Optimization of entanglement witnesses

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I. INTRODUCTION

Quantum entanglement, which is an essence of many fascinating quantum mechanical effects, is a very fragile phenomenon. It is usually very hard to create, maintain, and manipulate entangled states under laboratory conditions. In fact, any system is usually subjected to the effects of external noise and interactions with the environment. These effects turn pure state entanglement into mixed state, or noisy entanglement. The separability problem, that is, the characterization of mixed entangled states, is highly nontrivial and has not been accomplished so far. Even the apparently innocent question: Is a given state entangled and does it contain quantum correlations, or is it separable, and does not contain any quantum correlations? will, in general, be very hard (if not impossible!) to answer.

Mathematically, mixed state entanglement can be described as follows. A density operator \( \rho \geq 0 \) acting on a finite Hilbert space \( H = H_A \otimes H_B \) describing the state of two quantum systems \( A \) and \( B \) is called separable (or not entangled) if it can be written as a convex combination of product vectors; that is, in the form

\[
\rho = \sum_k p_k |e_k, f_k \rangle \langle e_k, f_k |,
\]

where \( p_k \geq 0 \), and \( |e_k, f_k \rangle \equiv |e_k \rangle_A \otimes |f_k \rangle_B \) are product vectors. Conversely, \( \rho \) is nonseparable (or entangled) if it cannot be written in this form. Physically, a state described by a separable (nonseparable) density operator \( \rho \) can always (never) be prepared locally. Most of the applications in quantum information are based on the nonlocal properties of quantum mechanics, and therefore on nonseparable states. Thus, a criterion to determine whether a given density operator is nonseparable, i.e., useful for quantum information purposes, or not is of crucial importance. On the other hand, PPTES are objects of special interest since they represent so-called bound entangled states, and therefore provide an evidence of irreversibility in quantum information processing.

For low dimensional systems there exist operationally simple necessary and sufficient conditions for separability. In fact, in \( H = \mathbb{C}^2 \otimes \mathbb{C}^2 \) and \( H = \mathbb{C}^2 \otimes \mathbb{C}^3 \) the Peres–Horodecki criterion establishes that \( \rho \) is separable iff its partial transpose is positive. Partial transpose means a transpose with respect to one of the subsystems. For higher dimensional systems all operators with non–positive partial transposition are entangled. However, there exist positive partial transpose entangled states (PPTES). Thus, the separability problem reduces to finding whether density operators with positive partial transpose are separable or not.

In the recent years there has been a growing effort in searching for necessary and sufficient separability criteria and checks which would be operationally simple. Several necessary or sufficient conditions for separability are known. A particularly interesting necessary condition is given by the so–called range criterion. According to this criterion, if the state \( \rho \) acting on a finite dimensional Hilbert space is separable then there must exist a set of product vectors \( \{ |e_k, f_k \rangle \} \) that spans the range \( R(\rho) \) such that the set of partial complex conjugated product states \( \{ |e_k, f_k^\dagger \rangle \} \) spans the range of the partial transpose of \( \rho \) with respect to the second system, i.e., \( \rho^{T_B} \). Among the PPTES that violate this criterion there are particular states with the property that if one subtracts a projector onto a product vector from them, the resulting operator is no longer a PPTES. In this sense, these states lie in the edge between PPTES and entangled states with non–positive partial transposition, and therefore we will call them “edge” PPTES. The analysis of the range of den-
sity operators initiated in Ref. [13] has turned out to be very fruitful. In particular, it has led to an algorithm for the optimal decomposition of mixed states into a separable and an inseparable part [12,22], and to a systematic method of constructing examples of PPTES using unextendible product bases [13,14]. For low rank operators it has allowed to show that one can reduce the separability problem to the one of determining the roots of certain complex polynomial equations [14,16].

From a different point of view, a very general approach to analyze the separability problem is based on the so-called entanglement witnesses (EW) and positive maps (PM). Entanglement witnesses [25] are operators that detect the presence of entanglement. Starting from these operators one can define PM’s [26] that also detect entanglement. An example of a PM is precisely partial transposition [10,27,28]. The importance of EW stems from the fact that a given operator is separable iff there exists an EW that detects it [11]. Thus, if one was able to construct all possible EW (or PM) one would have solve the problem of separability. Unfortunately, it is not known how to construct EW that detect PPTES in general. The only result in this direction so far has been given in Ref. [29], although some preliminary results exist in the mathematical literature [29]. Starting from a PPTES fulfilling certain properties (related to the existence of unextendible basis of product vectors [14]), it has been shown how to construct an EW (and the corresponding PM) that detects it. Perhaps, one of the most interesting goals regarding the separability problem is to develop a constructive and operational approach using EW and PM that allows us to detect mixed entanglement.

