Quantum states are the key mathematical objects in quantum mechanics [1], and entanglement lies at the heart of the nascent fields of quantum information processing and computation [2]. What determines whether an arbitrary quantum state is entangled or separable is therefore very important for investigating both fundamental physics and practical applications. Here we show that an arbitrary bipartite state can be divided into a unique purely entangled structure and a unique purely separable structure. We show that whether a quantum state is entangled or not is determined by the ratio of its weight of the purely entangled structure and its weight of the purely separable structure. We provide a general algorithm for the purely entangled structure and the purely separable structure, and a general algorithm for the best separable approximation (BSA) decomposition, that has been a long-standing open problem. Our result implies that quantum states exist as families in theory, and that the entanglement (separability) of family members can be determined by referring to a crucial member of the family.

Quantum entanglement almost fantastically accompanied the emergence of quantum mechanics. Since Einstein, Podolsky, and Rosen (EPR) initially wondered about the “spooky action at a distance” feature of entanglement, they posed the famous EPR pair [3]. A decade after Albert Einstein’s death, experiments confirmed this [4]. In 1989 Werner mathematically formulated the definition of separability, a notion that was to be the direct opposite of entanglement [5]. A quantum state in a composite system is called separable if it can be mathematically written as a convex combination of product states, and entangled otherwise. This definition provides an (external) boundary between entangled states and separable states. Here we reveal an internal boundary between entanglement and separability within an arbitrary bipartite quantum state.

Lewenstein and Sanpera investigated the internal structure and composition of a quantum state in 1998 [6]. They showed that an arbitrary quantum state $\rho$ can always be written in a form as $\rho = \lambda \rho_{\text{BSA}} + (1 - \lambda) \rho_{\text{OptPPT}}$, where $\rho_{\text{BSA}}$ is a separable state and the weight $\lambda$ of the separable part is maximal. Later, the form was proven to be unique [7, 8]. The separable state $\rho_{\text{BSA}}$ is called the BSA of $\rho$, and the convex decomposition is called the BSA decomposition (also called Lewenstein-Sanpera decomposition). Recently, Wang showed a framework where entangled states play the role of high-level witnesses [8, 9]. Instead of using a numerical value [10], Wang characterized the entanglement of an entangled state $\rho$ using a set of entanglement witnesses for detecting the entangled state $D_\rho = \{W | \text{tr}(W \rho) < 0\}$, where $W$ is the entanglement witness of $\rho$. Given two entangled states $\rho_1$ and $\rho_2$, it was said that $\rho_2$ is finer (more entangled) than $\rho_1$ if, and only if, all entanglement witnesses detecting $\rho_1$ can also detect $\rho_2$. It is determined that $\rho$ is optimal if there is no other entangled state which is finer. It was showed that the optimal entangled state just corresponds to the remainder of the BSA of a density matrix [8].

Here we show that an arbitrary bipartite quantum state can be divided into a purely entangled structure and a purely separable structure. It is determined by the ratio of the purely entangled structure and the purely separable structure whether a quantum state is entangled or separable. This ratio also determines whether the quantum state $\rho$ is a positive partial transposition (PPT) state or not a PPT state. We provide a general algorithm to obtain its purely entangled structure and its purely separable structure for an arbitrary quantum state. Furthermore, we provide a general algorithm to determine the BSA decomposition for an arbitrary quantum state, that has been a long-standing open problem, as well as best PPT approximation decomposition for an arbitrary entangled state in any finite-dimensional bipartite system.

The purely entangled structure and the purely separable structure of a quantum state. — Since the optimal entangled state doesn’t include any separable state, here we call it the purely entangled structure of a quantum state or, we call it the purely entangled state if we cannot subtract any projector onto a product vector from itself. Given a separable state (higher-level witness [8]) $\sigma$, define $D_\sigma = \{\Theta | \text{tr}(\Theta \sigma) < 0, \Theta = \Theta^\dagger\}$; that is the set of operators “witnessed” by $\sigma$. For our purpose, we restrict the not-block-positive Hermitian operator $\Theta$ in the “generally-normalized” scope with $-I \leq \Theta \leq I$ and the operator norm $\|\Theta\|_\infty = 1$, where $I$ is the identity matrix. Given two separable states, $\sigma_1$ and $\sigma_2$, we say that $\sigma_2$ is finer (more separable) than $\sigma_1$, if $D_{\sigma_1} \subseteq D_{\sigma_2}$; that is, if all the operators “witnessed” by $\sigma_1$, are also “witnessed” by $\sigma_2$. We say that $\sigma$ is an optimal separable state if there exists no other separable state which is finer. Following the definition above, unfortunately, the only way that $\sigma_2$ is finer than $\sigma_1$ is that they are exactly the same.
state. To make this partial order well-defined, we need to employ the entangled state.

**Lemma 1.** \( \sigma_2 \) is finer (more separable) than \( \sigma_1 \) if and only if there exists \( 1 > \epsilon > 0 \) such that \( \sigma_1 = (1 - \epsilon) \sigma_2 + \epsilon \Omega \), where \( \Omega \geq 0 \) is not finer than \( \sigma_1 \) or \( \Omega \) is a “negative separable state” such that \( \text{tr}(\Omega \Theta) \geq 0 \) with \( \text{tr}(\Theta \sigma_1) < 0 \) for all \( \Theta = \Theta^\dagger \).

**Corollary 1.** \( \sigma \) is optimal if and only if it does not exist a legitimate separable state \( \sigma' = (1 + \epsilon) \sigma - \epsilon \Omega \) being finer than \( \sigma \) for any \( \epsilon > 0 \) and \( \Omega \geq 0 \) with \( \text{tr}(\Omega \Theta) \geq 0 \) and \( \text{tr}(\Theta \sigma) < 0 \) for all \( \Theta = \Theta^\dagger \).

**Lemma 2.** If \( \{ |\psi_i\rangle \} \) is an orthogonal (partially or completely) product basis (PB) [11], \( \sigma = \sum_i p_i |\psi_i\rangle \langle \psi_i| \) \((p_i > 0)\) is an optimal separable state.

