satisfy

$$\left\| \mathcal{H}_\rho - \sum_{i=1}^R \mathbf{u}_i^{(1)} \circ \cdots \circ \mathbf{u}_i^{(m)} \circ \mathbf{u}_i^{(1)*} \circ \cdots \circ \mathbf{u}_i^{(m)*} \right\|_F = 0,$$

then we can get a positive Hermitian decomposition of $\mathcal{H}_\rho$, i.e.,

$$\mathcal{H}_\rho = \sum_{i=1}^R \mathbf{u}_i^{(1)} \circ \cdots \circ \mathbf{u}_i^{(m)} \circ \mathbf{u}_i^{(1)*} \circ \cdots \circ \mathbf{u}_i^{(m)*}.$$

Let $p_i = (\prod_{k=1}^m \|\mathbf{u}_i^{(k)}\|)^2$ and $\mathbf{v}_i^{(k)} = \frac{\mathbf{u}_i^{(k)}}{\|\mathbf{u}_i^{(k)}\|}$, $i \in [R]$, $k \in [m]$. Then

$$\mathcal{H}_\rho = \sum_{i=1}^R p_i \, \mathbf{v}_i^{(1)} \circ \cdots \circ \mathbf{v}_i^{(m)} \circ \mathbf{v}_i^{(1)*} \circ \cdots \circ \mathbf{v}_i^{(m)*}.$$

A natural question: $\sum_{i=1}^{R} p_i = 1$? If the answer is yes, then we obtain a decomposition of quantum mixed state ρ and determine that ρ is separable.

Theorem 4.1. Let the Hermitian tensor

$$\mathcal{H} = \sum_{i=1}^{s} \lambda_i \mathcal{X}_i \circ \mathcal{X}_i^*,$$

where $\lambda_i \geqslant 0$, $\sum_{i=1}^{s} \lambda_i = 1$, $\|\mathcal{X}_i\|_F = 1$, $\mathcal{X}_i \in \mathbb{C}^{n_1 \times \cdots \times n_m}$, $i \in [s]$. Assume that $\mathcal{H}$ is separable and has a positive Hermitian decomposition obtained by Algorithm 3.1 as

$$\mathcal{H} = \sum_{i=1}^{R} \mathbf{u}_i^{(1)} \circ \cdots \circ \mathbf{u}_i^{(m)} \circ \mathbf{u}_i^{(1)*} \circ \cdots \circ \mathbf{u}_i^{(m)*},$$

where $\mathbf{u}_i^{(k)} \in \mathbb{C}^{n_k}$ and $k \in [m]$. Let $p_i = (\prod_{k=1}^{m} \|\mathbf{u}_i^{(k)}\|)^2$ and $\mathbf{v}_i^{(k)} = \frac{\mathbf{u}_i^{(k)}}{\|\mathbf{u}_i^{(k)}\|}$, $i \in [R], k \in [m]$. Then

$$\mathcal{H} = \sum_{i=1}^{R} p_i \, \mathbf{v}_i^{(1)} \circ \cdots \circ \mathbf{v}_i^{(m)} \circ \mathbf{v}_i^{(1)*} \circ \cdots \circ \mathbf{v}_i^{(m)*},$$

with $p_i \geqslant 0$ and $\sum_{i=1}^{R} p_i = 1$.

Note. The proof of Theorem 4.1 is provided in Appendix B. If ρ is a density matrix of a separable quantum mixed state and $\mathcal{H}_\rho$ is its corresponding Hermitian tensor, then $\mathrm{Tr}_M(\mathcal{H}_\rho) = 1$ satisfying the condition of Theorem 4.1. On the other hand, we can obtain a positive Hermitian decomposition of $\mathcal{H}_\rho$ through Algorithm 3.1, which satisfies $p_i \geqslant 0$ and $\sum_{i=1}^{R} p_i = 1$ by Theorem 4.1. So, we can get a decomposition of quantum state ρ. Hence, we propose an algorithm in the following for the separability discrimination of a quantum mixed state ρ and calculating a decomposition of ρ if it is separable. If Algorithm 4.1 does not converge to zero, then we cannot guarantee that the output trace is equal to 1. In other words, if ρ is an entangled state and $\mathcal{H}_\rho$ is its corresponding Hermitian tensor, then some numerical results show that the matrix trace of approximate tensor $\hat{\mathcal{H}}$ of $\mathcal{H}_\rho$ is not 1. Refer to Example 5.1 and Example 5.3 for more details.

Algorithm 4.1. (Separability discrimination and decomposition of quantum mixed states)

Input: A quantum mixed state ρ, a Hermitian rank upper bound $R_{\max}$, an initial point $U^1 = (U_1^1, U_2^1, \ldots, U_m^1)$ and a small positive number ϵ.

Output: Answer whether ρ is separable. If it is separable, we give a decomposition, i.e., $\{p_i \geqslant 0 | i \in [R]\}$ and the state $\{|\phi_i^{(k)}\rangle | i \in [R], k \in [m]\}$.

Step 1: Obtain its corresponding tensor $\mathcal{H}_\rho$ for the mixed state ρ.

Step 2: Take $R = 1{:}R_{\max}$, we calculate the rank-R separable approximation of $\mathcal{H}_\rho$ by Algorithm 3.1. If $\|\mathcal{H}_\rho - \hat{\mathcal{H}}\|_F \geqslant \epsilon$, then we take $R = R + 1$. Loop until if $R = R_{\max}$ and $\|\mathcal{H}_\rho - \hat{\mathcal{H}}\|_F \geqslant \epsilon$, then go to Step 5. If there exists a suitable $R \leqslant R_{\max}$ such that $||\mathcal{H}_\rho - \hat{\mathcal{H}}||_F < \epsilon$, then go to the next step.

Step 3: Compute $p_i = (\prod_{k=1}^{m} \|\mathbf{u}_i^{(k)}\|)^2$ and the state $\{|\phi_i^{(k)}\rangle := \mathbf{v}_i^{(k)} = \frac{\mathbf{u}_i^{(k)}}{\|\mathbf{u}_i^{(k)}\|} | i \in [R], k \in [m]\}$.

Step 4: Return the mixed state ρ is separable, $\{p_i \geqslant 0 | i \in [R]\}$ and the state $\{|\phi_i^{(k)}\rangle | i \in [R], k \in [m]\}$.

Step 5: Return the mixed state ρ is entangled.