In this paper we realize this goal partially: we introduce a powerful technique to construct EW and PM that, among other things, allows us to study the separability of certain density operators. In particular, we show how to construct optimal EW; that is, operators that detect the presence of entanglement in an optimal way. We specifically concentrate on non-decomposable EW, which are those that detect the presence of PPTES. Furthermore, we present a way of constructing optimal EW for edge PPTES. Our method generalizes the one introduced by Terhal [23] to the case in which there are no unextendible basis of product vectors. When combined with our previous results [14,21] regarding subtracting product vectors from PPTES, the construction of non-decomposable optimal EW starting from “edge” PPTES gives rise to a novel sufficient criterion for non-separability of general density operators with positive partial transpose. We illustrate our method by constructing optimal EW that detect some known examples of PPTES [14] in \( H = \mathcal{A}^2 \otimes \mathcal{A}^3 \). The corresponding PM constitute the first examples of PM with minimal “qubit” domain, or – equivalently – minimal hermitian conjugate codomain.

This paper is organized as follows. In Section II we review the definition of EW and fix some notation. In Section III we study general EW. We define optimal witnesses and find a criterion to decide whether an EW is optimal or not. In Section IV we restrict the results of Section III to non-decomposable EW. In particular, we show how to optimize them by subtracting decomposable operators. In Section V we give an explicit method to optimize both, general and non-decomposable EW. We also show how to construct non-decomposable EW, and that this leads to a sufficient criterion of non-separability. The construction and optimization is based on the use of “edge” PPTES. In Section VI we extend our results to positive maps. In Section VII we illustrate our methods and results starting from the examples of PPTES given in Ref. [13]. The paper also contains two appendices. In Appendix A we describe in detail a method to check whether an EW is optimal or not. In Appendix B we discuss separately some important properties of the edge PPTES, and show that they provide a canonical decomposition of mixed states with positive partial transpose.

**II. DEFINITIONS AND NOTATION**

We say that an operator \( W = W^\dagger \) acting on \( H = \mathcal{H}_A \otimes \mathcal{H}_B \) is an EW if \( W \) satisfies the following properties:

1. **(I)** \( \langle e, f|W|e, f \rangle \geq 0 \) for all product vectors \( |e, f \rangle \);
2. **(II)** has at least one negative eigenvalue (i.e. is not positive);
3. **(III)** \( \text{tr}(W) = 1 \).

The first property (I) implies that \( \langle \rho \rangle_W \equiv \text{tr}(W \rho) \geq 0 \) for all \( \rho \) separable. Thus, if we have \( \langle \rho \rangle_W < 0 \) for some \( \rho \geq 0 \), then \( \rho \) is nonseparable. In that case we say that \( W \) detects \( \rho \). The second one (II) implies that every EW detects something, since in particular it detects the projector on the subspace corresponding to the negative eigenvalues of \( W \). The third property (III) is just normalization condition that we need in order to compare the action of different EW [30].

In this paper we will denote by \( K(\rho) \) and \( R(\rho) \) the kernel and range of \( \rho \), respectively. The partial transposition of an operator \( X \) will be denoted by \( X^T \). On the other hand, we will encounter several kinds of operators (EW, positive operators, decomposable operators, etc) and vectors. In order to help to identify the kind of operators and vectors we use, and not to overwhelm the reader by specifying at each point their properties, we will use the following notation:

- \( W \) will denote an EW.
- \( P, Q \) will denote positive operators. Unless specified they will have unit trace \( \text{tr}(P) = \text{tr}(Q) = 1 \).
- \( D \) will denote a decomposable operator. That is, \( D = aP + bQ^T \), where \( a, b \geq 0 \). Unless stated, all decomposable operators that we use will have unit trace (i.e., \( b = 1 - a \)).
• ρ will denote a positive operator (not necessarily of trace 1).
• |e, f⟩ will denote product vectors with |e⟩ ∈ HA and |f⟩ ∈ HB. Unless specified, they will be normalized.

III. GENERAL ENTANGLEMENT WITNESSES

In this Section we first give some definitions directly related to EW. Then we introduce the concept of optimal EW. We derive a criterion to determine when an EW is optimal. This criterion will serve us to find an optimization procedure for these operators.

A. Definitions

Given an EW, W, we define:

• DW = {ρ ≥ 0, such that ⟨ρ⟩W < 0}; that is, the set of operators detected by W.
• Finer: Given two EW, W1 and W2, we say that W2 is finer than W1, if DW1 ⊆ DW2; that is, if all the operators detected by W1 are also detected by W2.
• Optimal entanglement witness (OEW): We say that W is an OEW if there exist no other EW which is finer.
• PW = {⟨e, f|W|e, f⟩ = 0}; that is, the set of product vectors on which W vanishes. As we will show, these vectors are closely related to the optimality property.