We attach the properties and characterization and their proofs in the Supplemental Materials. We can easily conclude that the maximally mixed state is an optimal separable state by Corollary 2.

The previous result tells us that a separable state is optimal when we subtract any operator from it, the resulting operator is not finer than the separable state any more. To compare the optimization of entangled states [8] and the optimization of entanglement witnesses [12], the optimization of separable states should subtract the block operator. Both of them were shown that an entanglement witness can be written as a pseudo-mixture of local projectors (product states) [13], and that an entangled state can be represented by negative quasi-probabilities of product states [14]. To subtract the “negative separable state” and to keep the positivity of the resulting operator, one can only subtract the entangled state by Lemma 1. Exactly, the entangled state excluding any separable state, namely the purely (optimal) entangled state should be subtracted. However, it is still not practical. The weight of the purely entangled state cannot easily be known because it is not the maximum number to keep the positivity of the resulting operator even if the subtracted purely entangled state is known. Fortunately, we have an algorithm to obtain its optimal separable state and its purely (optimal) entangled state for an arbitrary state.

To be consistent with this concept purely entangled state, we call the optimal separable state, the purely separable structure of a quantum state or the purely separable state. Note that different from the purely (optimal) entangled state, the resulting operator may be a quantum state if we subtract a purely (optimal) entangled state from a purely (optimal) separable state, but there exists no finer (more separable) relation between the original purely (optimal) separable state and the resulting state.

Before we proceed, we need a Lemma.

**Lemma 2 [8].** There exists an (common) entanglement witness \( W \) detected by an entangled state \( \rho_1 \) and an entangled state \( \rho_2 \) if and only if for any \( k \in [0, 1] \),

\[
\rho = k \rho_1 + (1 - k) \rho_2
\]

is an entangled state.

**Corollary 3.** For an orthogonal (partially or completely) entangled basis \( \{ |\psi_i\rangle \} \), if the convex mixture \( \rho = \sum_{i=1}^m k_i |\psi_i\rangle \langle \psi_i| \) is separable for any \( k_i > 0 \), and

\[
\sum_{i=1}^m k_i = 1, \quad \rho \text{ is (separable) optimal.}
\]

**Proof.** Without loss of generality, suppose \( m \) equals 2. By Lemma 2, there exist a \( k > 0 \) such that \( \rho_k = k |\psi_1\rangle \langle \psi_1| + (1 - k) |\psi_2\rangle \langle \psi_2| \) is separable.

Suppose \( k_0 \) is the minimum number such that \( \rho_{k_0} = k_0 |\psi_1\rangle \langle \psi_1| + (1 - k_0) |\psi_2\rangle \langle \psi_2| \) is separable. If it is not optimal, there exists at least an optimal entangled state \( \Theta \) such that \( \text{tr}(\rho_{k_0} |\psi_1\rangle \langle \psi_1| + (1 - k_0) |\psi_2\rangle \langle \psi_2| - c \Omega \Theta) < 0 \) for all \( \Theta = \Theta^\dagger \). Therefore, \( \text{tr}(\rho_\Theta) > 0 \).

Without loss of generality, suppose \( \Theta = t_1 \rho_0 + t_2 T_1 \), where \( T_1 \) is a non-negative operator (normalized state) and \( T_1 \) is contained in \( \{ \rho_{k_0} \} \). By \( \text{tr}(\rho_{k_0} \Theta) < 0, t_1 < 0 \). Suppose \( \Omega = q_1 \rho_{k_0} + q_2 T_2 \). Clearly, \( q_1 > 0 \) and \( q_2 < 0 \). So \( \rho \) is not positive or it is entangled. Therefore, \( \rho_{k_0} \) is optimal.

**Algorithm 1.** A general method for the purely entangled state and the purely separable state

(i) Split the eigen-ensemble [13] of \( \rho \) into two parts, the entangled eigenvectors (marked as \( \{ |\psi_i^E\rangle \} \), with eigenvalues \( \{ \lambda_i^E \} \)) and the separable eigenvectors (marked as \( \{ |\psi_i^S\rangle \} \), with eigenvalues \( \{ \lambda_i^S \} \)).

(ii) If there exists at least one common entanglement witness for all entangled eigenvectors, the (unnormalized) purely entangled state of \( \rho \), \( \rho^E \), is the purely entangled part of the state \( \rho \), \( \rho^E = \sum_i \lambda_i^E |\psi_i^E\rangle \langle \psi_i^E| \) and the (unnormalized) purely separable state of \( \rho \), \( \rho^S \), is \( \sum_i \lambda_i^S |\psi_i^S\rangle \langle \psi_i^S| \).

(iii) Divide all the entangled eigenvectors into subsets, each containing all entangled eigenvectors without any common entanglement witness (some subsets probably contain only one entangled eigenvector). Note that there exists at least one common entanglement witness for the eigenvectors in different subsets.

(iv) Split each subset into the purely entangled part and the purely separable part according to Corollary 3.

Without loss of generality, suppose there are two (normalized) eigenvectors \( |\psi_1^E\rangle, |\psi_2^E\rangle \) with eigenvalues \( \lambda_1^E, \lambda_2^E \), respectively in certain a subset. Suppose \( t_0 \) is the minimum number such that \( \rho_{t_0} = t_0 |\psi_1^E\rangle \langle \psi_1^E| + (1 - t_0) |\psi_2^E\rangle \langle \psi_2^E| \) is separable. If \( \lambda_1^E > t_0 \lambda_2^E \), \( \{ \lambda_1^E |\psi_1^E\rangle \langle \psi_1^E| + \lambda_2^E |\psi_2^E\rangle \langle \psi_2^E| \} \) is the purely separable part of the subset, else if \( \lambda_1^E < t_0 \lambda_2^E \), \( \{ \lambda_1^E |\psi_1^E\rangle \langle \psi_1^E| + \lambda_2^E |\psi_2^E\rangle \langle \psi_2^E| \} \) is the purely separable part of the subset, else if \( \lambda_1^E \leq t_0 \lambda_2^E \), \( \{ \lambda_1^E |\psi_1^E\rangle \langle \psi_1^E| + \lambda_2^E |\psi_2^E\rangle \langle \psi_2^E| \} \) is the purely separable part of the subset.