TABLE I. The matrix trace $\mathrm{Tr}_M(\hat{\mathcal{H}}_{\rho(\alpha)})$ of approximate tensors $\hat{\mathcal{H}}_{\rho(\alpha)}$.

α	0.3	0.6	1
$\mathrm{Tr}_M(\hat{\mathcal{H}}_{\rho(\alpha)})$	1.2	1.1	1.5

V. NUMERICAL EXAMPLES

For a quantum mixed state, we use Algorithm 4.1 to detect its separability. If it is separable, we give its decomposition. To test the effectiveness of Algorithm 4.1, we study several quantum mixed states. From Ref. [19], we know that $R_{\max} \leqslant \binom{n+m-1}{m}^2$ if $\mathcal{H}_\rho$ is a symmetric Hermitian tensor. Let $\hat{\mathcal{H}}$ be a separable Hermitian tensor defined by Eq. (3). The relative error of $\mathcal{H}_\rho$ and $\hat{\mathcal{H}}$ is defined as

$$\delta := \frac{\|\mathcal{H}_\rho - \hat{\mathcal{H}}\|_F}{\|\mathcal{H}_\rho\|_F}.$$

Example 5.1 [20]. Consider the quantum mixed state

$$\rho(\alpha) = \alpha|\psi_1\rangle\langle\psi_1| + (1-\alpha)|\psi_2\rangle\langle\psi_2|,$$

where $|\psi_1\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$, $|\psi_2\rangle = \frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|10\rangle$, $\alpha \in (0, 1)$.

By calculating the geometric measure of $\rho(\alpha)$, Hu *et al.* showed that $\rho(\frac{1}{2})$ is separable and the rest are entangled. $\rho(\frac{1}{2})$ corresponds to a fourth-order two-dimensional Hermitian tensor $\mathcal{H}_{\rho(\frac{1}{2})}$ and its nonzero elements are $(\mathcal{H}_{\rho(\frac{1}{2})})_{1111} = (\mathcal{H}_{\rho(\frac{1}{2})})_{2211} = (\mathcal{H}_{\rho(\frac{1}{2})})_{1221} = (\mathcal{H}_{\rho(\frac{1}{2})})_{2121} = (\mathcal{H}_{\rho(\frac{1}{2})})_{1212} = (\mathcal{H}_{\rho(\frac{1}{2})})_{2112} = (\mathcal{H}_{\rho(\frac{1}{2})})_{1122} = (\mathcal{H}_{\rho(\frac{1}{2})})_{2222} = \frac{1}{4}$. To verify the correctness of Algorithm 4.1, we conduct an experiment for the mixed state $\rho(\frac{1}{2})$.

Using Algorithm 4.1 ten times, we compute the rank-R separable approximation of $\mathcal{H}_{\rho(\frac{1}{2})}$ for all $R = 1, 2, \ldots, 7$. In most cases, we get all relative errors $\delta_{\rho(\frac{1}{2})}$ as 0.7071, $5.7941e-07$, $2.0223e-05$, $5.4682e-05$, $9.4914e-05$, $8.9762e-05$, $2.5051e-04$, respectively. It is clear that $\rho(\frac{1}{2})$ is separable. We obtain a decomposition of $\rho(\frac{1}{2})$ in Appendix C 1.

Take $\alpha = 0.3$, $\alpha = 0.6$, and $\alpha = 1$. which correspond to Hermitian tensors $\mathcal{H}_{\rho(0.3)}$, $\mathcal{H}_{\rho(0.6)}$, and $\mathcal{H}_{\rho(1)}$. Since $\mathcal{H}_{\rho(0.3)}$, $\mathcal{H}_{\rho(0.6)}$, and $\mathcal{H}_{\rho(1)}$ are symmetric Hermitian tensors, we take $R_{\max} = \binom{3}{2}^2 = 9$. When $R = R_{\max} = 9$, we calculate the relative errors $\delta_{\rho(0.3)} = 0.2626$, $\delta_{\rho(0.6)} = 0.1387$, and $\delta_{\rho(1)} = 0.5$ by Algorithm 4.1. Hence $\rho(0.3)$, $\rho(0.6)$, and $\rho(1)$ are entangled.

If we take α equal to 0.3, 0.6, or 1, numerical results indicate that the matrix traces of approximate tensors $\hat{\mathcal{H}}_{\rho(\alpha)}$ of $\mathcal{H}_{\rho(\alpha)}$ are not equal to 1. The results are shown in Table I.

Finally, we plot $\delta^2[\rho(\alpha)]$ for the mixed states $\rho(\alpha)$ with parameter $\alpha \in [0, 1]$. The result is shown in Fig. 1.

Example 5.2 [17]. Consider mixtures of three-qubit $|GHZ\rangle$, $|W\rangle$, and inverted-$|W\rangle$ states as

$$\rho\left(\tfrac{1}{4}, \tfrac{3}{8}\right) = \tfrac{1}{4}|GHZ\rangle\langle GHZ| + \tfrac{3}{8}|W\rangle\langle W| + \tfrac{3}{8}|\tilde{W}\rangle\langle\tilde{W}|,$$

where $|GHZ\rangle, |W\rangle, |\tilde{W}\rangle$ are defined as follows: $|GHZ\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$, $|W\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$, $|\tilde{W}\rangle = (|110\rangle + |101\rangle + |011\rangle)/\sqrt{3}$.

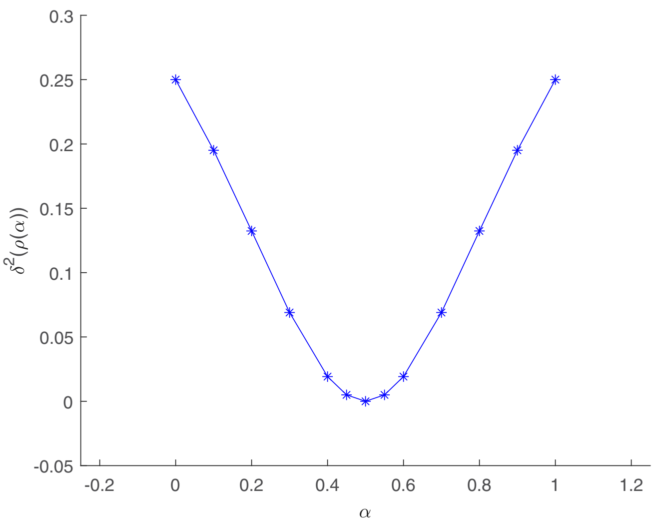

FIG. 1. The $\delta^2[\rho(\alpha)]$ for the mixed states $\rho(\alpha)$ in Example 5.1.