Note the important role that the vectors in PW play regarding entanglement (for a method to determine PW in practice, see Appendix A). If we have an EW, W, which detects a given operator ρ, then the operator ρ′ = ρ + ρw where

\[ \rho_w = \sum_k p_k|e_k, f_k⟩⟨e_k, f_k| \]

with pk ≥ 0, and |e_k, f_k⟩ ∈ PW is also detected by W. In fact, this means that any operator of the form (2) is in the border between separable states and non-separable states, in the sense that if we add an arbitrarily small amount of ρ to it we obtain a non-separable state. Thus, the structure of the sets PW characterizes the border between separable and non-separable states. In fact, from the results of this Section it will become clear that we can restrict ourselves to the structure of the sets of PW corresponding to OEW’s.

B. Optimal entanglement witnesses

According to Ref. [1] ρ is nonseparable iff there exists an EW which detects it. Obviously, we can restrict ourselves to the study of OEW. For that, we need criteria to determine when an EW is optimal. In this subsection we will derive a necessary and sufficient condition for this to happen (Theorem 1 below). In order to do that, we first have to introduce some results that tell us under which conditions an EW is finer than another one.

Lemma 1: Let W2 be finer than W1 and

\[ \lambda \equiv \inf_{\rho_1 \in D_{W_1}} \left| \frac{⟨\rho_1⟩_{W_2}}{⟨\rho_1⟩_{W_1}} \right|. \]

Then we have:

(i) If ⟨ρ⟩W1 = 0 then ⟨ρ⟩W2 ≤ 0.
(ii) If ⟨ρ⟩W1 < 0, then ⟨ρ⟩W2 ≤ ⟨ρ⟩W1.
(iii) If ⟨ρ⟩W1 > 0 then λ(⟨ρ⟩W1 ≥ ⟨ρ⟩W2.
(iv) λ ≥ 1. In particular, λ = 1 iff W1 = W2.

Proof: Since W2 is finer than W1 we will use the fact that for all ρ ≥ 0 such that ⟨ρ⟩W1 < 0 then ⟨ρ⟩W2 < 0. (i) Let us assume that ⟨ρ⟩W2 > 0. Then we take any ρ1 ∈ DW1 so that for all x ≥ 0, 0 ≤ ⟨x⟩W2 ∈ DW1. But for sufficiently large x we have that ⟨x⟩W2 is positive, which cannot be since then ⟨x⟩W2 < 0. (ii) We define ρ = ρ + |⟨ρ⟩W2⟩| ≥ 0. We have that ⟨ρ⟩W1 = 0. Using (i) we have that 0 ≥ ⟨ρ⟩W2 + |⟨ρ⟩W1|. (iii) We take ρ1 ∈ DW1, and define ρ = ⟨ρ⟩W1 + |⟨ρ⟩W1| ≥ 0, so that ⟨ρ⟩W1 = 0. Using (i) we have |⟨ρ⟩W1| |⟨ρ⟩W2 ≤ |⟨ρ⟩W1| ⟨ρ⟩W1. Dividing both sides by ⟨ρ⟩W2 > 0 we obtain

\[ \frac{⟨ρ⟩W2}{⟨ρ⟩W1} ≤ \frac{|⟨ρ⟩W1|}{⟨ρ⟩W1}. \]

Taking the infimum with respect to ρ1 ∈ DW1 in the rhs of this equation we obtain the desired result.

(iv) From (ii) immediately follows that λ ≥ 1. On the other hand, we just have to prove that if λ = 1 then W1 = W2 (the only if part is trivial). If λ = 1, using (i) and (iii) we have that |⟨ρ⟩W1| ≥ |⟨ρ⟩W2| for all ρ = |e, f⟩⟨e, f| projector on a product vector. Since tr(W1) = tr(W2) we must have tr([W1 − W2]ρv) = 0 for all ρv, since we can always find a product basis in which we can take the trace. But now, for any given ρ ≥ 0 we can define ρ(x) = ρ + xI such that for large enough x, ρ(x) is separable [8]. In that case we have ⟨ρ(x)⟩W1 = ⟨ρ(x)⟩W2 which implies that ⟨ρ⟩W1 = ⟨ρ⟩W2, i.e. W1 = W2. □

Corollary 1: DW1 = DW2 iff W1 = W2.

Proof: We just have to prove the only if part. For that, we define λ as in (1). On the other hand, defining

\[ \bar{\lambda} \equiv \inf_{\rho_2 \in D_{W2}} \left| \frac{⟨\rho_2⟩_{W1}}{⟨\rho_2⟩_{W2}} \right|. \]

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we have that $\lambda \geq 1$ since $W_1$ is finer than $W_2$ (Lemma 1(iv)). Equivalently,

$$1 \geq \sup_{\rho_1 \in D_{W_1}} \frac{|\langle \rho_1 | W_2 \rangle|}{|\langle \rho_1 | W_1 \rangle|} \geq \lambda \geq 1,$$

(6)

where for the last inequality we have used that $W_2$ is finer than $W_1$. Now, since $\lambda = 1$ we have that $W_1 = W_2$ according to Lemma 1(iv). □

Next, we introduce one of the basic results of this paper. It basically tells us that EW is finer than another one if they differ by a positive operator. That is, if we have an EW and we want to find another one which is finer, we have to subtract a positive operator.