(v) Mix all the purely entangled parts of all subset into a mixture. The mixture just denotes the purely entangled part of the state \( \rho \). Mix all the purely separable parts of all subset and all separable eigenvectors in Step 1 into the purely separable part of the state \( \rho \).

Note that it is not easy for Step (iv) in Algorithm 1. It is the procedure that, by “consuming” entangled ensembles without any common entanglement witness,
produces purely separable states and leaves the entangled eigen-ensembles being purely entangled states which cannot “counteract” each other’s entanglement into separability. Note that if the eigenvalues of a density matrix are degenerate, its spectral decomposition is not unique. However, the eigenspace of degenerate eigenvalues is unique. Therefore, the result of Algorithm 1 is unique (see also Theorem 1 below).

To illustrate the algorithm, consider the Werner state. The spectral decomposition for $\rho_p$ in Eq. (7) reads

$$
\rho_p = \frac{1-p}{4} |\psi_0\rangle\langle \psi_0 | + \frac{1-p}{4} |\psi_1\rangle\langle \psi_1 |
+ \frac{1-p}{4} |\psi_2\rangle\langle \psi_2 | + \frac{1+3p}{4} |\psi_3\rangle\langle \psi_3 |,
$$

(1)

where $|\psi_0\rangle = |00\rangle$ and $|\psi_1\rangle = |01\rangle$ are separable, while $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$ and $|\psi_3\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ are entangled. However, $|\psi_2\rangle$ and $|\psi_3\rangle$ do not have any common entanglement witness since $1 \cdot |\psi_2\rangle\langle \psi_2 | + 1 \cdot |\psi_3\rangle\langle \psi_3 | = |00\rangle \otimes |00\rangle + |11\rangle \otimes |11\rangle$ is separable. The latter half of the Eq. (1) on the right, $\frac{1-p}{4} |\psi_2\rangle\langle \psi_2 | + \frac{1}{4} |\psi_3\rangle\langle \psi_3 |$, can be decomposed into $(\frac{1-p}{4} |\psi_2\rangle\langle \psi_2 | + \frac{1}{4} |\psi_3\rangle\langle \psi_3 | = \frac{1-p}{4} (|00\rangle \langle 00 | + |11\rangle \langle 11 |))$ (the purely separable) + $p|\psi_3\rangle\langle \psi_3 |$ (the purely entangled).

Thus, Eq. (1) can be decomposed into

$$
\rho_p = \frac{1-p}{4} |\psi_0\rangle\langle \psi_0 | + \frac{1-p}{4} |\psi_1\rangle\langle \psi_1 |
+ \frac{1-p}{4} |\psi_2\rangle\langle \psi_2 | + \frac{1}{4} |\psi_3\rangle\langle \psi_3 | + p|\psi_3\rangle\langle \psi_3 |.
$$

(2)

where $\frac{1}{4}$ is the purely separable state with the weight $1-p$ and $|\psi_3\rangle\langle \psi_3 | \equiv |\psi^+\rangle\langle \psi^- |$ is the purely entangled with the weight $p$.

Generally, the orthogonal product basis is not unique for an optimal (purely) separable state. For example, the maximally mixed qubit state $\frac{1}{4}(|00\rangle \langle 00 | + |01\rangle \langle 01 | + |10\rangle \langle 10 | + |11\rangle \langle 11 |)$ can be decomposed into $\frac{1}{2}(|00\rangle \langle 00 | + |11\rangle \langle 11 |)$, $\frac{1}{2}(|00\rangle \langle 01 | + |01\rangle \langle 10 |)$, and $\frac{1}{2}(|10\rangle \langle 01 | + |11\rangle \langle 10 |)$ constitute an orthogonal product basis. Surprisingly, both the purely entangled part and the purely separable part are unique for an arbitrary bipartite quantum state.

**Theorem 1.** An arbitrary bipartite density matrix $\rho$ has a unique **general** decomposition in the form

$$
\rho = \Lambda \rho^{PS} + (1 - \Lambda) \rho^{PE}; \Lambda \in [0, 1],
$$

(3)

where (normalized) $\rho^{PS}$ denotes the purely separable state of $\rho$ and (normalized) $\rho^{PE}$ denotes the purely entangled state of $\rho$.

**Proof.**— Case (i): $\rho$ is separable. By Lemma 1 and Corollary 1, $\rho = \Lambda \rho^{PS} + (1 - \Lambda) \Omega$, where $\Omega \geq 0$ is a “negative separable state” (an entangled state) such that $tr(\Omega) \geq 0$ with $tr(\Theta \sigma_i) < 0$ for all $\Theta = \Theta^\dagger$. If $\rho$ is purely separable, $\Lambda$ equals to 1. Without loss of generality, suppose $\Lambda$ denotes the maximum weight $[7, 8]$ such that $\Omega$ is positive. Suppose $\Omega$ is not optimal (purely entangled). There exists at least a product state $P$ and a nonnegative number $t > 0$, such that $\rho = \Omega - tP \geq 0$ by Ref. [8]. By Lemma 1, (normalized) $\sigma = \frac{1}{\sqrt{\lambda}} (\Lambda \rho^{PS} + tP)$ is finer than $\rho$. Since $\rho^{PS}$ is the optimal separable state of $\rho$, $\rho^{PS}$ is finer than $\sigma = \frac{1}{\sqrt{\lambda}} (\rho^{PS} + tP)$. By Corollary 1, there does not exist any $\Theta' \in \mathbb{H}_{AB}$ such that $tr(\sigma \Theta') < 0$ with $tr(\rho^{PS} \Theta') > 0$, and there must exist at least one $\Theta$ to satisfy $tr(\Theta \rho^{PS}) < 0$ and $tr(\Theta \sigma) \geq 0$. We can obtain $tr(\Theta \sigma) > 0$, and $tr((\Theta + (1 - r)P)P) \geq 0$ for any $0 \leq r \leq 1$. Let $\Theta_r = -(r \Theta + (1 - r)P)$. There must exist a $r_0$ such that $tr(\Theta_r, \rho^{PS}) < 0$ with $tr(\Theta_r, \rho^{PS}) \geq 0$. It is impossible because $\rho^{PS}$ is optimal.