Wei and Goldbart said that $\rho(\frac{1}{4}, \frac{3}{8})$ is separable. However, they did not show its decomposition. $\rho(\frac{1}{4}, \frac{3}{8})$ corresponds to a Hermitian tensor $\mathcal{H}_{\rho(\frac{1}{4},\frac{3}{8})}$ of size sixth-order two dimensions. Next, we verify whether Algorithm 4.1 can distinguish whether the mixed state $\rho(\frac{1}{4}, \frac{3}{8})$ is separable.

Using Algorithm 4.1 five times, we calculate the rank-R separable approximation of $\mathcal{H}_{\rho(\frac{1}{4},\frac{3}{8})}$ for all $R = 1, 2, \ldots, 7$. we obtain all mean relative error values as $0.81009,\ 0.56565,\ 2.2225e-06,\ 6.8205e-05,\ 1.486e-04,\ 2.0062e-04,\ 1.5276e-04$, respectively. So $\rho(\frac{1}{4}, \frac{3}{8})$ is separable and its Hermitian rank is 3. We obtain a decomposition of $\rho(\frac{1}{4}, \frac{3}{8})$ in Appendix C 2.

When $R = 3$, we run the Algorithm 4.1 five times. For fixed R, Algorithm 4.1 takes different initial values, and its running time, iteration number, and relative error are slightly different as in Table II.

Example 5.3 [21]. Consider the quantum mixed state

$$\rho(x) = x|\psi\rangle\langle\psi| + \frac{1-x}{16}\mathbb{I}_{16},$$

where $|\psi\rangle = \frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)$ and $\mathbb{I}_{16}$ is defined as

$$(\mathbb{I}_{16})_{i_1i_2i_3i_4j_1j_2j_3j_4} = \begin{cases} 1, & \text{if } i_l = j_l, \quad l = 1, 2, 3, 4, \\ 0, & \text{otherwise.} \end{cases}$$

Zhao *et al.* said that these mixed states are entangled when x are $\frac{3}{4}$, $\frac{4}{5}$, and $\frac{6}{7}$. $\mathcal{H}_{\rho(x)}$ is the tensor corresponding to state $\rho(x)$.

TABLE II. Running time and iteration number of rank-3 separable approximation for $\rho(\frac{1}{4}, \frac{3}{8})$.

	$R = 3$		
No.	Time(s)	Iterations	Relative error
1	0.5820	57	2.1242×10^{-06}
2	0.5380	51	2.5548×10^{-06}
3	0.6990	67	1.9185×10^{-06}
4	0.6130	59	1.9701×10^{-06}
5	0.7820	77	2.5447×10^{-06}

TABLE III. The matrix trace $\mathrm{Tr}_M(\hat{\mathcal{H}}_{\rho(x)})$ of approximate tensors $\hat{\mathcal{H}}_{\rho(x)}$.

x	$\frac{3}{4}$	$\frac{4}{5}$	$\frac{6}{7}$
$\mathrm{Tr}_M(\hat{\mathcal{H}}_{\rho(x)})$	1.6289	1.6781	1.7344

Because $\mathcal{H}_{\rho(\frac{3}{4})}$, $\mathcal{H}_{\rho(\frac{4}{5})}$, and $\mathcal{H}_{\rho(\frac{6}{7})}$ are symmetric Hermitian tensors, we take $R_{\max} = \binom{5}{4}^2 = 25$. When $R = R_{\max} = 25$, we calculate that $\delta_{\rho(\frac{3}{4})} = 0.6190$, $\delta_{\rho(\frac{4}{5})} = 0.6298$, and $\delta_{\rho(\frac{6}{7})} = 0.6405$. Hence, the mixed states $\rho(\frac{3}{4})$, $\rho(\frac{4}{5})$, and $\rho(\frac{6}{7})$ are entangled.

If we take x equal to $\frac{3}{4}$, $\frac{4}{5}$, or $\frac{6}{7}$, numerical results indicate that the matrix traces of approximate tensors $\hat{\mathcal{H}}_{\rho(x)}$ of $\mathcal{H}_{\rho(x)}$ are not equal to 1. The results are shown in Table III.

Example 5.4. (Comparison with E-Truncated K-Moment semi-definite relaxation (ETKM-SDR) method) ETKM-SDR method is a method that converts the separability discrimination problem to a moment optimization problem, and solves it using the semi-definite relaxation method. We compare the stability and computing speed of the BFGS method and ETKM-SDR method. Consider the 2-partite isotropic states $\rho_{\mathrm{iso}}(F)$ [17],

$$\rho_{\mathrm{iso}}(F) = \frac{1-F}{3}(\mathbb{I} - |\Phi^+\rangle\langle\Phi^+|) + F|\Phi^+\rangle\langle\Phi^+|,$$

where $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ and $\mathbb{I}_{1111} = \mathbb{I}_{1212} = \mathbb{I}_{2121} = \mathbb{I}_{2222} = 1$. M. Horodecki and P. Horodecki indicated that $\rho_{\mathrm{iso}}(F)$ is separable for $F \in [0, \frac{1}{2}]$. Take $F = \frac{1}{2}$. We calculate the rank-R separable approximation of $\mathcal{H}_{\rho_{\mathrm{iso}}(\frac{1}{2})}$, for all $R = 1, 2, \ldots, 7$. We get all relative error values as $0.8165,\ 0.57735,\ 0.33333,\ 1.9959e-04,\ 1.8132e-04,\ 1.6908e-04,\ 1.2228e-04$, respectively. It is clear that $\mathcal{H}_{\rho_{\mathrm{iso}}(\frac{1}{2})}$ is separable and its Hermitian rank is 4. When $R = 4, 5, 6$, we obtain numerical decompositions of $\rho_{\mathrm{iso}}(\frac{1}{2})$ in Appendix C 3.

We do ten numerical experiments by the BFGS method and the ETKM-SDR method for the quantum mixed state $\rho_{\mathrm{iso}}(\frac{1}{2})$, respectively. We obtain running time and the relative error in Table IV. From Table IV, we see that the BFGS algorithm has

TABLE IV. Comparison of BFGS method and ETKM-SDR method for $\rho_{\mathrm{iso}}(\frac{1}{2})$.

