Universal methods for extending any entanglement witness from the bipartite to the multipartite case

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Any bipartite entanglement witness $W$ can be written as $W = c_\sigma I - \sigma$, where $\sigma$ is a quantum state, $I$ is the identity matrix, and $c_\sigma$ is a non-negative real number. We present a general method to extend the given entanglement witness to multipartite cases via purification, partial purification, and direct tensor of the quantum state $\sigma$. Our methods extend $\sigma$ but leave the parameter $c_\sigma$ untouched. This is very valuable since the parameter is generally not easy to compute.

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I. INTRODUCTION

It is well established that entanglement plays an essential role in many applications of quantum information science [1, 2]. The detection of entanglement has become one of the central problems in the field. The notion of an entanglement witness (in short, witness), which is formulated in terms of a positive, but not completely positive map via the Jamiołkowski-Choi isomorphism [3], is arguably the most powerful method for entanglement detection. An observable $W$ is a witness if it has non-negative expectation value for an arbitrary separable state; and it has at least one negative eigenvalue (see, e.g., [4]). A witness is said to be weakly optimal if its expectation value vanishes on at least one product state [5, 6].

There is substantial literature on the topic. Bipartite witnesses, i.e., witnesses for bipartite quantum systems, have been exhaustively studied in a number of works [4, 7–14]. However, multipartite witnesses for partial and genuine entanglement are more difficult to approach [15–19]. Of course, such witnesses are important because multipartite entanglement has been shown to be an essential resource in a variety of contexts, including applications in quantum computing [20], interferometry [21], and in metrological tasks [22]. We refer the reader to Ref. [23] for a recent and extensive review on entanglement witnesses.

In the present paper, we consider the general form of a witness, $W = c_\sigma I - \sigma$, where $c_\sigma$ is a non-negative real number, $I$ is the identity matrix, and $\sigma$ is a quantum state. Given $W$, we propose methods for purifying, partially purifying, or directly tensor the quantum state $\sigma$, and in this way extending the witness from the bipartite to the multipartite case. Our methods modify $\sigma$ but leave the parameter $c_\sigma$ unchanged. This is valuable since $c_\sigma$ is in general not easy to compute.

The remainder of the paper is organized as follows. In Section II, we introduce a general form of bipartite entanglement witnesses from density matrices of states. In Section III, we extend any witness in bipartite to witnesses in multipartite by purification and by partial purification. In Section IV, we show the extension by extending states to mixed states. Section V is a summary.

II. PRELIMINARIES

For our purposes, we can consider a finite dimensional composite Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$. Let $\sigma$ be a density matrix for such a system. The quantum state $\sigma$ is said to be separable if it can be written as

\begin{equation}
\sigma = \sum_k p_k |\psi^k_1\rangle \langle \psi^k_1| \otimes |\psi^k_2\rangle \langle \psi^k_2| \otimes \cdots \otimes |\psi^k_n\rangle \langle \psi^k_n|, \tag{1}
\end{equation}

where $p_k$ is a probability distribution and each $|\psi^k_i\rangle$ is a pure state of $\mathcal{H}_i$, for $i = 1, 2, \ldots, n$. If a quantum state $\rho$ cannot be written as the form of Eq. (1), it is referred to as multipartite entangled.

On the basis of this definition, a multipartite entanglement witness, $W \in \mathcal{H}$, is a Hermitian operator such that: (i) $\text{tr}(W \sigma) \geq 0$ for all separable states $\sigma$; (ii) $\text{tr}(W \rho) < 0$ for at least one state $\rho$.

Wang and Long [6, 24] showed that any (possibly unnormalized) bipartite witness $W \in \mathcal{H}_A \otimes \mathcal{H}_B$ can be written as

\begin{equation}
W = \rho - c_\rho I, \tag{2}
\end{equation}

where $\rho$ is a (separable) density matrix and

\begin{equation}
\lambda_{0\rho} < c_\rho \leq c_\rho^{\max} \tag{3}
\end{equation}

is a real number related to $\rho$. Here, $\lambda_{0\rho}$ is the smallest eigenvalue of $\rho$. The parameter $c_\rho^{\max}$ is the maximum $c_\rho$ for which $W$ is a witness, and it is given by

\begin{equation}
c_\rho^{\max} = \inf_{\|\mu_A\| = 1, \|\mu_B\| = 1} \langle \mu_A \mu_B | \rho | \mu_A \mu_B \rangle, \tag{4}
\end{equation}

where $| \mu_A \mu_B \rangle$ is any unit product state. A witness $W = \rho - c_\rho I$ is weakly optimal if and only if $c_\rho = c_\rho^{\max}$.