Case (ii): $\rho$ is entangled. By the BSA decomposition [7, 8], $\rho = \Lambda \rho^{BSA} + (1 - \Lambda) \rho^{PE}$, where $\Lambda$ denotes the maximal number such that $\rho^{BSA}$ is separable. By case (i), $\rho^{BSA} = \Lambda (\rho^{PSA})^{PS} + (1 - \Lambda) (\rho^{BSA})^{PE}$ since $\rho^{BSA}$ is separable. Therefore, $\rho = \Lambda \Lambda (\rho^{BSA})^{PS} + \Lambda (1 - \Lambda) (\rho^{PSA})^{PE} + (1 - \Lambda) \rho^{PE}$. We can conclude that $\Lambda (1 - \Lambda) (\rho^{BSA})^{PE} + (1 - \Lambda) \rho^{PE}$ must be an optimal (purely) unnormalized entangled state, otherwise $(1 - \Lambda) \rho^{PE}$ can be “consumed” and $\Lambda$ is not the maximal number such that $\rho^{BSA}$ is separable. That is, despite the case the mixture of two different optimal (purely) entangled states might not be an optimal (purely) entangled state, it is not the case here. By the uniqueness of the optimal (purely) entangled state of an entangled state [8], $\rho^{PE} = (\rho^{BSA})^{PE}$.

By Case (i) and Case (ii), we can draw our conclusion. □

**Remark 1.** The set of bipartite quantum states is composed of disjoint families. Each family contains a single purely entangled state and a single purely separable state, and the other members of the family are obtained by mixing this purely entangled state with the purely separable state, as shown in Fig. 1.

This result means that bipartite quantum states can be classified into purely entangled states, purely separable states, and their convex mixtures.

**What determines whether an arbitrary quantum state is entangled or separable.**— Generally, it is very difficult to calculate the exact BSA decomposition for an arbitrary entangled state. Despite the fact that methods for the BSA decomposition in $\mathbb{C}^2 \otimes \mathbb{C}^2$ were provided [16], how to calculate the BSA in high-dimension systems still remains open.

Consider the family (convex mixture) of the purely entangled state $\rho^{PE}$ of $\rho$ and the purely separable state $\rho^{PS}$ of $\rho$.

$$
\rho_t = t \rho^{PE} + (1 - t) \rho^{PS}
$$

(4)

with the weight $t$ varying from 0 to 1.

**Lemma 3.** An arbitrary entangled state $\rho$ has the
BSA decomposition

\[ \rho = \Lambda \rho^{PE} + (1 - \Lambda) \rho^{BSA}, \]

(5)

where the BSA of \( \rho \), \( \rho^{BSA} = \frac{\Lambda - \Lambda^2}{1 - \Lambda} \rho^{PE} + \frac{1 - \Lambda}{1 - \Lambda} \rho^{PS} \) and \( \Lambda \) is the threshold (the minimum real number) such that \( \rho^{BSA} \) is separable.

**Proof.** — By theorem 1, an arbitrary entangled state \( \rho \) has the unique general decomposition

\[ \rho = \Lambda \rho^{PE} + (1 - \Lambda) \rho^{PS}; \Lambda \in [0, 1]. \]

(6)

By Ref. [9], \( \rho^{PE} \) is just the remainder of the BSA decomposition of \( \rho \). It is clear that \( \rho^{BSA} \) is separable because \( \Lambda \) is the threshold to which \( \rho_\Lambda = \Lambda \rho^{PE} + (1 - \Lambda) \rho^{PS} \) is just separable with \( \Lambda \) increasing from 0. If we subtract any projector onto a product vector after we subtract \( (1 - \Lambda) \rho^{BSA} \) from \( \rho \), then the resulting operator is no longer an entangled state. By the Lemma 1 in Ref. [17], any product vector in the decomposition of separability on \( \rho^{BSA} \) must belong to the range of \( \rho \). By the uniqueness of the BSA decomposition [7, 9], we know Eq. (5) is the BSA decomposition of \( \rho \). \( \Box \)

**Remark 2.** The mixed member of the purely entangled state and the purely separable state will be entangled when the ratio of their weights goes beyond a threshold, while the mixed member will be separable when the ratio within the threshold, as shown in Fig. 1.

![Diagram showing quantum states classification](image)

FIG. 1. (Color online) Quantum states are classified into purely entangled states, purely separable states, and their convex mixtures. The boundary between separable states and entangled states is marked as “∂”. And the boundary between PPT states and NPPT states is marked as “□”.

To illustrate this result, we sketch the proof (calculation) of the threshold \( p = \frac{1}{3} \) for the Werner state

\[ \rho_p = p|\psi^+\rangle\langle\psi^+| + (1-p)\frac{I}{4}, \]

(7)

where \( |\psi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \) and \( 0 \leq p \leq 1 \) [5].

**Proof (Calculation).** — Let \( \sigma_2 \equiv \frac{1}{4}, \sigma_1 \equiv \rho_p, \) and \( \Omega \equiv |\psi^+\rangle\langle\psi^+| \). By Lemma 1, \( tr(\rho_p \Theta) = p|\psi^+\rangle\langle\psi^+|\Theta|\psi^+\rangle + (1-p)tr(\Theta) < 0 \) and \( tr(|\psi^+\rangle\langle\psi^+|\Theta) \geq 0 \). Therefore, \( tr(\Theta) < 0 \). Without loss of generality, suppose \( \Theta = t|\psi^+\rangle\langle\psi^+| + (-t - \epsilon)T, \) where \( T \in \{|\psi^+\rangle\langle\psi^+|\} \) and \( \{|\psi^+\rangle\langle\psi^+|\} \) denotes the (orthogonal) complementary subspace of \( \{|\psi^+\rangle\langle\psi^+|\} \). We can obtain \( t > 0 \) and \( \epsilon > 0 \) since \( tr(\Theta) < 0 \).