	BFGS method			ETKM-SDR method		
No.	Time(s)	Relative error	R	Time(s)	Relative error	R
1	6.3650	$2.2137\times^{-04}$	7	125.4763	0.0011	7
2	5.1110	$1.8103\times^{-04}$	6	133.9843	0.0594	6
3	8.5330	$1.5636\times^{-04}$	5	123.7532	$4.4168\times^{-05}$	5
4	5.1030	$1.7343\times^{-04}$	7	117.6680	0.0014	7
5	10.9620	$1.6389\times^{-04}$	5	138.9516	$6.6597\times^{-04}$	5
6	2.7550	$1.2883\times^{-04}$	6	131.7422	0.0013	6
7	6.2630	$1.7412\times^{-04}$	6	123.6200	0.0048	6
8	2.6810	$1.4525\times^{-04}$	7	135.5775	0.0117	7
9	13.5510	$2.0537\times^{-04}$	4	120.3903	$2.8345\times^{-05}$	4
10	2.7570	$1.5629\times^{-04}$	6	129.8795	$3.4562\times^{-04}$	6

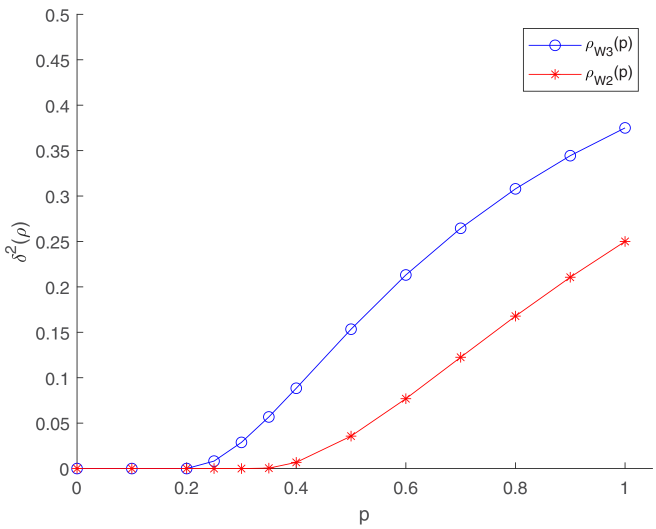

FIG. 2. The $\delta^2(\rho)$ for Werner states of three qubits which is compared to the two-qubits case.

better performance than the ETKM-SDR algorithm in terms of running time, relative error, and stability.

Example 5.5 [22]. In this example, we consider the Werner states of three qubits which have the following form:

$$\rho_{W3}(p) = p|GHZ\rangle\langle GHZ| + \frac{1-p}{8}\mathbb{I}_8, \tag{10}$$

where $|GHZ\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ and $\mathbb{I}_8$ is

$$(\mathbb{I}_8)_{i_1i_2i_3j_1j_2j_3} = \begin{cases} 1, & \text{if } i_l = j_l, \quad l = 1, 2, 3, \\ 0, & \text{otherwise.} \end{cases}$$

This is a generalization of the Werner states to three qubits, known as the generalized Werner states. These mixed states are very classical. Next, we will study whether these states are entangled.

Through Algorithm 4.1, they are found that when $0 \leqslant p \leqslant \frac{1}{5}$, the mixed states $\rho_{W3}(p)$ are completely separable, and when $\frac{1}{5} < p \leqslant 1$, the mixed states $\rho_{W3}(p)$ are entangled. The result is shown in Fig. 2. Figure 2 can be compared to the $\delta^2(\rho)$ for Werner states of two qubits with parameter $p \in [0, 1]$, where the Werner states of two qubits are defined as

$$\rho_{W2}(p) = p|\phi^+\rangle\langle\phi^+| + \frac{1-p}{4}\mathbb{I}_4,$$

with the state $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$.

Example 5.6 [23]. We consider the Werner states generated by the Bell states

$$\rho_W(F) = F|\psi^-\rangle\langle\psi^-| + \frac{1-F}{3}(|\psi^+\rangle\langle\psi^+| + |\phi^+\rangle\langle\phi^+| + |\phi^-\rangle\langle\phi^-|),$$

where $|\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$, $|\psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$, $|\phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$, and $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. We apply Algorithm 4.1 to this Werner states $\rho_W(F)$. The parameter F that describes the degree of mixing is called fidelity.

When $F = \frac{1}{2}$, $\rho_W(\frac{1}{2})$ corresponds to a fourth-order two-dimensional Hermitian tensor $\mathcal{H}_{\rho_W(\frac{1}{2})}$. By Algorithm 4.1, we calculate the rank-R separable approximation of $\mathcal{H}_{\rho_W(\frac{1}{2})}$ for all $R = 1, 2, \ldots, 7$. We obtain all relative error values as 0.817, 0.577, 0.333, $1.251e-04$, $1.269e-04$, $1.106e-04$, $9.902e-05$, respectively. Hence, the Werner state $\rho_W(\frac{1}{2})$ is separable and its Hermitian rank is 4.

When F are $\frac{2}{3}$ and $\frac{4}{5}$, $\rho_W(\frac{2}{3})$ and $\rho_W(\frac{4}{5})$ correspond to Hermitian tensors $\mathcal{H}_{\rho_W(\frac{2}{3})}$ and $\mathcal{H}_{\rho_W(\frac{4}{5})}$. We take $R_{\max} = \binom{3}{2}^2 = 9$. When $R = R_{\max} = 9$, we calculate the relative errors $\delta_{\rho_W(\frac{2}{3})} = 0.2402$ and $\delta_{\rho_W(\frac{4}{5})} = 0.3712$ by Algorithm 4.1. Hence, $\rho_W(\frac{2}{3})$ and $\rho_W(\frac{4}{5})$ are entangled.

VI. CONCLUSION

In this paper, we study the separability criterion and decomposition problem of quantum mixed states. First, we convert the separability determination problem of quantum mixed states to the positive Hermitian decomposition problem of Hermitian tensors. Then we consider a rank-R separable approximation model of Hermitian tensors and introduce a BFGS algorithm for rank-R separable approximation. It is known that the corresponding Hermitian tensor is separable if a mixed state is separable. Moreover, we prove that a positive Hermitian decomposition of the Hermitian tensor obtained by the algorithm corresponds to a decomposition of the mixed state. Hence, we design a BFGS algorithm for separability determination and decomposition of quantum mixed states. Numerical examples show the effectiveness and correctness of the BFGS algorithm. Meanwhile, we compare the BFGS algorithm with the semi-definite relaxation algorithm. Numerical examples show that the BFGS algorithm has better stability and faster computing speed than the semi-definite relaxation algorithm. Reference [24] is the program code for Algorithm 4.1, used to calculate from Example 5.1 to Example 5.6. However, the BFGS algorithm is a numerical algorithm, and the termination condition is given according to the calculation requirements, which cannot be infinitely small. Hence, no matter how small the termination condition is, we can always construct an entangled state such that its distance from a separable state is less than this termination condition. However, it does not mean that the algorithm is ineffective.