Remark 1. Let $W = \rho - c_\rho I$ be a witness such that $\rho$ has spectral decomposition $\rho = \sum_i \lambda_i |e_i\rangle \langle e_i|$, with
orthonormal basis \( \{ |e_1 \rangle, |e_2 \rangle, \ldots, |e_n \rangle \} \). We have one of the following two cases: (i) \( \rho \) has zero nullity; The basis spans \( \mathcal{H}_{AB} \) and \( |e_0 \rangle \) is an entangled state corresponding to the minimum eigenvalue \( \lambda_0 \neq 0 \); (ii) \( \rho \) has nonzero nullity. The complementary space of the basis is a completely entangled subspace (for short, CES). A CES does not contain any product state. [25–28].

Similarly to Refs. [6, 24], we can obtain the dual witnesses’ form of Eq. (2),

\[
W = c_\rho I - \rho, \\
\]

where \( \rho \) is a (separable) density matrix and

\[
c_\rho_{\text{min}} \leq c_\rho < \lambda_{M\rho} \\
\]

is a real number related to \( \rho \). The maximum eigenvalue of \( \rho \) is denoted by \( \lambda_{M\rho} \) and

\[
c_\rho_{\text{min}} = \sup_{\|\mu\|_2 = 1, \|\mu\|_2 = 1} \langle \mu_A \mu_B | \rho | \mu_A \mu_B \rangle \\
\]

is the minimum \( c_\rho \) such that \( W \) is a witness; \( |\mu_A \mu_B \rangle \) is any unit product state.

**Remark 2.** If \( W = c_\rho I - \rho \) is a witness with spectral decomposition of \( \rho = \sum_{i=0}^k \lambda_i |e_i \rangle \langle e_i | \), the eigenspace of the maximum eigenvalue \( \lambda_{M\rho} \) is a CES.

It is easy to conclude that any multipartite witness can be constructed from a (separable) state of the form given in Eq. (2) or Eq. (5).

### III. PURIFICATION AND PARTIAL PURIFICATION

#### A. Purification

Purification is a fundamental tool [29]. We recall it for the sake of completeness. Let \( \rho_A \) be a state in Hilbert space \( \mathcal{H}_A \). We introduce another system, with space denoted by \( \mathcal{H}_B \), and define a pure state \( \psi_{AB} \) for the joint system \( \mathcal{H}_A \otimes \mathcal{H}_B \) such that \( \rho_A = \text{tr}_B (|\psi_{AB} \rangle \langle \psi_{AB}|) \).

More precisely, suppose \( \rho_A \) has an orthonormal decomposition \( \rho_A = \sum_i |i^A \rangle \langle i^A| \). To purify \( \rho_A \), we introduce a system \( \mathcal{H}_B \) which has the same state space as \( \rho_A \) and an orthonormal basis \( |i^B \rangle \). We define a pure state for the combined system by \( |\psi_{AB} \rangle = \sum_i \sqrt{p_i} |i^A \rangle |i^B \rangle \). This state is said to be a purification of \( |\psi_{AB} \rangle \). The reduced density matrix for \( \mathcal{H}_A \) corresponding to the state \( \psi_{AB} \) is

\[
\text{tr}_B (|\psi_{AB} \rangle \langle \psi_{AB}|) = \sum_{ij} \sqrt{p_i p_j} |i^A \rangle \langle j^A| \delta_{ij} \\
= \sum_{ij} \sqrt{p_i p_j} |i^A \rangle \langle j^A| \\
= \sum_i p_i |i^A \rangle \langle i^A| \\
= \rho_A. \\
\]

We are now ready to state our first result.

**Theorem 1.** If \( W_{12} = c_{\sigma_{12}} I - \sigma_{12} \) is a bipartite witness, then

\[
W_{123} = c_{\sigma_{12}} I_{123} - |\psi_{123} \rangle \langle \psi_{123}| \\
\]

is a tripartite witness, where \( |\psi_{123} \rangle \) is any purification of \( \sigma_{12} \).

In fact, this extension is the inverse process of the cascaded structure in [19]. We give two proofs of the statement in our language: The first proof is lengthy; the second one is much shorter. We believe that both proofs are instructive.

**Lemma 1.** [29] Suppose \( |AB_1 \rangle \) and \( |AB_2 \rangle \) are two purifications of the state \( \rho^A \) to a composite system \( \mathcal{H}_A \otimes \mathcal{H}_B \). There exists a unitary transformation \( U_B \) acting on \( \mathcal{H}_B \) such that \( |AB_1 \rangle = (I_A \otimes U_B) |AB_2 \rangle \).