**Lemma 2:** $W_2$ is finer than $W_1$ iff there exists a $P$ and $1 > \epsilon \geq 0$ such that $W_1 = (1 - \epsilon)W_2 + \epsilon P$.

**Proof:** (If) For all $\rho \in D_{W_1}$, we have that $0 > |\langle \rho | W_1 \rangle| = (1 - \epsilon)|\langle \rho | W_2 \rangle| + \epsilon |\langle \rho | P \rangle|$, which implies $\langle \rho | W_2 \rangle < 0$ and therefore $\rho \notin D_{W_2}$. (Only if) We define $\lambda$ as in (3). Using Lemma 1(iv) we have $W_1$ has $\lambda \geq 1$. First, if $\lambda = 1$ then according to Lemma 1(iv) we have $W_1 = W_2$ (i.e., $\epsilon = 0$). For $\lambda > 1$, we define $P = (\lambda - 1)^{-1}(\lambda W_1 - W_2)$ and $\epsilon = 1 - 1/\lambda > 0$. We have that $W_1 = (1 - \epsilon)W_2 + \epsilon P$, so that it only remains to be shown that $P \geq 0$. But this follows from Lemma 1(i–iii) and the definition of $\lambda$, $\lambda = \inf_{\rho_1 \in D_{W_1}} \frac{|\langle \rho_1 | W_2 \rangle|}{|\langle \rho_1 | W_1 \rangle|}$. □

The previous lemma provides us with a way of determining when an EW is finer than another one. With this result, we are now at the position of fully characterizing OEW.

**Theorem 1:** $W$ is optimal iff for all $P$ and $\epsilon > 0$, $W' = (1 + \epsilon)W - \epsilon P$ is not an EW (does not fulfill (I)).

**Proof:** (If) According to Lemma 2, there is no EW which is finer than $W$, and therefore $W$ is optimal. (Only if) If $W'$ is an EW, then according to Lemma 2 $W$ is not optimal. □

The previous theorem tells us that $W$ is optimal iff when we subtract any positive operator from it, the resulting operator is not positive on product vectors. This result is not very practical because of two reasons: (1) for a given $P$ it is typically very hard to check whether there exists some $\epsilon > 0$ such that $W - \epsilon P$ is positive on all product vectors; (2) it may be difficult to find a particular $P$ that can be subtracted from $W$ among all possible positive operators. In Appendix A we show how to circumvent these two drawbacks in practice: we give a simple criterion to determine when a given $P$ can be subtracted from $W$. This allows us to determine which are the positive operators which can be subtracted from a given EW.

In the rest of this subsection we will present some simple results related to these two questions. First, it is clear that not every positive operator $P$ can be subtracted from an EW, $W$. In particular, the following lemma tells us that it must vanish on $P_W$.

**Lemma 3:** If $PP_W \neq 0$ then $P$ cannot be subtracted from $W$.

**Proof:** There exists some $|e_0, f_0 \rangle \in P_W$ such that $\langle e_0, f_0 | P | e_0, f_0 \rangle > 0$. Substituting this product vector in the condition I for any $W - \epsilon P$ we see that the inequality is not fulfilled for any $\epsilon > 0$, i.e. $P$ cannot be subtracted. □

**Corollary 2:** If $P_W$ spans $H$ then $W$ is optimal.

Note that, as announced at the beginning of this Section, the set $P_W$ plays an important role in determining the properties of the separable states which lie on the border with the entangled states. We see here, that this set also plays an important role in determining whether an EW is optimal or not.

On the other hand, in order to check whether a given operator $P$ can be subtracted or not from $W$, one has to check whether there exists some $\epsilon > 0$ such that $\langle e, f | W - \epsilon P | e, f \rangle > 0$ for all $|e, f \rangle$. The following lemma gives an alternative way to do this. In fact, it gives a necessary and sufficient criterion for an EW to be optimal. For a given $|e \rangle \in H_A$, we will denote by $W_e = \langle e | W | e \rangle$.