ACKNOWLEDGMENTS

The authors would like to thank the editor and two anonymous referees for their valuable suggestions, which helped us to improve this paper. The research is supported by the National Natural Science Foundation of China (Grant No. 12371315).

APPENDIX A: PROOF OF THEOREM 3.1

Proof. Since

$$F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*) = ||\mathcal{H} - \hat{\mathcal{H}}||_F^2 = \langle \mathcal{H} - \hat{\mathcal{H}}, \mathcal{H} - \hat{\mathcal{H}}\rangle$$
$$= \langle \mathcal{H}, \mathcal{H}\rangle - \langle \mathcal{H}, \hat{\mathcal{H}}\rangle - \langle \hat{\mathcal{H}}, \mathcal{H}\rangle + \langle \hat{\mathcal{H}}, \hat{\mathcal{H}}\rangle.$$

Let $F_0 = \langle \mathcal{H}, \mathcal{H}\rangle$, $F_1 = \langle \mathcal{H}, \hat{\mathcal{H}}\rangle$, $F_2 = \langle \hat{\mathcal{H}}, \mathcal{H}\rangle$ and $F_3 = \langle \hat{\mathcal{H}}, \hat{\mathcal{H}}\rangle$. Thus

$$F_{\mathcal{H}}(U_k, U_k^*) = F_0 - F_1 - F_2 + F_3.$$

Note that F_0 is a real constant and $(\frac{\partial F_0}{\partial U_k^*})_{j_k t_k} = 0,\ j_k \in [n_k]$, $t_k \in [R]$. Hence,

$$\frac{\partial F}{\partial U_k^*} = -\frac{\partial F_1}{\partial U_k^*} - \frac{\partial F_2}{\partial U_k^*} + \frac{\partial F_3}{\partial U_k^*}.$$

Next we have

$$\begin{aligned}\left(\frac{\partial F_1}{\partial U_k^*}\right)_{j_k t_k} &= \frac{\partial(\mathcal{H}^* \cdot \hat{\mathcal{H}})}{\partial[(U_k^*)_{j_k t_k}]} \\ &= \sum_{I,J\in E,\ j_k \text{ is fixed}} \mathcal{H}_{IJ}^* \cdot \left(\mathbf{u}_{t_k}^{(1)}\right)_{i_1} \cdots \left(\mathbf{u}_{t_k}^{(m)}\right)_{i_m} \\ &\quad \times \left(\mathbf{u}_{t_k}^{(1)*}\right)_{j_1} \cdots \left(\mathbf{u}_{t_k}^{(k-1)*}\right)_{j_{k-1}} \left(\mathbf{u}_{t_k}^{(k+1)*}\right)_{j_{k+1}} \\ &\quad \cdots \left(\mathbf{u}_{t_k}^{(m)*}\right)_{j_m}.\end{aligned}$$

Then

$$\begin{aligned}\frac{\partial F_1}{\partial U_k^*} &= \mathcal{H}_{(k+m)}^* \left(U_m^* \odot \cdots \odot U_{k+1}^*\right. \\ &\quad \left.\odot U_{k-1}^* \odot \cdots \odot U_1^* \odot U_m \odot \cdots \odot U_1\right).\end{aligned}$$

Similarly, we can get

$$\begin{aligned}\frac{\partial F_2}{\partial U_k^*} &= \mathcal{H}_{(k)} \left(U_m \odot \cdots \odot U_1\right. \\ &\quad \left.\odot U_m^* \odot \cdots \odot U_{k+1}^* \odot U_{k-1}^* \odot \cdots \odot U_1^*\right).\end{aligned}$$

Finally, we deduce the partial derivatives of F_3.

$$\begin{aligned}\left(\frac{\partial F_3}{\partial U_k^*}\right)_{j_k t_k} &= \frac{\partial\left(\sum_{I,J}(\hat{\mathcal{H}}^*)_{IJ} \cdot (\hat{\mathcal{H}})_{IJ}\right)}{\partial[(U_k^*)_{j_k t_k}]} \\ &= \sum_{I,J\in E,\ j_k \text{ is fixed}} \hat{\mathcal{H}}_{IJ}^* \cdot \left(\mathbf{u}_{t_k}^{(1)}\right)_{i_1} \cdots \left(\mathbf{u}_{t_k}^{(m)}\right)_{i_m} \\ &\quad \times \left(\mathbf{u}_{t_k}^{(1)*}\right)_{j_1} \cdots \left(\mathbf{u}_{t_k}^{(k-1)*}\right)_{j_{k-1}} \left(\mathbf{u}_{t_k}^{(k+1)*}\right)_{j_{k+1}} \\ &\quad \cdots \left(\mathbf{u}_{t_k}^{(m)*}\right)_{j_m} + \sum_{I,J\in E,\ i_k \text{ is fixed}} \hat{\mathcal{H}}_{IJ} \cdot \left(\mathbf{u}_{t_k}^{(1)*}\right)_{i_1} \\ &\quad \cdots \left(\mathbf{u}_{t_k}^{(k-1)*}\right)_{i_{k-1}} \left(\mathbf{u}_{t_k}^{(k+1)*}\right)_{i_{k+1}} \\ &\quad \cdots \left(\mathbf{u}_{t_k}^{(m)*}\right)_{i_m} \left(\mathbf{u}_{t_k}^{(1)}\right)_{j_1} \cdots \left(\mathbf{u}_{t_k}^{(m)}\right)_{j_m}.\end{aligned}$$

Then

$$\begin{aligned}\frac{\partial F_3}{\partial U_k^*} &= \hat{\mathcal{H}}_{(k+m)}^* \left(U_m^* \odot \cdots \odot U_{k+1}^*\right. \\ &\quad \left.\odot U_{k-1}^* \odot \cdots \odot U_1^* \odot U_m \odot \cdots \odot U_1\right) \\ &\quad + \hat{\mathcal{H}}_{(k)}\left(U_m \odot \cdots \odot U_1\right. \\ &\quad \left.\odot U_m^* \odot \cdots \odot U_{k+1}^* \odot U_{k-1}^* \odot \cdots \odot U_1^*\right).\end{aligned}$$