Thus, \( tr(\rho_p \Theta) = pt + \frac{1}{4}(-t - \epsilon) - \frac{1}{4}t < 0 \) for any \( t > 0 \) and \( \epsilon > 0 \). Therefore, \( \frac{4p}{4} - \frac{1}{4} \leq 0, \) and \( 1 \leq p \leq \frac{1}{3} \). In other words, \( \frac{1}{3} \) is finer (more separable) than \( p_0 \) for \( 0 \leq p \leq \frac{1}{3} \). \( \Box \)

Interestingly, if a single purely entangled state is mixed with a single purely separable state, usually the purely entangled state (the purely separable state) of the resulting state is not the original purely entangled state (the purely separable state). Consider mixing a purely entangled state \(|\psi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)\) with a purely separable state \(|\phi\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |11\rangle)\), \( \rho_m = \frac{1}{2}|\psi^+\rangle\langle\psi^+| + \frac{1}{2}|\phi\rangle\langle\phi|\). The purely entangled state of \( \rho_m \) reads \( \rho_m^{PE} = |\phi\rangle\langle\phi| \) with the weight \( \frac{3}{4} \) and the purely separable state of \( \rho_m \) reads \( \rho_m^{PS} = |\phi\rangle\langle\phi| \) with the weight \( \frac{1}{4} \), where \( \rho_m^{PE} = \frac{3}{2} \rho_m^{PS} + |\phi\rangle\langle\phi| \) and \( \rho_m^{PS} = \frac{2}{2} \rho_m^{PE} + |\phi\rangle\langle\phi| \).

Let \( \tau \) and \( \sigma \) be the quantum states acting on a bipartite system \( \mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d \). Vidal and Tarrach [18] defined the robustness of \( \tau \) relative to \( \sigma \), \( R(\tau|\sigma) \), to be the minimum nonnegative number \( t \) such that the state \( \rho = \frac{1}{1+t\tau} + \frac{t}{1+t\tau} \sigma \) is separable. By Lemma 3, we have the following result.

**Theorem 2.** An arbitrary bipartite density matrix \( \rho \) has the BSA decomposition

\[ \rho = \Lambda \rho^{PE} + (1 - \Lambda) \rho^{PS}, \]

(8)

if \( R(\rho^{PE} \parallel \rho^{PS}) \) is infinite, otherwise it has the BSA decomposition

\[ \rho = \Lambda \rho^{PE} + (1 - \Lambda) \rho^{BSA}, \Lambda \in [0, 1], \]

(9)

where \( \Lambda = \frac{\Lambda(1 + R(\rho^{PE} \parallel \rho^{PS})) - 1}{R(\rho^{PE} \parallel \rho^{PS}) + 1}, \rho^{BSA} = \frac{1 + R(\rho^{PE} \parallel \rho^{PS}) R(\rho^{PS} \parallel \rho^{PE})}{1 + R(\rho^{PE} \parallel \rho^{PS}) + 1 R(\rho^{PS} \parallel \rho^{PE})} \rho^{PS} \), and \( R(\rho^{PE} \parallel \rho^{PS}) \) denotes the robustness of \( \rho^{PE} \) relative to \( \rho^{PS} \) [18].

Therefore, to get the BSA of a quantum state, we can use results about the robustness of entanglement.

**Lemma 4 [19].** The random robustness of a pure entangled state \(|\psi\rangle\) acting on a bipartite system \( \mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d \),

\[ R_e(|\psi\rangle) = r_1 r_2 d_A d_B, \]

(10)

where \( |\psi\rangle = \sum_j r_j |j\rangle|j\rangle \) is the Schmidt decomposition of \(|\psi\rangle\) with \( r_1 \geq r_2 \geq \cdots \geq 0 \).

**Corollary 4.** For an arbitrary bipartite density matrix \( \rho = \Lambda |\psi\rangle\langle\psi| + (1 - \Lambda) \frac{I}{d_1d_2} \), the BSA of \( \rho \) is

\[ \rho^{BSA} = \Lambda |\psi\rangle\langle\psi| + (1 - \Lambda) \frac{I}{d_1d_2}, \]

(11)

where \(|\psi\rangle\langle\psi|\) is a pure (entangled) state, \( d_1d_2 \) is the dimension of the state space, and \( \Lambda = \frac{d_1d_2 r_1r_2}{d_1d_2 + r_1r_2} \).
We can get the exact BSA decomposition by the following steps.

**Algorithm 2** A general method for the BSA decomposition
(i) Obtain the purely entangled state and the purely separable state by Algorithm 1.
(ii) Calculate the threshold between the separable states and the entangled states and obtain the exact BSA decomposition by the robustness of the purely entangled state to the purely separable state for a given entangled state or by other separability criteria (such as, PPT criterion [20], the cross-norm or realignment (CCNR) criterion [21, 22], and so on).
(iii) Obtain the BSA decomposition.

What determines whether an entangled state is free or PPT.— Next, we consider the PPT boundary, as shown in Fig. 1 marked as “□”. We can define the best positive partial transposition approximation (BPPTA) [23, 24].

**Theorem 3.** An arbitrary (normalized) entangled density matrix $\rho$ has a unique decomposition in the form

$$\rho = \Lambda_B \rho^{PE} + (1 - \Lambda_B) \rho^{BPPTA}; \Lambda \in [0, 1],$$

where $\rho^{PE}$ denotes the purely entangled state of $\rho$, $\rho^{BPPTA}$ denotes the best positive partial transposition approximation (BPPTA) of the entangled density matrix, and $\Lambda_B$ is the threshold (the minimum real number) such that $\rho^{BPPTA}$ is entangled.

In analogy to the analysis of the BSA, we can describe the properties and characterization of the BPPTA. The BPPTA can naturally serve as a quantification of entanglement. We can easily conclude that the boundary between the positive partial transposition states and the NPPT (entangled) states overlaps with the threshold of the BPPTA. Moreover, the separable boundary and the PPT boundary, overlap in some cases. In particular, the two boundaries completely overlap in the case of low dimension (no positive partial transposition entangled state and no BPPTA). A fact worth mentioning is that PPT purely entangled states exist [9].