**Proof:** Let us consider the spectral decomposition \( \sigma_{12} = \sum_i p_i |\psi_{12} \rangle \langle \psi_{12}| \). The state \( |\psi_{123} \rangle = \sum_i \sqrt{p_i} |\psi_{12} \rangle |e_3 \rangle \) is a purification of \( \sigma_{12} \), where \( |e_3 \rangle \) is any orthonormal basis states in \( \mathcal{H}_3 \). Suppose

\[
c_{\text{min}}^{12} = \max_{\|\mu_1\|_2 = 1, \|\mu_2\|_2 = 1, \|\mu_3\|_2 = 1} \langle \mu'_1 \mu'_2 \mu'_3 | \psi_{123} \rangle \langle \psi_{123}| \mu'_1 \mu'_2 \mu'_3 \rangle \\
= \langle \mu_1 \mu_2 \mu_3 | \psi'_{123} \rangle \langle \psi'_{123}| \mu_1 \mu_2 \mu_3 \rangle \\
= r r^* \\
\]

and \( |\mu_3 \rangle = \sum_i t_i |e_3 \rangle \), where \( r \) and \( t_i \) are complex numbers. Then,

\[
r = \langle \mu_1 \mu_2 | \mu_3 \rangle \sum_i \sqrt{p_i} |\psi_{12} \rangle |e_3 \rangle \\
= \langle \mu_1 \mu_2 \sum_j t_j^* |e_3 \rangle \sum_i \sqrt{p_i} |\psi_{12} \rangle |e_3 \rangle \\
= \langle \mu_1 \mu_2 \sum_i \sqrt{p_i} t_i^* |e_3 \rangle \\
\]

It follows that

\[
\sum_i \sqrt{p_i} t_i^* = 1. \\
\]

Let \( t_i = \sqrt{p_i} (\mu_1 \mu_2 |\psi_{12}) \). Since \( \sum_i t_i t_i^* = 1 \), we have

\[
|\mu_3 \rangle = \sum_i \frac{\sqrt{p_i}}{r} (\mu_1 \mu_2 |\psi_{12}) |e_3 \rangle \\
\]

Similarly, suppose

\[
c_{\text{min}}^{12} = \langle \mu_1 \mu_2 | \sigma_{12} | \mu_1 \mu_2 \rangle. \\
\]
We can write
\[
\sigma_{\text{min}}(c_{12}) = \langle \mu_1 \mu_2 \rangle = \sum_i p_i \langle \psi_{12}^i | \psi_{12}^i \rangle \langle \psi_{12}^i | \mu_1 \mu_2 \rangle
\]
(19)
\[
= \sum_i \sqrt{p_i} \langle \mu_1 \mu_2 | \psi_{12}^i \rangle \sum_j \sqrt{p_j} \langle \psi_{12}^j | \mu_1 \mu_2 \rangle \langle \psi_{12}^j | \mu_3 \rangle
\]
(20)
\[
= r \sum_i \sqrt{p_i} \langle \mu_1 \mu_2 | \psi_{12}^i \rangle \left( \sum_j \sqrt{p_j} \langle \mu_1 \mu_2 | \psi_{12}^j \rangle \langle \psi_{12}^j | \mu_3 \rangle \right)
\]
(21)
\[
= r \sum_i \sqrt{p_i} \langle \mu_1 \mu_2 | \psi_{12}^i \rangle \langle \psi_{12}^i | \mu_3 \rangle
\]
(22)
\[
= r \langle \psi_{12}^{123} | \mu_1 \mu_2 \mu_3 \rangle
\]
(23)
\[
= c_{\text{min}}(\psi_{12}^{123}) \langle \psi_{12}^{123} | \psi_{12}^{123} \rangle
\]
(24)
\[
= c_{\text{min}}(\psi_{12}^{123}) \langle \psi_{12}^{123} | \psi_{12}^{123} \rangle
\]
(25)
\[
\text{since}
\]
\[
\sigma_{\text{min}}(\psi_{12}^{123}) = \langle \mu_1 \mu_2 | \psi_{12}^{123} \rangle \langle \psi_{12}^{123} | \mu_3 \rangle
\]
(26)
\[
\text{where}
\]
\[
\langle \psi_{12}^{123} | \psi_{12}^{123} \rangle = \langle \mu_1 \mu_2 | \psi_{12}^{123} \rangle \langle \psi_{12}^{123} | \mu_3 \rangle
\]
(27)
\[
\text{since}
\]
\[
|\psi_{12}^{123} \rangle = \langle \mu_1 \mu_2 | \psi_{12}^{123} \rangle
\]
(28)
\[
\text{is a bipartite witness.}
\]