**Lemma 4:** $W$ is optimal iff for all $\Psi$ orthogonal to $P_W$

$$\epsilon \equiv \inf_{|e \rangle \in H_A} \left(\langle \Psi | W_e^{-1} \langle e | \Psi \rangle\right)^{-1} = 0.$$

(7)

**Proof:** (If) Let us assume that $W$ is not optimal: that is, there exists $W' \neq W$, finer than $W$. Then, according to Lemma 2 we have that there exists $\epsilon_0 > 0$ and $P \geq 0$ such that $W' = (W - \epsilon_0 P)/(1 - \epsilon_0)$. Imposing that $W'$ is positive on product vectors (i.e., $W'_e \geq 0$ for all $|e \rangle \in H_A$) we obtain $0 \leq \langle e | W - \epsilon_0 P | e \rangle \leq W_e - \epsilon_0 \lambda_\Psi \langle e | \Psi \rangle \langle \Psi | e \rangle$, where $|\Psi\rangle$ is any eigneastate of $P$ with nonzero eigenvalue $\lambda_\Psi$. According to Ref. [22], this last operator is positive iff both: (i) $\langle e | \Psi \rangle$ is in the range of $\langle e | W | e \rangle$, which imposes that $|\Psi\rangle$ is orthogonal to $P_W$; (ii) $\lambda_\Psi \epsilon_0 \leq \left(\langle e | W_e^{-1} \langle e | \Psi \rangle\right)^{-1}$, which imposes that $\epsilon \geq \lambda_\Psi \epsilon_0 > 0$ for that given $|\Psi\rangle$. (Only if) Let us assume that there exists some $|\Psi\rangle$ orthogonal to $P_W$ such that $\epsilon > 0$. Then, using the same arguments one can show that $W' \equiv (W - \epsilon \langle \Psi | W \langle \Psi | \rangle)/(1 - \epsilon) \neq W$ is an EW. According to Lemma 2, $W'$ is finer than $W$, so that $W$ is not optimal. □

**C. Decomposable entanglement witnesses**

There exists a class of EW which is very simple to characterize, namely the decomposable entanglement witnesses (d-EW) [28]. Those are EW that can be written in the form

$$W = aP + (1 - a)Q^T,$$

(8)

where $a \in [0, 1]$. As it is well known (see next section), these EW cannot detect PPTES. In any case, for the sake of completeness, we will give some simple properties of optimal d-EW.
Theorem 2: Given a d–EW, \( W \), if it is optimal then it can be written as \( W = Q^T \), where \( Q \geq 0 \) contains no product vector in its range.

Proof: Since \( W \) is decomposable, it can be written as \( W = aP + (1 - a)Q^T \). \( W' \propto W - aP \) is also a witness, which according to Lemma 2 is finer than \( W \), and therefore \( W \) is not optimal. On the other hand, if \( |e, f\rangle \in R(Q) \) then for some \( \lambda > 0 \) we have that \( W \propto (Q - \lambda |e, f\rangle \langle e, f|)^T \) is finer than \( W \), and therefore this last is not optimal. \( \Box \)

This previous result can be slightly generalized as follows:

Theorem 2': Given a d–EW, \( W \), if it is optimal then it can be written as \( W = Q^T \), where \( Q \geq 0 \) and there is no operator \( P \in R(Q) \) such that \( P^T \geq 0 \).

Proof: Is the same as in previous theorem. \( \Box \)

Corollary 3: Given a d–EW, \( W \), if it is optimal then \( W^T \) is not an EW [does not fulfill (II)].

Proof: Using Theorem 2 we have that \( W = Q^T \) with \( Q \geq 0 \). Then \( W^T = Q \geq 0 \), which does not satisfy property (ii). \( \Box \)

IV. NON–DECOMPOSABLE ENTANGLEMENT WITNESSES

In the previous section we have been concerned with EW in general. As mentioned above, when studying separability we just have to consider those EW that can detect PPTES. In order to characterize them, one defines non–decomposable witnesses (nd–EW) as those EW which cannot be written in the form \( (8) \). This section is devoted to this kind of witnesses. The importance of nd–EW in order to detect PPTES is reflected in the following

Theorem 3: An EW is non–decomposable iff it detects PPTES.

Proof: (If) Let us assume that the EW is decomposable. Then it cannot detect PPT, since if \( \rho, \rho^T \geq 0 \) we have \( \text{tr}(aP + (1 - a)Q^T)\rho = a\text{tr}(P\rho) + (1 - a)\text{tr}(Q\rho^T) \geq 0 \). (Only if) The set of decomposable witnesses is convex and closed, and \( W \), as a set containing one point, is a closed convex set itself. Thus, from Hahn–Banach theorem \( \Box \) it follows that there exists an operator \( p \) such that: (i) \( \text{tr}[aP + (1 - a)Q^T]p \geq 0 \) for all \( P, Q \geq 0 \), \( a \in [0,1] \); (ii) \( \text{tr}(W^T) < 0 \). From (i), taking \( a = 1 \) we infer that \( \rho \geq 0 \), taking \( a = 0 \) we obtain that \( \text{tr}(p^TQ) \geq 0 \) for all \( Q \geq 0 \), and therefore \( \rho^T \geq 0 \). Thus, \( W \) detects \( \rho \) which is a PPTES. \( \Box \)

Corollary 4: Given an operator \( D \), it is decomposable iff \( \text{tr}(D\rho) \geq 0 \) for all \( \rho, \rho^T \geq 0 \).