**Remark 3.** As the weight $t$ increases from 0 to 1 in Eq. (4), the quantum state $\rho_t$ changes. A quantitative change of the weight $t$ in the mixture produces a qualitative change of the resulting state. When the weight $t$ is beyond a threshold (denoted as $t_S$, marked as “o”, as shown in Fig. 1), the separability of the quantum state will change. When the weight $t$ from $t_S$ to 1 is beyond another threshold (denoted as $t_{PPT}$, marked as “□”, as shown in Fig. 1), the PPT property of $\rho_t$ will change.

We illustrate our results using the Horodecki states [25]. It is known that

$$\sigma_\alpha = \frac{2}{7} |\Psi_+\rangle \langle \Psi_+| + \frac{\alpha}{7} \sigma_+ + \frac{5 - \alpha}{7} \sigma_-,$$

are separable for $2 \leq \alpha \leq 3$, bound entangled for $3 < \alpha \leq 4$ and free entangled for $4 < \alpha \leq 5$, where $|\Psi_+\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle + |22\rangle), \sigma_+ = \frac{1}{2} (|01\rangle \langle 01| + |12\rangle \langle 12| + |20\rangle \langle 20|), \sigma_- = \frac{1}{2} (|01\rangle \langle 01| + |21\rangle \langle 21| + |10\rangle \langle 10| |20\rangle \langle 20|).$

Rewriting Eq. (13), we have

$$\sigma_\alpha = \frac{2}{7} P_{\Psi_+} + \frac{5}{7} \Omega_\alpha,$$

where $P_{\Psi_+} = |\Psi_+\rangle \langle \Psi_+|$ and $\Omega_\alpha = \frac{\alpha}{7} \sigma_+ + \frac{5 - \alpha}{7} \sigma_-$. It is clear that $P_{\Psi_+}$ is just the purely entangled state of $\sigma_\alpha$, and $\Omega_\alpha$ is the purely separable states of $\sigma_\alpha$.

**Figure 2.** (Color online) The Separable Boundary and the PPT Boundary in the Horodecki States Family.

Considering the family of the Horodecki states

$$\sigma_\alpha^t = t P_{\Psi_+} + (1 - t) \Omega_\alpha, t \in [0, 1],$$

we can compute the two boundaries at $t_{1,2}^\alpha = \frac{2 \alpha^2 - 10 \alpha + 25 + 5 \sqrt{4 \alpha^4 - 20 \alpha^2 + 25}}{2 (\alpha^2 - 5 \alpha + 25)}$ for $0 \leq \alpha \leq 5$ by realigning $\sigma_\alpha^t$ according to the CCNR [21, 22]. We can obtain the PPT boundary at $t = \frac{\alpha^2 - 5 \alpha + 5 \sqrt{\alpha (5 - \alpha)}}{\alpha^2 - 5 \alpha + 25}$ by positive partial transposing $\sigma_\alpha^t$ according to the PPT criterion [20]. Note that from the perspective of the purely entangled state, all states in Eq. (15) belong to the family of the purely entangled state $P_{\Psi_+}$, but from the perspective of the purely separable states, states in Eq. (15) belong to different families with the different purely separable states $\Omega_\alpha$ for different variables $\alpha$.

Letting $\alpha = 2.5$, the separable boundary overlaps with the PPT boundary, and both the BSA and the BPPTA of $\sigma_{2.5}^t$ are $\frac{1}{2} P_{\Psi_+} + \frac{3}{2} \Omega_{2.5}$ for all $t \geq \frac{4}{7}$. Letting $\alpha = 3$, $t_{1}^3 = \frac{2}{7}$ and $t_{2}^3 = \frac{3}{8}$, the BSA of $\sigma_3^t$ is just $\frac{2}{7} P_{\Psi_+} + \frac{5}{7} \Omega_3$ (one of the Horodecki states, as shown in Fig. 2) for $t \geq \frac{4}{7}$, and the BPPTA of $\sigma_3^t$ is $\frac{3}{8} P_{\Psi_+} + \frac{5}{8} \Omega_3$ for $t \geq \frac{3}{8}$. Letting $\alpha = 5$, $\sigma_5^t = t |\Psi_+\rangle \langle \Psi_+| + (1 - t) \sigma_+$, (16)
are both the BSA decomposition and the BPPTA decomposition of $\sigma_1$ because the robustness of $|\Psi_+\rangle\langle\Psi_+|$ relative to $\sigma_1$ is infinite. Fig. 2 illustrates the schematic picture.

Discussions and conclusions. — The internal structure of entanglement and separability can naturally be extended to the multiparty setting because the definition and characterization of $m$-partite (full) separability in terms of positive, but not completely positive, maps and witnesses were generalized in a natural way [26]. Thus, we can introduce the concept of $m$-partite (full) finer and purely (optimal) entangled states as well as $m$-partite (full) finer and purely (optimal) separable states. However, it is not a trivial extension of the internal structure of entanglement and separability of bipartite systems. As far as the simplest case where there are only three systems $A, B, C$, i.e., $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, there exist three categories of optimal product and bipartite entangled state $(A - BC, B - AC, C - AB)$. The classification, boundaries, thresholds in the multiparty setting are left for further study.

In this paper we mainly considered the case of discrete systems on the finite dimensional Hilbert space. Our results in infinite-dimensional systems might be significantly different from the case of the discrete systems because there is no separable neighbourhood of any mixed state in infinite-dimensional systems [27]. Our results in continuous variable systems also might be significantly different from the case of the discrete systems, because the precondition of the Hahn-Banach theorem continuous variable systems is different from the one in discrete systems [8, 28]. These systems have not been discussed here.