Proof: The proof uses two points:

(i) Suppose \( \mu_i \) is any unit pure state of a system with Hilbert space \( \mathcal{H}_i \), for \( i = 1, 2, 3 \). We have
\[
\langle \mu_1 \mu_2 \mu_3 | W_{123} | \mu_1 \mu_2 \mu_3 \rangle
\]
(29)
\[
\geq c_{\text{min}}(\psi_{12}^{123}) \langle \psi_{12}^{123} | \psi_{12}^{123} \rangle \langle \psi_{12}^{123} | \mu_1 \mu_2 \mu_3 \rangle
\]
(30)
\[
= \langle \psi_{12}^{123} | \mu_1 \mu_2 \mu_3 \rangle
\]
(31)
\[
= 0
\]
(32)
\[
\text{since } W_{12} \text{ is a bipartite witness.}
\]

(ii) By Eq. (6), \( W_{123} < 0 \) since \( c_{\sigma_{12}} < 1 \).

Combining together (i) and (ii), \( W_{123} \) is a tripartite witness.

**Corollary 1.** If \( W_{12} = c_{\sigma_{12}} I - \sigma_{12} \) is a bipartite witness, then
\[
W_{12n} = c_{\sigma_{12}} I - \sigma_{12}
\]
(33)
\[
is a n\text{-partite witness, where } |\psi_{123} \rangle \text{ is any purification of } \sigma_{12} \text{ and } |\psi_i \rangle \text{ is a pure state in } \mathcal{H}_i.
\]

We illustrate our results for the case of the isotropic qubit state. It is known that
\[
\sigma_q = \begin{pmatrix}
\frac{1+q}{4} & 0 & 0 & \frac{q}{2} \\
0 & 1-q & 0 & 0 \\
0 & 0 & 1-q & 0 \\
\frac{q}{2} & 0 & 0 & \frac{1+q}{4}
\end{pmatrix}
\]
(34)
is the (separable) density matrix of
\[
\sigma_q = q |\psi \rangle \langle \psi | + (1-q) I/4,
\]
where \( |\psi \rangle = \frac{1}{\sqrt{2}} (|00 \rangle + |11 \rangle) \text{ and } 0 < q < \frac{1}{3} \).

By computing \( c_{\sigma_q} = \frac{1+3q}{4} \text{ [24],} \)
\[
W_{12} = \frac{1+q}{4} I - \sigma_q
\]
(35)
is a bipartite witness for \( 0 < q < \frac{1}{3} \). It works for
\[
\sigma_p = p |\psi \rangle \langle \psi | + (1-p) I/4,
\]
where \( p > \frac{1}{3} \). Since the maximum eigenvalue of \( \sigma_q \) is \( \lambda_{M} = \frac{1+3q}{4} \),
\[
W_{12} = c_{\sigma_q} I - \sigma_q
\]
(36)
is a bipartite witness for \( \frac{1+q}{4} \leq c_{\sigma_q} < \frac{1+3q}{4} \).

The spectral decomposition for \( \sigma_q \) is
\[
\sigma_q = \frac{1-q}{4} |\psi_{12}^0 \rangle \langle \psi_{12}^0 | + \frac{1-q}{4} |\psi_{12}^1 \rangle \langle \psi_{12}^1 | + \frac{1-q}{4} |\psi_{12}^2 \rangle \langle \psi_{12}^2 | + \frac{1-q}{4} |\psi_{12}^3 \rangle \langle \psi_{12}^3 |,
\]
where \( |\psi_{12}^0 \rangle = |00 \rangle \text{ and } |\psi_{12}^1 \rangle = |01 \rangle \text{ are separable, while }|\psi_{12}^2 \rangle = \frac{1}{\sqrt{2}} (|00 \rangle - |11 \rangle) \text{ and } |\psi_{12}^3 \rangle = \frac{1}{\sqrt{2}} (|00 \rangle + |11 \rangle) \text{ are entangled.}