A. Definitions

In this subsection we introduce some definitions which are parallel to those given in the previous section. Given a nd–EW, \( W \), we define:

- \( d_W = \{ \rho \geq 0, \text{ such that } \rho^T \geq 0 \text{ and } (\rho)_W < 0 \} \);
- Non–decomposable-finer (nd–finer): Given two nd–EW, \( W_1 \) and \( W_2 \), we say that \( W_2 \) is nd–finer than \( W_1 \), if \( d_{W_1} \subseteq d_{W_2} \); that is, if all the operators detected by \( W_1 \) are also detected by \( W_2 \).
- Non–decomposable optimal entanglement witness (nd–OEW): We say that \( W \) is an nd–OEW if there exist no other nd–EW which is nd–finer.
- \( p_W = \{ |e, f\rangle \in H, \text{ such that } \langle e, f|W|e, f\rangle = 0 \} \); that is, the product vectors on which \( W \) vanishes.

Note again the important role that the vectors in \( p_W \) play regarding PPTES. If we have a nd–EW, \( W \), which detects a given PPTES \( \rho \), then the operator \( \rho' = \rho + \rho_w \) where \( \rho_w \) has the form \( (9) \) with \( p_w \geq 0 \), and \( \langle e_k, f_k| \in p_W \) also describes a PPTES. Thus, any operator of the form \( (9) \) lies in the border between separable states and PPTES.

B. Optimal non–decomposable entanglement witness

The goal of this section is to find a necessary and sufficient condition for a nd–EW to be optimal. We start by proving a similar result to the one given in Lemma 1, but for nd–EW:

Lemma 1b: Let \( W_2 \) be nd–finer than \( W_1 \),

\[
\lambda \equiv \inf_{\rho \in d_{W_1}} \frac{\text{tr}(W_2\rho)}{\text{tr}(W_1\rho)},
\]

and now both, \( \rho, \rho^T \geq 0 \). Then we have have (i–iv) as in Lemma 1.

Proof: The proof is basically the same as in Lemma 1 and will be omitted here.

Corollary 1b: Given two nd–EW, \( W_{1,2} \), then \( d_{W_1} = d_{W_2} \) iff \( W_1 = W_2 \).

Proof: The proof is basically the same as Corollary 1 and will be omitted here.

Lemma 2b: Given two nd–EW, \( W_{1,2} \), \( W_2 \) is nd–finer than \( W_1 \) iff there exists a decomposable operator \( D \) and \( 1 > \epsilon \geq 0 \) such that \( W_1 = (1 - \epsilon)W_2 + \epsilon D \).

Proof: (If) Given any \( \rho, \rho^T \geq 0 \), we have that if \( \rho \in d_{W_1} \), then \( 0 > \langle \rho|W_1 = (1 - \epsilon)|\rho\rangle_{W_2} + \epsilon|\rho\rangle_D \geq (\rho)_W_2 \), where in the last inequality we have used that \( (\rho)_D \geq 0 \) since \( D \) is decomposable (see Corollary 4). Therefore \( \rho \in d_{W_2} \). (Only if) We define \( \lambda \) as in \( (9) \), so that \( \lambda \geq 1 \) according to Lemma 1b(iv). If \( \lambda = 1 \) we have \( W_1 = W_2 \). If \( \lambda > 1 \) we define \( D = (\lambda - 1)^{-1}(\lambda W_1 - W_2 ) \) and \( \epsilon = 1 - 1/\lambda \). We have that \( W_1 = (1 - \epsilon)W_2 + \epsilon D \), so that it only remains to be shown that \( D \) is decomposable. But from Lemma 1b(i–iii) and the definition of \( \lambda \) it follows
that \( \langle \rho \rangle_D \geq 0 \) for all \( \rho, \rho^T \geq 0 \). Using Corollary 4 we then have that \( D \) is decomposable. \( \square \)

Now we are able to fully characterize nd–OEW.

**Theorem 1b:** Given an nd–EW, \( W \), it is nd–optimal iff for all decomposable operators \( D \) and \( \epsilon > 0 \), \( W' = (1 + \epsilon)W - \epsilon D \) is not an EW [does not fulfill (I)].