In summary, we showed that the separability (entanglement) of a quantum state is determined by the weight of its purely entangled state and the weight of its purely separable state, though the determination of an arbitrary quantum state entangled or not is a nondeterministic polynomial-time (NP) hard problem [29]. We provided a general algorithm to obtain the purely entangled state and the purely separable state of an arbitrary state. We also provided a general operational algorithm to calculate the BSA decomposition for any finite-dimensional bipartite quantum state. How to calculate the BSA in high-dimensional systems was previously an open question. We gave a state-of-the-art classification of all bipartite quantum states. Our results can be generalized to general convex resource theories [30] and the operator theory. Quantum entanglement was shown being at the centre of a new mathematical proof recently [31]. We expected that our findings will stimulate further investigation on the quantum theory and practical applications in other fields.

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Supplementary Information

A. Proofs of properties of separable states in the role of witnesses

We show the proofs of properties of separable states in the role of witnesses.

The following results and proofs follow from Ref. [1–3] with minor modification. Note the difference between the results and proofs and the ones in Ref. [1–3].

Lemma A1: Let σ2 be finer than σ1 and

\[ \delta = \inf_{\Theta_1 \in D_{\sigma_1}} \frac{\text{tr}(\Theta_1 \sigma_2)}{\text{tr}(\Theta_1 \sigma_1)} \]. \hspace{1cm} (17)

Then we have the following:

(i): If \( \text{tr}(\Theta \sigma_1) = 0 \), then \( \text{tr}(\Theta \sigma_2) \leq 0 \).

(ii): If \( \text{tr}(\Theta \sigma_1) < 0 \), then \( \text{tr}(\Theta \sigma_2) \leq \text{tr}(\Theta \sigma_1) \).

(iii): If \( \text{tr}(\Theta \sigma_1) > 0 \), then \( \delta \text{tr}(\Theta \sigma_1) \geq \text{tr}(\Theta \sigma_2) \).

(iv): \( \delta \geq 1 \). In particular, \( \delta = 1 \) iff \( \sigma_1 = \sigma_2 \).

Proof: Since \( \sigma_2 \) is finer than \( \sigma_1 \) we will use the fact that for all \( \Theta \not\in 0 \) such that \( \text{tr}(\Theta \sigma_1) < 0 \) then \( \text{tr}(\Theta \sigma_2) < 0 \).

(i) Let us assume that \( \text{tr}(\Theta \sigma_2) > 0 \). Then we take any \( \Theta_1 \in D_{\sigma_1} \), so that for all \( x \geq 0 \), \( \Theta(x) = \Theta_1 + x\Theta \in D_{\sigma_1} \). But for sufficiently large \( x \) we have that \( \text{tr}(\Theta_1 \sigma_2) > 0 \) is possible, which cannot be since then \( \Theta(x) \not\in D_{\sigma_2} \).

(ii) We define \( \tilde{\Theta} = \Theta + |\text{tr}(\Theta \sigma_1)|I \), where I is the identity matrix. We have that \( \text{tr}(\tilde{\Theta} \sigma_1) = 0 \). Using (i) we have that \( 0 \geq \text{tr}(\Theta_2 \sigma_2) + |\text{tr}(\Theta_1 \sigma_1)| \).

(iii) We take \( \Theta_1 \in D_{\sigma_1} \) and define \( \tilde{\Theta} = \text{tr}(\Theta_1 \sigma_1) \Theta_1 + |\text{tr}(\Theta_1 \sigma_1)| \Theta \), so that \( \text{tr}(\tilde{\Theta} \sigma_1) = 0 \). Using (i) we have \( |\text{tr}(\Theta_1 \sigma_1)| |\text{tr}(\Theta_2 \sigma_2) \leq |\text{tr}(\Theta_1 \sigma_2)\text{tr}(\Theta_1 \sigma_1) \text{tr}(\Theta_2 \sigma_1)\text{tr}(\Theta_1 \sigma_1) \text{tr}(\Theta_2 \sigma_1) | \). Dividing both sides by \( |\text{tr}(\Theta_1 \sigma_1)| > 0 \) and \( \text{tr}(\Theta_1 \sigma_1) > 0 \) we obtain

\[ \frac{\text{tr}(\Theta_2 \sigma_2)}{\text{tr}(\Theta_2 \sigma_1)} \leq \frac{\text{tr}(\Theta_1 \sigma_2)}{\text{tr}(\Theta_1 \sigma_1)} \]. \hspace{1cm} (18)

Taking the infimum with respect to \( \Theta_1 \in D_{\sigma_1} \) on the right hand side of this equation we obtain the desired result.

(iv) By (ii), it immediately follows that \( \delta \geq 1 \). The “only if” part is trivial. We prove that if \( \lambda = 1 \) then \( \sigma_1 = \sigma_2 \).

For any positive operator \( \Theta \), we have \( \text{tr}(\Theta \sigma_1) \geq 0 \).

Case (1): If \( \text{tr}(\Theta \sigma_1) = 0 \) then, by (i), \( \text{tr}(\Theta \sigma_2) = 0 \).

Case (2): If \( \text{tr}(\Theta \sigma_1) > 0 \), then by (iii)

\[ \text{tr}(\Theta \sigma_2) \leq \text{tr}(\Theta \sigma_1) \]. \hspace{1cm} (19)

Let \( \hat{\Theta} = -\Theta \). Then \( \text{tr}(\hat{\Theta} \sigma_1) < 0 \); by Lemma A1 (ii), we have

\[ \text{tr}(\Theta \sigma_2) \leq \text{tr}(\Theta \sigma_1) \]. \hspace{1cm} (20)

Hence

\[ \text{tr}(\Theta \sigma_2) \geq \text{tr}(\Theta \sigma_1) \]. \hspace{1cm} (21)

By Eq. (19) and Eq. (21), we have \( \text{tr}(\Theta \sigma_2) = \text{tr}(\Theta \sigma_1) \).

According to case (1) and (2), we have, for any positive operator \( \Theta \)

\[ \text{tr}(\Theta \sigma_1) = \text{tr}(\Theta \sigma_2) \]. \hspace{1cm} (22)

Hence \( \sigma_1 = \sigma_2 \). □

Corollary A1: \( D_{\sigma_1} = D_{\sigma_2} \), if and only if \( \sigma_1 = \sigma_2 \).