Thus, it can be obtained from the above

$$\begin{aligned}\frac{\partial F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)}{\partial\, U_k^*} &= -(\mathcal{H}_{(k+m)} - \hat{\mathcal{H}}_{(k+m)})^* \left(U_m^* \odot \cdots\right. \\ &\quad \odot U_{k+1}^* \odot U_{k-1}^* \odot \cdots \odot U_1^* \odot U_m \odot \\ &\quad \left.\cdots \odot U_1\right) - (\mathcal{H}_{(k)} - \hat{\mathcal{H}}_{(k)}) \left(U_m \odot \cdots \odot U_1\right. \\ &\quad \left.\odot U_m^* \odot \cdots \odot U_{k+1}^* \odot U_{k-1}^* \odot \cdots \odot U_1^*\right).\end{aligned}$$

In addition,

$$\begin{aligned}&(\mathcal{H}_{(k+m)} - \hat{\mathcal{H}}_{(k+m)})^* \left(U_m^* \odot \cdots \odot U_{k+1}^*\right. \\ &\quad \left.\odot U_{k-1}^* \odot \cdots \odot U_1^* \odot U_m \odot \cdots \odot U_1\right) \\ &\quad = (\mathcal{H}_{(k)} - \hat{\mathcal{H}}_{(k)}) \left(U_m \odot \cdots \odot U_1 \odot U_m^*\right. \\ &\quad \left.\odot \cdots \odot U_{k+1}^* \odot U_{k-1}^* \odot \cdots \odot U_1^*\right).\end{aligned}$$

It follows that

$$\begin{aligned}\frac{\partial F_{\mathcal{H}}(\hat{\mathcal{H}}, \hat{\mathcal{H}}^*)}{\partial U_k^*} &= -2(\mathcal{H}_{(k+m)} - \hat{\mathcal{H}}_{(k+m)})^* \left(U_m^* \odot \cdots \odot U_{k+1}^*\right. \\ &\quad \left.\odot U_{k-1}^* \odot \cdots \odot U_1^* \odot U_m \odot \cdots \odot U_1\right).\end{aligned}$$

This completes the proof. ■

APPENDIX B: PROOF OF THEOREM 4.1

Proof. It is easy to know that $p_i \geqslant 0$, $i \in [R]$. In addition,

$$\mathcal{H} = \sum_{i=1}^{R} p_i \mathbf{v}_i^{(1)} \circ \cdots \circ \mathbf{v}_i^{(m)} \circ \mathbf{v}_i^{(1)*} \circ \cdots \circ \mathbf{v}_i^{(m)*},$$

where $\|\mathbf{v}_i^{(k)}\| = 1$, $p_i \geqslant 0$, $\mathbf{v}_i^{(k)} \in \mathbb{C}^{n_k}$, $k \in [m]$, $i \in [R]$. In the remainder of the paper, we only prove that $\sum_{i=1}^{R} p_i = 1$. On one hand,

$$\begin{aligned}\mathrm{Tr}_M(\mathcal{H}) &= \sum_{i=1}^{R} p_i \mathrm{Tr}_M\left(\mathbf{v}_i^{(1)} \circ \cdots \circ \mathbf{v}_i^{(m)} \circ \mathbf{v}_i^{(1)*} \circ \cdots \circ \mathbf{v}_i^{(m)*}\right) \\ &= \sum_{i=1}^{R} p_i \sum_{i_1,\cdots,i_m=1}^{n_1,\cdots,n_m} \left(\mathbf{v}_i^{(1)}\right)_{i_1} \cdots \left(\mathbf{v}_i^{(m)}\right)_{i_m} \left(\mathbf{v}_i^{(1)}\right)_{i_1}^* \cdots \left(\mathbf{v}_i^{(m)}\right)_{i_m}^* \\ &= \sum_{i=1}^{R} p_i \sum_{i_1=1}^{n_1} \left(\mathbf{v}_i^{(1)}\right)_{i_1} \left(\mathbf{v}_i^{(1)}\right)_{i_1}^* \cdots \sum_{i_m=1}^{n_m} \left(\mathbf{v}_i^{(m)}\right)_{i_m} \left(\mathbf{v}_i^{(m)}\right)_{i_m}^* \\ &= \sum_{i=1}^{R} p_i \left(\prod_{k=1}^{m} \|\mathbf{v}_i^{(k)}\|^2\right) = \sum_{i=1}^{R} p_i.\end{aligned}$$

On the other hand,

$$\begin{aligned}\mathrm{Tr}_M(\mathcal{H}) &= \sum_{i=1}^{s} \lambda_i \mathrm{Tr}_M(\mathcal{X}_i \circ \mathcal{X}_i^*) \\ &= \sum_{i=1}^{s} \lambda_i \sum_{i_1,\ldots,i_m=1}^{n_1,\ldots,n_m} (\mathcal{X}_i)_{i_1\ldots\, i_m} (\mathcal{X}_i)_{i_1\ldots\, i_m}^* \\ &= \sum_{i=1}^{s} \lambda_i \|\mathcal{X}_i\|_F^2 \\ &= \sum_{i=1}^{s} \lambda_i = 1.\end{aligned}$$

Hence, we have $\mathrm{Tr}_M(\mathcal{H}) = \sum_{i=1}^{R} p_i = 1$. This completes the proof. ■

APPENDIX C: NUMERICAL DECOMPOSITIONS OF EXAMPLES

1. Numerical decomposition of Example 5.1

In Example 5.1, we obtain a decomposition of the mixed state $\rho(\frac{1}{2})$,

$$\rho\left(\frac{1}{2}\right) = \sum_{i=1}^{2} p_i \left|\phi_i^{(1)}\phi_i^{(2)}\right\rangle\!\left\langle\phi_i^{(1)}\phi_i^{(2)}\right|,$$

where $p = [0.5, 0.5]^\top$,

$$\left|\phi_1^{(1)}\right\rangle = (-0.0728 + 0.7034i)|0\rangle + (0.0728 - 0.7034i)|1\rangle,$$
$$\left|\phi_2^{(1)}\right\rangle = (0.1889 + 0.6814i)|0\rangle + (0.1889 + 0.6814i)|1\rangle,$$
$$\left|\phi_1^{(2)}\right\rangle = (-0.4440 - 0.5503i)|0\rangle + (0.4440 + 0.5503i)|1\rangle,$$
$$\left|\phi_2^{(2)}\right\rangle = (0.5729 + 0.4145i)|0\rangle + (0.5729 + 0.4145i)|1\rangle.$$