**Proof:** Is the same as for Theorem 1. \( \square \)

Theorems 1 and 1b allow us to relate OEW and nd–OEW. In this way we can directly translate the results for general OEW to nd–OEW. We have

**Theorem 4:** Given a nd–EW, \( W, W \) is a nd–EW iff both \( W \) and \( W^T \) are OEW.

**Proof:** (If) Let us assume that \( W \) is not a nd–EW. Then, according to Theorem 1b there exists \( \epsilon > 0 \) and a decomposable operator \( D \) such that \( W' = (1 + \epsilon)W - \epsilon D \) is a nd–EW. We can write \( D = aP + (1 - a)Q^T \), with \( a \in [0, 1] \). If \( a = 0 \), then \( W_1 = (1 + \epsilon a)W - \epsilon a P \) fulfills \( \langle e, f | W_1 | e, f \rangle \geq \langle e, f | W' | e, f \rangle \geq 0 \), and therefore, according to Lemma 2, \( W \) is not optimal. If \( a = 1 \) then \( W_2 = [1 + (1 - \epsilon)]W - (1 - \epsilon)Q \) fulfills \( \langle e, f | W_2 | e, f \rangle \geq \langle e, f | (W')^T | e, f \rangle \geq 0 \). If \( \epsilon > 0 \), \( W \) is an EW and therefore \( W' \) is not optimal. (Only if) According to Theorem 1b, if \( W \) is nd–optimal then for all \( D = aP + (1 - a)Q^T \), with \( a \in [0, 1] \), and all \( \epsilon > 0 \) we have that \( W' = (1 - \epsilon)W - \epsilon D \) does not satisfy (I). Taking \( a = 1 \) we have for all \( P \) and \( \epsilon > 0 \), \( W_1 = (1 - \epsilon)W - \epsilon P \) does not fulfill (I), and therefore (Theorem 1) \( W \) is optimal; analogously, taking \( a = 0 \) we have that \( W^T \) is optimal also. \( \square \)

**Corollary 5:** \( W \) is a nd–EW iff \( W^T \) is an nd–EW.

**V. OPTIMIZATION**

In this Section we give a procedure to optimize EW which is based on the results of the previous Sections.

**A. Optimization of general entanglement witnesses**

Our method is based in the following lemma. It tells us how much we can subtract from an EW. Here we will denote by \( W_e = \langle e | W | e \rangle \) and \( P_e = \langle e | P | e \rangle \) where \( | e \rangle \in H_A \) by \( [\ldots]_{\min} \) the minimum eigenvalue, and by \( [\ldots]_{\max} \) the maximum eigenvalue. On the other hand, \( X^{1/2} \) will denote the square root of the pseudoinverse of \( X \) [35].

**Lemma 5:** If there exists some \( P \) such that \( PP_W = 0 \) and

\[
\lambda_0 \equiv \inf_{| e \rangle \in H_A} \left[ D_e^{-1/2} W_e D_e^{-1/2} \right]_{\min}
\]

\[
= \left( \sup_{| e \rangle \in H_A} \left[ W_e^{-1/2} P_e W_e^{-1/2} \right]_{\max} \right)^{-1} > 0.
\]

then

\[
W'(\lambda) \equiv (W - \lambda D)/(1 - \lambda)
\]

with \( \lambda > 0 \) is an EW iff \( \lambda \leq \lambda_0 \).

**Proof:** Let us find out for which values of \( \lambda \geq 0 \), \( W'(\lambda) \) is an EW. We have to impose condition (I), which can be written as \( \langle e | W'(\lambda) | e \rangle \geq 0 \), i.e.

\[
W_e - \lambda P_e \geq 0.
\]

Multiplying by \( P_e^{-1/2} \) on the right and left of this equation we obtain \( P_e^{-1/2} W_e P_e^{-1/2} \geq \lambda P_e \), which immediately gives that \( \lambda \leq \lambda_0 \) given in the first part of Eq. (10).

On the other hand, multiplying by \( W_e^{-1/2} \) on the right and left of Eq. (12) we obtain \( W_e^{-1/2} P_e W_e^{-1/2} \leq 1/\lambda \), which immediately gives that \( \lambda \leq \lambda_0 \) given in the second equality of Eq. (10). \( \square \)

Lemma 5 provides us with a direct method to optimize EW by subtracting positive operators for which the elements of \( P_W \) are contained in their kernels. The method thus consists of: (1) determining \( P_W \); (2) choosing an operator \( P \) so that \( PP_W = 0 \) and determining \( \lambda \) using (10); (3) if \( \lambda \neq 0 \) then we subtract the operator \( P \) according to Lemma 5. Continuing in the same vein we will reach an OEW. In Appendix A we show how to accomplish steps (1) and (2) in practice.

**B. Optimization of non–decomposable entanglement witnesses**

For nd–EW we have the following generalization of Lemma 5:

**Lemma 5b:** Given a nd–EW, \( W \), if there exists some decomposable operator \( D \) such that \( DP_W = 0 \) and

\[
\lambda_0 \equiv \inf_{| e \rangle \in H_A} \left[ D_e^{-1/2} W_e D_e^{-1/2} \right]_{\min}
\]

\[
= \left( \sup_{| e \rangle \in H_A} \left[ W_e^{-1/2} P_e W_e^{-1/2} \right]_{\max} \right)^{-1} > 0.
\]

then

\[
W'(\lambda) \equiv (W - \lambda D)/(1 - \lambda)
\]

with \( \lambda > 0 \) is a nd–EW iff \( \lambda \leq \lambda_0 \).