Proof: We prove the only if part. The if part is trivial. We define \( \delta \) as in Eq. (17) and define

\[ \tilde{\delta} = \inf_{\Theta_2 \in D_{\sigma_2}} \frac{\text{tr}(\Theta_2 \sigma_1)}{\text{tr}(\Theta_2 \sigma_2)} \]. \hspace{1cm} (23)

By Lemma A1 (iv), we have that \( \tilde{\delta} \geq 1 \) since \( \sigma_1 \) is finer than \( \sigma_2 \).

Equivalently, since \( \sigma_2 \) is finer than \( \sigma_1 \), we have
Lemma A1 (iv). Phys. Rev. A 1 separable state such that \(\|B-H.\) Wang, 20050302(R) (2018).

\[1 \geq \sup_{\theta_1 \in D_{\sigma_1}} \left| \frac{tr(\theta_1 \sigma_2)}{tr(\theta_1 \sigma_1)} \right| \geq \delta \geq 1. \] (24)

Therefore, we have \(\sigma_1 = \sigma_2\) since \(\delta = 1\) according to Lemma A1 (iv).

Lemma 1. \(\sigma_2\) is finer (more separable) than \(\sigma_1\) if and only if there exists \(1 > \epsilon \geq 0\) such that \(\sigma_1 = (1-\epsilon)\sigma_2 + \epsilon \Omega\), where \(\Omega > 0\) is not finer than \(\sigma_1\) or \(\Omega\) is a “negative separable state” such that \(tr(\Omega \Theta) \geq 0\) for all \((tr(\Theta \sigma_1)) < 0 \) and \(\Theta = \Theta^d\).

Proof: (If) For all \(\Theta \in D_{\sigma_1}\), we have that \(0 > tr(\Theta \sigma_1) = (1-\epsilon)tr(\Theta \sigma_2) + \epsilon tr(\Theta \Omega)\) which implies \(tr(\Theta \sigma_2) < 0\) and therefore \(\Theta \in D_{\sigma_2}\). (Only if) We define \(\delta\) as in Eq. (17). Using Lemma A1(iv) we have \(\delta \geq 1\). First, if \(\delta = 1\) then according to Lemma A1(iv) we have \(\sigma_1 = \sigma_2\) (i.e., \(\epsilon = 0\)).

For \(\delta > 1\), we define

\[\delta = \sup_{\theta_1 \in D_{\sigma_1}} \left| \frac{tr(\theta_1 \sigma_2)}{tr(\theta_1 \sigma_1)} \right| \geq 1. \] (25)

\(\Omega = (\delta - 1)^{-1}(\hat{\delta} \sigma_1 - \sigma_2)\) and \(\epsilon = 1 - 1/\delta > 0\). We have that \(\sigma_1 = (1-\epsilon)\sigma_2 + \epsilon \Omega\) and \(\hat{\delta} > 1\). We can easily know that \(\Omega\) is not finer than \(\sigma_1\) or \(\Omega\) is a “negative separable state” such that \(tr(\Omega \Theta) \geq 0\) with \(tr(\Theta \sigma_1) < 0\) for all \(\Theta\).

Next, we prove that \(\Omega\) is positive. For any \(\langle \psi \rangle, \langle \psi | \Omega | \psi \rangle = (\hat{\delta} - 1)^{-1}(\delta (\psi | \sigma_2 | \psi) - (\psi | \sigma_2 | \psi)).\) Let \(\Theta = -|\psi \rangle \langle \psi|= (\hat{\delta} - 1)^{-1}(\delta - 1)\left| \frac{tr(\sigma_2 \Theta)}{tr(\sigma_2 \sigma_1)} \right| (\hat{\delta} - 1)^{-1}(\hat{\delta} - 1)\left| \frac{tr(\sigma_2 \Theta)}{tr(\sigma_2 \sigma_1)} \right| \geq 0. \]

Corollary 1. \(\sigma\) is optimal if and only if it does not exist a legitimate separable state \(\sigma' = (1+\epsilon)\sigma - \Omega\) being finer than \(\sigma\) for any \(\epsilon > 0\) and \(\Omega \geq 0\) with \(tr(\Omega \Theta) \geq 0\) and \(tr(\Theta \sigma) < 0\) for all \(\Theta = \Theta^d\).

Proof: (If) According to Lemma 1, there is no separable state which is finer than \(\sigma\), and therefore \(\sigma\) is optimal. (Only if) If \(\sigma'\) is a separable state, then according to Lemma 1, \(\sigma\) is not optimal. □

Consider

\[q_a = \frac{1}{8a + 1} \left( \begin{array}{cccccc} a & 0 & 0 & 0 & 0 & 0 \\ 0 & a & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & 0 \\ 0 & 0 & 0 & 0 & a & 0 \\ 0 & 0 & 0 & 0 & 0 & a \end{array} \right) \] (26)

\[\text{where} 0 = a < \frac{1}{2} \] [17]. We can know that \(q_a\) was constructed from \(q_a = \frac{8a}{8a+1} \hat{q}_{\text{insep}} + P_{\phi_a}\), where \(|\phi_a\rangle = \frac{1}{\sqrt{2}}(|0\rangle + \sqrt{\frac{1-a}{a+1}} |1\rangle) \hat{q}_{\text{insep}} = \frac{1}{2} P_{\phi_a} + \frac{1}{2} Q,\) and \(Q = I - (\sum_{i=0}^{a-1} |i\rangle \langle i| \otimes |i\rangle \langle i| + |0\rangle \langle 0| \otimes |2\rangle \langle 2|).\)

Rewriting Eq. (26), we have

\[q_a = \frac{3a}{8a + 1} P_{\phi_a} + \frac{5a + 1}{8a + 1} Q_a, \] (27)

where \(Q_a = \frac{5a}{8a+1} + \frac{1}{8a+1} P_{\phi_a}\) is the purely separable part of \(q_a\). We can obtain the state of Eq. (26) family

\[q_a^t = t P_{\phi_a} + (1-t) Q_a, t \in [0, 1]. \] (28)