A purification of \( \sigma_q \) in \( C^2 \otimes C^2 \otimes C^4 \) is
\[
|\psi_{123} \rangle = \sqrt{\frac{1-q}{4}} |\psi_{12}^0 \rangle + \sqrt{\frac{1-q}{4}} |\psi_{12}^1 \rangle + \sqrt{\frac{1-q}{4}} |\psi_{12}^2 \rangle + \sqrt{\frac{1-q}{4}} |\psi_{12}^3 \rangle
\]
(37)
\[
\text{where } \{|i\rangle \}_{i=0}^{3} \text{ is the orthogonal basis in } C^4. \text{ Hence,}
\]
\[
W_{123} = \frac{1+q}{4} I_{123} - |\psi_{123} \rangle \langle \psi_{123} |
\]
(38)
is a tripartite witness in \( C^2 \otimes C^2 \otimes C^4 \) for \( 0 < q < \frac{1}{3} \).
B. Partial purification

The dimension of $\mathcal{H}_3$ is the same as the dimension of $\mathcal{H}_1 \otimes \mathcal{H}_2$ (or it is equal to the rank of $\sigma_{12}$) because of the demand of purification. There exists a large gap. There also exists a restriction to the dimension of $\mathcal{H}_3$ for the extension. One would hope that $\mathcal{H}_3$ can be of any dimension. Here we need to extend the notion of purification. The joint system $(A, B)$ will be on a space $\mathcal{H}_A \otimes \mathcal{H}_B$.

Suppose the spectral decomposition for $\rho_A$ is

$$\rho_A = \lambda_0 |\phi_0^A\rangle \langle \phi_0^A| + \lambda_1 |\phi_1^A\rangle \langle \phi_1^A| + \cdots + \lambda_M |\phi_M^A\rangle \langle \phi_M^A|,$$

with $\lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_M$, where $\lambda_0$ and $\lambda_M$ are the minimum and maximum eigenvalue, respectively. To purify $\rho_A$ to the system $B$, whose dimension is less than the rank of $\rho_A$, we define a (unnormalized) pure state $|\phi_{AB}\rangle$ for the joint system such that

$$|\phi_{AB}\rangle = \sum_i \sqrt{\lambda_i} |\phi_i^A\rangle |e_i^B\rangle,$$

This state is said to be a partial purification of $\rho_A$. The states $|e_i^B\rangle$ form an orthonormal basis in $\mathcal{H}_B$. Moreover, $\lambda_i$ and $|\phi_i^A\rangle$ are selected from the eigenvalues and eigenvectors of $\rho_A$. When $\lambda_M$ and $|\phi_M^A\rangle$ (respectively, $\lambda_0$ and $|\phi_0^A\rangle$) are selected, the state $|\phi_{AB}\rangle$ is said to be a partial purification with maximum eigenvalue (respectively minimum eigenvalue).

Generally, a partial purification $|\phi_{AB}\rangle$ is unnormalized and $\text{tr}_B(|\phi_{AB}\rangle \langle \phi_{AB}|) \leq \rho_A^3$. For example, if the spectral decomposition for $\sigma_{12} \in \mathbb{C}^2 \otimes \mathbb{C}^2$ is

$$\sigma_{12} = p_0 |\phi_0^{12}\rangle \langle \phi_0^{12}| + p_1 |\phi_1^{12}\rangle \langle \phi_1^{12}| + p_2 |\phi_2^{12}\rangle \langle \phi_2^{12}| + p_3 |\phi_3^{12}\rangle \langle \phi_3^{12}|,$$

where $|\phi_i^{12}\rangle$ is the orthonormal basis state in $\mathbb{C}^2 \otimes \mathbb{C}^2$. Partial purifications of $\sigma_{12}$ are

$$|\phi_{123}\rangle = \sqrt{p_0} |\phi_0^{12}\rangle |\phi_0^{12}\rangle + \sqrt{p_1} |\phi_1^{12}\rangle |\phi_1^{12}\rangle + \sqrt{p_2} |\phi_2^{12}\rangle |\phi_2^{12}\rangle + \sqrt{p_3} |\phi_3^{12}\rangle |\phi_3^{12}\rangle,$$

and

$$|\phi'_{123}\rangle = \sqrt{p_0} |\phi_0^{12}\rangle |\phi_0^{12}\rangle + \sqrt{p_1} |\phi_1^{12}\rangle |\phi_1^{12}\rangle + \sqrt{p_2} |\phi_2^{12}\rangle |\phi_2^{12}\rangle + \sqrt{p_3} |\phi_3^{12}\rangle |\phi_3^{12}\rangle.$$  

Theorem 2. If $W_{12} = c_{\sigma_{12}} I - \sigma_{12}$ is a bipartite witness, then

$$W_{123} = c_{\sigma_{12}} I_{123} - |\phi_{123}\rangle \langle \phi_{123}|$$

is a tripartite witness, where the (unnormalized) pure state $|\phi_{123}\rangle$ is a partial purification of $\sigma_{12}$ with maximum eigenvalue.