2. Numerical decomposition of Example 5.2

In Example 5.2, we get a decomposition of the mixed state $\rho(\frac{1}{4}, \frac{3}{8})$, i.e.,

$$\rho\left(\frac{1}{4}, \frac{3}{8}\right) = \sum_{i=1}^{3} p_i \left|\phi_i^{(1)}\phi_i^{(2)}\phi_i^{(3)}\right\rangle\!\left\langle\phi_i^{(1)}\phi_i^{(2)}\phi_i^{(3)}\right|,$$

where $p = [p_1, p_2, p_3]^\top = [\frac{1}{3}, \frac{1}{3}, \frac{1}{3}]^\top$,

$$\left|\phi_1^{(1)}\right\rangle = (0.5042 + 0.4958i)|0\rangle + (0.5042 + 0.4958i)|1\rangle,$$
$$\left|\phi_2^{(1)}\right\rangle = (-0.2161 + 0.6733i)|0\rangle + (0.6911 - 0.1495i)|1\rangle$$
$$, \left|\phi_3^{(1)}\right\rangle = (0.6739 + 0.2141i)|0\rangle + (-0.5224 + 0.4766i)|1\rangle,$$
$$\left|\phi_1^{(2)}\right\rangle = (-0.4236 - 0.5662i)|0\rangle + (-0.4236 - 0.5662i)|1\rangle,$$
$$\left|\phi_2^{(2)}\right\rangle = (0.0666 + 0.7040i)|0\rangle + (0.5763 - 0.4097i)|1\rangle,$$
$$\left|\phi_3^{(2)}\right\rangle = (-0.6347 - 0.3118i)|0\rangle + (0.5873 - 0.3937i)|1\rangle,$$
$$\left|\phi_1^{(3)}\right\rangle = (-0.6709 - 0.2232i)|0\rangle + (-0.6709 - 0.2232i)|1\rangle,$$
$$\left|\phi_2^{(3)}\right\rangle = (0.5649 + 0.4253i)|0\rangle + (0.0859 - 0.7019i)|1\rangle,$$

3. Numerical decompositions of Example 5.4

In Example 5.4, we consider the mixed state $\rho_{\text{iso}}(F)$, $F = \frac{1}{2}$. When $R = 4$, we get a numerical decomposition of the mixed state $\rho_{\text{iso}}(\frac{1}{2})$,

$$\rho_{\text{iso}}\left(\frac{1}{2}\right) = \sum_{i=1}^{4} p_i \left|\phi_i^{(1)}\phi_i^{(2)}\right\rangle\!\left\langle\phi_i^{(1)}\phi_i^{(2)}\right|,$$

where $p = [0.25, 0.25, 0.25, 0.25]^\top$,

$$`\left|\phi_1^{(1)}\right\rangle = (0.0487 + 0.4264i)|0\rangle + (0.8569 + 0.2855i)|1\rangle,$$
$$\left|\phi_2^{(1)}\right\rangle = (0.3357 - 0.3861i)|0\rangle + (0.5284 + 0.6775i)|1\rangle,$$
$$\left|\phi_3^{(1)}\right\rangle = (0.7965 - 0.2641i)|0\rangle + (-0.5435 - 0.0215i)|1\rangle,$$
$$\left|\phi_4^{(1)}\right\rangle = (0.8300 + 0.4012i)|0\rangle + (0.3018 + 0.2431i)|1\rangle,$$
$$\left|\phi_1^{(2)}\right\rangle = (0.4154 - 0.0392i)|0\rangle + (0.4756 + 0.7744i)|1\rangle,$$
$$\left|\phi_2^{(2)}\right\rangle = (-0.4667 + 0.1748i)|0\rangle + (0.4572 + 0.7366i)|1\rangle,$$
$$\left|\phi_3^{(2)}\right\rangle = (-0.8468 + 0.0287i)|0\rangle + (0.4920 - 0.2000i)|1\rangle,$$
$$\left|\phi_4^{(2)}\right\rangle = (0.8772 + 0.3003i)|0\rangle + (0.3719 + 0.0454i)|1\rangle.$$

When $R = 5$, we obtain a numerical decomposition of the mixed state $\rho_{\text{iso}}(\frac{1}{2})$,

$$\rho_{\text{iso}}\left(\frac{1}{2}\right) = \sum_{i=1}^{5} p_i \left|\phi_i^{(1)}\phi_i^{(2)}\right\rangle\!\left\langle\phi_i^{(1)}\phi_i^{(2)}\right|,$$

where $p = [0.2341, 0.1913, 0.1261, 0.2001, 0.2484]^\top$,

$$\left|\phi_1^{(1)}\right\rangle = (-0.3447 - 0.6169i)|0\rangle + (-0.6910 + 0.1523i)|1\rangle$$
$$\left|\phi_2^{(1)}\right\rangle = (0.4555 + 0.2936i)|0\rangle + (0.4211 + 0.7274i)|1\rangle,$$
$$\left|\phi_3^{(1)}\right\rangle = (-0.5163 - 0.6940i)|0\rangle + (0.2530 - 0.4334i)|1\rangle,$$
$$\left|\phi_4^{(1)}\right\rangle = (-0.9552 - 0.2044i)|0\rangle + (0.2129 + 0.0235i)|1\rangle,$$
$$\left|\phi_5^{(1)}\right\rangle = (-0.2195 - 0.3457i)|0\rangle + (0.6273 + 0.6624i)|1\rangle,$$
$$\left|\phi_1^{(2)}\right\rangle = (-0.7050 - 0.0394i)|0\rangle + (-0.1768 - 0.6857i)|1\rangle,$$
$$\left|\phi_2^{(2)}\right\rangle = (-0.3454 - 0.4211i)|0\rangle + (-0.7570 - 0.3610i)|1\rangle,$$
$$\left|\phi_3^{(2)}\right\rangle = (-0.8284 - 0.2190i)|0\rangle + (-0.3036 + 0.4167i)|1\rangle,$$
$$\left|\phi_4^{(2)}\right\rangle = (-0.9453 + 0.2424i)|0\rangle + (0.2147 - 0.0405i)|1\rangle,$$
$$\left|\phi_5^{(2)}\right\rangle = (-0.0286 + 0.4170i)|0\rangle + (0.2502 - 0.8733i)|1\rangle.$$