Proof: We proceed as follows:

(i) By Theorem 1,

$$c_{\sigma_{12}}^\text{min} \leq c_{\sigma_{12}}^\text{min} \leq c_{\sigma_{12}}^\text{min} \leq c_{\sigma_{12}}.$$

(ii) By the definition of partial purification, the maximum eigenvalue of $|\phi_{123}\rangle$ is equal to the sum of eigenvalues selected to partially purify. Since we select the maximum eigenvalue $\lambda_{M\sigma_{12}}$, we have then

$$\lambda_{M\sigma_{12}} \leq \lambda_{M|\phi_{123}\rangle} |\phi_{123}|.$$
with one of the partial purification of $\sigma_q$ with maximum eigenvalue

$$|\psi_{123}\rangle = \sqrt{\frac{1+3q}{4}}|\psi_{123}\rangle |0\rangle + \sqrt{\frac{1-q}{4}}|\psi_{123}\rangle |1\rangle.$$  

Also,

$$W_{123}^2 = \frac{1+q}{4}I_{123} - |\psi_{123}\rangle\langle\psi_{123}|$$

with one of the partial purification of $\sigma_q$ with maximum eigenvalue

$$|\psi'_{123}\rangle = \sqrt{\frac{1+3q}{4}}|\psi_{123}\rangle |0\rangle + \sqrt{\frac{1-q}{4}}|\psi_{123}\rangle |1\rangle.$$  

Finally,

$$W_{123}^3 = \frac{1+q}{4}I_{123} - |\psi''_{123}\rangle\langle\psi''_{123}|,$$

where

$$|\psi''_{123}\rangle = \sqrt{\frac{1+3q}{4}}|\psi_{123}\rangle |1\rangle + \sqrt{\frac{1-q}{4}}|\psi_{123}\rangle |0\rangle,$$

and so on.

### C. Bipartite witnesses

In standard quantum mechanics, there is no entanglement and no witness for a single system. However, it is interesting that we can consider a witness $W_1 = 0$ for a single system. We can extend $W_1$ to bipartite witnesses. Then,

$$W_1 = 0 = \frac{1}{2}I - \frac{1}{2}I$$

in a 2-level system, can be extended to a bipartite witness $W_{12}$ in $\mathbb{C}^2 \otimes \mathbb{C}^2$. We purify

$$\frac{1}{2}I = \frac{1}{2}(|0\rangle \langle 0| + |1\rangle \langle 1|)$$

to the pure state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle)$$

in the composite system

$$W_{12} = \frac{1}{2}I_{12} - |\psi\rangle\langle\psi|.$$  

We can also purify $\frac{1}{2}I$ to

$$|\phi\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle),$$

and obtain the bipartite witness

$$W_{12} = \frac{1}{2}I_{12} - |\phi\rangle\langle\phi|.$$  

### IV. Mixed States Extension

We begin the section with a question: can we extend bipartite witnesses by transforming states into mixed states in Eq. (5)? The following result answers the question:

**Theorem 3.** If $W_{12} = c_{\sigma_{12}} I_{12} - \sigma_{12}$ is a bipartite witness then

$$W_{12\cdots n} = c_{\sigma_{12}} I_{12\cdots n} - \sigma_{12} \otimes \frac{1}{\lambda_{M\sigma_3}} \sigma_3 \otimes \cdots$$

$$\otimes \frac{1}{\lambda_{M\sigma_n}} \sigma_n$$  

(45)

is a $n$-partite witness, where $\sigma_i$ is any (normalized, mixed or pure) state in $\mathcal{H}_i$ with maximum eigenvalue $\lambda_{M\sigma_i}$.

**Proof:** (i) Firstly,

$$c_{\min}^{\min}$$  

\begin{align*}
\sigma_{12} & \otimes \frac{1}{\lambda_{M\sigma_3}} \sigma_3 \otimes \cdots \otimes \frac{1}{\lambda_{M\sigma_n}} \sigma_n
\end{align*}

$$= \max_{||\mu'_1||=1, ||\mu'_2||=1, \ldots} \langle \mu'_1 | \mu'_2 | \cdots | \mu'_n \rangle
\sigma_{12} \otimes \frac{1}{\lambda_{M\sigma_3}} \sigma_3 \otimes \cdots \otimes \frac{1}{\lambda_{M\sigma_n}} \sigma_n | \mu'_1 | \mu'_2 | \cdots | \mu'_n \rangle
$$  

(46)

$$= \lambda_{M\sigma_1} e_{e_1} \cdots \langle e_n | \lambda_{M\sigma_n} e_n | \langle e_1 | \lambda_{M\sigma_1} e_1 \cdots \langle e_n | \lambda_{M\sigma_n} e_n
$$  

(47)

$$c_{\min}^{\min},$$

where $|e_i\rangle$ is the eigenvector corresponding to the maximum eigenvalue of $\sigma_i$, with $3 < i \leq n$.

(ii) Then, since in these cases the maximum eigenvalue of $\frac{1}{\lambda_{M\sigma_i}} \sigma_i$ is 1, we have

$$\lambda_{M\sigma_1} = \lambda_{M\sigma_2} \cdots \frac{1}{\lambda_{M\sigma_3}} \sigma_3 \otimes \cdots \otimes \frac{1}{\lambda_{M\sigma_n}} \sigma_n \otimes \cdots \otimes \frac{1}{\lambda_{M\sigma_3}} \sigma_3.$$  

By (i) and (ii), $W_{12\cdots n}$ is an $n$-partite witness. \hfill \blacksquare

Can we extend the bipartite witness by purification or partial purification in the form given by Eq. (2) [the dual form of Eq. (5)]? The answer is negative, since the minimum eigenvalue is 0 after the process of purification and then the space spanned by the eigenvectors generally is not a CES if we purify the state $\sigma_{12}$. The following extension, however, can be done by extending pure states to mixed states from both Eqs. (2) and (5).

**Corollary 4.** If $W_{12} = c_{\sigma_{12}} I_{12} - \sigma_{12}$ is a bipartite witness then

$$W_{12\cdots n} = c_{\sigma_{12}} I_{123} - \sigma_{12} \otimes \sigma_3 \otimes \cdots$$

$$\otimes \sigma_n$$  

(49)

is a $n$-partite witness in $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$.

If $\rho_{12}$ is the entangled state witnessed by $W_{12}$, $tr(W_{12\cdots n} I_{12\cdots n}) < 0$ by Corollary 4, where $\rho_{12\cdots n} = \rho_{12} \otimes \rho_3 \otimes \cdots \otimes \rho_n$ and $\rho_i$ is any state in $\mathcal{H}_i$. This result indicates that all states can be witnessed by $W_{12\cdots n}$, and that this is given by the tensor product of any state witnesses by $W_{12}$ and any state in $\mathcal{H}_i$.

By Corollary 4, we can thus extend Eq. (34) to

$$W_{123}^q = \frac{1+q}{4} I_{123} - \sigma_{123}^q$$
where
\[
\sigma_{123}^q = \left(1 - \frac{q}{4}\right) (|\psi_{123}^0\rangle\langle\psi_{123}^0| + |\psi_{123}^1\rangle\langle\psi_{123}^1| + |\psi_{123}^2\rangle\langle\psi_{123}^2|)
+ \frac{1 + 3q}{4} |\psi_{123}^3\rangle\langle\psi_{123}^3|) \otimes (|0\rangle\langle0| + |1\rangle\langle1| + |2\rangle\langle2| + |3\rangle\langle3|)
\]
(50)
in \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^4.

We can extend Eq. (34) to
\[
W_{123}^q = \frac{1 + q}{4} I_{123} - \sigma_{123}^q
\]
(51)
where
\[
\sigma_{123}^q = \left(1 - \frac{q}{4}\right) (|\psi_{123}^0\rangle\langle\psi_{123}^0| + |\psi_{123}^1\rangle\langle\psi_{123}^1| + |\psi_{123}^2\rangle\langle\psi_{123}^2|)
+ \frac{1 + 3q}{4} |\psi_{123}^3\rangle\langle\psi_{123}^3|) \otimes (|0\rangle\langle0| + |1\rangle\langle1|)
\]
(52)
in \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2.