When $R = 6$, we obtain a numerical decomposition of the mixed state $\rho_{\text{iso}}(\frac{1}{2})$,

$$\rho_{\text{iso}}\left(\frac{1}{2}\right) = \sum_{i=1}^{6} p_i \left|\phi_i^{(1)}\phi_i^{(2)}\right\rangle\!\left\langle\phi_i^{(1)}\phi_i^{(2)}\right|,$$

where $p = [0.0272, 0.2472, 0.2471, 0.2294, 0.2373, 0.0119]^\top$,

$$\left|\phi_1^{(1)}\right\rangle = (-0.5647 + 0.2368i)|0\rangle + (-0.2667 - 0.7443i)|1\rangle,$$
$$\left|\phi_2^{(1)}\right\rangle = (-0.0991 + 0.9275i)|0\rangle + (0.3361 - 0.1302i)|1\rangle,$$
$$\left|\phi_3^{(1)}\right\rangle = (-0.3606 - 0.4593i)|0\rangle + (-0.6972 - 0.4159i)|1\rangle,$$
$$\left|\phi_4^{(1)}\right\rangle = (0.5201 - 0.6481i)|0\rangle + (0.4670 + 0.3023i)|1\rangle,$$
$$\left|\phi_5^{(1)}\right\rangle = (-0.3565 + 0.0752i)|0\rangle + (0.9119 - 0.1889i)|1\rangle,$$
$$\left|\phi_6^{(1)}\right\rangle = (-0.0869 + 0.2033i)|0\rangle + (0.9716 + 0.0849i)|1\rangle,$$
$$\left|\phi_1^{(2)}\right\rangle = (-0.0774 - 0.6082i)|0\rangle + (-0.7744 + 0.1564i)|1\rangle,$$
$$\left|\phi_2^{(2)}\right\rangle = (-0.7068 + 0.6067i)|0\rangle + (-0.0687 - 0.3572i)|1\rangle,$$
$$\left|\phi_3^{(2)}\right\rangle = (-0.4143 - 0.4051i)|0\rangle + (-0.3601 - 0.7311i)|1\rangle,$$
$$\left|\phi_4^{(2)}\right\rangle = (0.0781 + 0.8307i)|0\rangle + (0.5507 + 0.0227i)|1\rangle,$$
$$\left|\phi_5^{(2)}\right\rangle = (0.0387 - 0.3651i)|0\rangle + (-0.0571 + 0.9284i)|1\rangle,$$
$$\left|\phi_6^{(2)}\right\rangle = (-0.1981 - 0.1241i)|0\rangle + (0.7232 - 0.6499i)|1\rangle.$$

[1] E. Schrödinger, Die gegenwärtige Situation in der Quantenmechanik, Naturwissenschaften **23**, 823 (1935).

[2] A. Einstein, B. Podolsky, and N. Rosen, Can quantum-mechanical description of physical reality be considered complete? Phys. Rev. **47**, 777 (1935).

[3] A. Vesperini, G. Bel-Hadj-Aissa, and R. Franzosi, Entanglement and quantum correlation measures for quantum multipartite mixed states, Sci. Rep. **13**, 2852 (2023).

[4] O. Gühne, Characterizing entanglement via uncertainty relations, Phys. Rev. Lett. **92**, 117903 (2004).

[5] Y. Li and G. Ni, Separability discrimination and decomposition of m-partite quantum mixed states, Phys. Rev. A **102**, 012402 (2020).

[6] L. Gurvits, Classical deterministic complexity of edmonds' problem and quantum entanglement, in *Annual ACM Symposium on Theory of Computing* (ACM Press, New York, 2003).

[7] S. Gharibian, Strong NP-hardness of the quantum separability problem, Quantum Inf. Comput. **10**, 343 (2010).

[8] S. Halder and U. Sen, Separability and entanglement in superpositions of quantum states, Phys. Rev. A **107**, 022413 (2023).

[9] M. Horodecki, P. Horodecki, and R. Horodecki, Separability of mixed states: necessary and sufficient conditions, Phys. Lett. A **223**, 1 (1996).

[10] A. Peres, Separability criterion for density matrices, Phys. Rev. Lett. **77**, 1413 (1996).

[11] G. Vidal and R. F. Werner, Computable measure of entanglement, Phys. Rev. A **65**, 032314 (2002).

[12] M. Lewenstein, B. Kraus, J. I. Cirac, and P. Horodecki, Optimization of entanglement witnesses, Phys. Rev. A **62**, 052310 (2000).

[13] O. Gühne, P. Hyllus, O. Gittsovich, and J. Eisert, Covariance matrices and the separability problem, Phys. Rev. Lett. **99**, 130504 (2007).

[14] G. Ni, Hermitian tensor and quantum mixed state, arXiv:1902.02640.

[15] G. Ni, L. Qi, and M. Bai, Geometric measure of entanglement and U-eigenvalues of tensors, SIAM J. Matrix Anal. Appl. **35**, 73 (2014).

[16] G. Ni, Y. Li, and M. Zhang, *Complex Tensor Optimization and its Application in Quantum Information*, 1st ed. (Science Press, Beijing, 2022).

[17] T.-C. Wei and P. M. Goldbart, Geometric measure of entanglement and applications to bipartite and multipartite quantum states, Phys. Rev. A **68**, 042307 (2003).

[18] Y. Bo, L. Ying, N. Guyan, and Z. Mengshi, Rank-*R* positive Hermitian approximation algorithms and positive Hermitian decompositions of Hermitian tensors (in Chinese), Sci. Sin. Math. **53**, 1125 (2023).

[19] G. Ni and B. Yang, Symmetric Hermitian decomposability criterion, decomposition, and its applications, Front. Math. China **17**, 961 (2022).

[20] S. Hu, L. Qi, Y. Song, and G. Zhang, Geometric measure of quantum entanglement for Multipartite Mixed States, Int. J. Softw. Inf. **8**, 317 (2014).

[21] H. Zhao, Y. Liu, N. Jing, and Z. Wang, Detection of genuine entanglement for multipartite quantum states, Quantum Inf. Process. **21**, 315 (2022).

[22] A. Streltsov, H. Kampermann, and D. Bruß, Simple algorithm for computing the geometric measure of entanglement, Phys. Rev. A **84**, 022323 (2011).

[23] Z. Zhang, Y. Dai, Y.-L. Dong, and C. Zhang, Numerical and analytical results for geometric measure of coherence and geometric measure of entanglement, Sci. Rep. **10**, 12122 (2020).

[24] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevA.108.052217 for the program code for Algorithm 4.1, used to calculate from Example 5.1 to Example 5.6.