Consider the same witness (unnormalized)
\[
W_{12} = \frac{1}{2} W_{12}^{\psi}\text{ as (normalized) } W_{12}^{\psi} = |\psi\rangle\langle\psi|^{\Gamma},
\]
where \(\psi = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)\) and \(\Gamma\) refers to partial transposition. We can write \(W_{12}\) in the form given in Eq. (2)
\[
W_{12} = \frac{1}{4} |\psi\rangle\langle\psi|^{\Gamma} = \sigma_{12} - \frac{3}{16} I_{12},
\]
where
\[
\sigma_{12} = \begin{pmatrix}
\frac{5}{16} & 0 & 0 & 0 \\
0 & \frac{3}{16} & \frac{1}{16} & 0 \\
0 & \frac{1}{16} & \frac{3}{16} & 0 \\
0 & 0 & 0 & \frac{5}{16}
\end{pmatrix}.
\]

Hence, we have the spectral decomposition
\[
\sigma = \frac{1}{16} |\psi_{12}^0\rangle\langle\psi_{12}^0| + \frac{5}{16} |\psi_{12}^1\rangle\langle\psi_{12}^1| + \frac{5}{16} |\psi_{12}^2\rangle\langle\psi_{12}^2| + \frac{5}{16} |\psi_{12}^3\rangle\langle\psi_{12}^3|
\]
(53)
where \(|\psi_{12}^0\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)\) and \(|\psi_{12}^1\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)\) are entangled, while \(|\psi_{12}^2\rangle = |00\rangle\) and \(|\psi_{12}^3\rangle = |11\rangle\) are separable. We can extend \(\sigma_{12}\) to
\[
\sigma_{123} = \frac{1}{16} |\psi_{123}^0\rangle\langle\psi_{123}^0| + \frac{5}{16} |\psi_{123}^1\rangle\langle\psi_{123}^1| + \frac{5}{16} |\psi_{123}^2\rangle\langle\psi_{123}^2| + \frac{5}{16} |\psi_{123}^3\rangle\langle\psi_{123}^3|
\]
+ \frac{5}{16} |\psi_{123}^4\rangle\langle\psi_{123}^4| \otimes (|0\rangle\langle0| + |1\rangle\langle1| + |2\rangle\langle2| + |3\rangle\langle3|)
\]
(54)
which is full rank in \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^4, and
\[
W_{123} = \sigma_{123} - \frac{3}{16} I_{123}
\]
(55)
is a tripartite witness. Similarly, we can extend \(\sigma_{12}\) to
\[
\sigma'_{123} = \frac{1}{16} |\psi_{123}^0\rangle\langle\psi_{123}^0| + \frac{5}{16} |\psi_{123}^1\rangle\langle\psi_{123}^1| + \frac{5}{16} |\psi_{123}^2\rangle\langle\psi_{123}^2|
+ \frac{5}{16} |\psi_{123}^3\rangle\langle\psi_{123}^3| \otimes (|0\rangle\langle0| + |1\rangle\langle1|),
\]
(56)
which is full rank in \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2, and
\[
W_{123}' = \sigma'_{123} - \frac{3}{16} I_{123}
\]
(57)
is a tripartite witness.

Similar to the proof of Theorem 1, we can show \(\lambda_{0\sigma_{123}} < \frac{3}{16} \leq c_{\sigma_{123}}^{\text{max}}\) in Eq. (55) and \(\lambda_{0\sigma'_{123}} < \frac{3}{16} \leq c_{\sigma'_{123}}^{\text{max}}\) in Eq. (57), and that Eqs. (55) and (57) give tripartite witnesses.

Note that we can also extend \(\sigma_{12}\) to tripartite states by selecting partial bases in \(\mathcal{H}_3\), but cannot for the extending from the form of Eq. (2). The simplest extension is just the following easy but still useful result, which can be also directly drawn from Theorem 3.

**Corollary 5.** If \(W_{12} = c_{\sigma_{12}} I_{12} - \sigma_{12}\) is a bipartite witness then
\[
W_{12\ldots n} = c_{\sigma_{12}} I_{12\ldots n} - \sigma_{12} \otimes |\psi_3\rangle\langle\psi_3| \cdots \otimes |\psi_n\rangle\langle\psi_n|
\]
is an \(n\)-partite witness, where \(|\psi_i\rangle\langle\psi_i|\) is a pure state in \(\mathcal{H}_i\).

\section{Summary}

Based on the general form of a witness \(W_{12} = c_{\sigma_{12}} I_{12} - \sigma_{12}\), we extend a bipartite witness to tripartite witnesses \(W_{123} = c_{\sigma_{123}} I_{123} - |\psi_{123}\rangle\langle\psi_{123}|\) by purifying or partially purifying \(\sigma_{12}\) to \(|\psi_{123}\rangle\langle\psi_{123}|\). We extend a bipartite witness \(W_{12} = c_{\sigma_{12}} I_{12} - \sigma_{12}\) to tripartite witnesses by extending \(\sigma_{12}\) to mixed product states in \(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3\). For all methods, we do not need to change the parameter \(c_{\sigma_{12}}\). Our methods are universal and generalizable to extend a bipartite witness to the multipartite case.

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