**Proof:** Is the same as for Lemma 5.

With the help of Lemma 5b we can optimize nd–EW by subtracting decomposable operators as follows: (1) determining \( p_W \) and \( p_{W^T} \); (2) choosing an operator \( P \) so that \( PP_W = 0 \) and \( Q_{pW^T} = 0 \), building \( D = aP + (1 - a)Q^T \) with \( a \in [0, 1] \), and determining \( \lambda_0 \) using (13); (3) if \( \lambda_0 \neq 0 \) then we subtract the operator \( P \) according to Lemma 5b.

**C. Detectors of “edge” PPTES**

In the previous subsections we have have given two optimization procedures. In both of them, starting from a general EW one can obtain one which is optimal (or nd–optimal). It may well happen that the EW found in this
way is non–decomposable even though the original one was decomposable. To check that one simply has to use Corollary 3; that is, check whether $W^T$ is an EW or not. In case it is, then the OEW $W$ is non–decomposable. However, nothing guarantees that the final EW is non–decomposable if the original one is not. In this subsection we describe a general method to construct nd–EW using the optimization procedures introduced earlier. This method generalizes the one presented in Ref. 25.

We are going to use the results presented in Ref. 24,21. There, we have already used and discussed the “edge” PPTES, without naming them, however. Let us now introduce the following definition:

**Definition:** [see Ref. 24] A PPTES $\delta$ is an “edge” PPTES if for all product vector $|e,f\rangle$ and $\epsilon > 0$, $\delta - \epsilon|e,f\rangle\langle e,f|$ is not a PPTES.

This definition implies that that the “edge” states lie on the boundary between the PPTES and entangled states with non–positive partial transpose. In this subsection we will show how, out of an “edge” PPTES, we can construct a nd–OEW that detects it. As we mentioned in the introduction, “edge” PPTES are of special importance. In particular, they allow to provide a canonical form to write PPTES in arbitrary Hilbert spaces. For these reasons, some of the properties of the “edge” PPTES are discussed in Appendix B.

In order to check whether a PPTES $\delta$ is an “edge” PPTES we can use the range criterion (see also 24). That is, $\delta$ is an “edge” PPTES iff for all $|e,f\rangle \in R(\delta)$, $|e,f^*\rangle \not\in R(\delta^T)$.

Let $\delta$ be an “edge” PPTES, and let us denote by $P_1$ the projector onto $K(\delta)$ and by $Q_1$ the projector onto $K(\delta^T)$. We define

$$W_\delta = a(P_1 + Q_1^T),$$

where $a = 1/\text{tr}(P_1 + Q_1)$. Let us also define

$$\epsilon_1 \equiv \inf_{|e,f\rangle} \langle e,f|W_\delta|e,f\rangle.$$

Then we have

**Lemma 6:** Given an “edge” PPTES $\delta$, then $W_1 \propto W_2 - \epsilon_1 1$ is a nd–EW, where $\epsilon_1$ and $W_2$ are defined in section II, respectively.

**Proof:** We have that $\langle e,f|W_\delta|e,f\rangle = a\langle e,f|P_1|e,f\rangle + \langle e,f^*|Q_1|e,f^*\rangle \geq 0$. This quantity is zero iff $\langle e,f|P_1|e,f\rangle = \langle e,f^*|Q_1|e,f^*\rangle = 0$. But this is not possible since $\delta$ is an “edge” PPTES. Thus, $\langle e,f|W_\delta|e,f\rangle > 0$ for all $|e,f\rangle$. Defining $\epsilon_1$ as in (14), and taking into account that $\langle e,f|W_\delta|e,f\rangle$ is a continuous function of (the coefficients of) $|e,f\rangle$ and that the set in which we are taken the infimum is compact, we obtain $\epsilon_1 > 0$. Then we obviously have that $W_1$ fulfills properties (I) and (III). On the other hand, $\langle \delta|W_1 \propto a(\langle \delta|P_1 + (\delta^T)Q_1\rangle - \epsilon_1 < 0$, since $P_1\delta = Q_1\delta^T = 0$. Thus, $W_1$ detects a PPTES, and therefore, according to Theorem 3 is non–decomposable.

Note that Lemma 6 provides an important generalization of the method of Terhal 25, based on the use of unextendible product bases 13. Our method works in Hilbert spaces of arbitrary dimensions, and in particular when $\dim(H_1) = 2$ (in $2 \times N$ dimensional systems) for which unextendible product basis do not exist. By combining Lemma 6 and the optimization procedure introduced earlier, we obtain a way of creating nd–OEW. Once we have $W_1$ we find $p_{W_1}$ and $p_{W_1^T}$. We denote by $P_2$ and $Q_2$ the projector operators orthogonal to these two sets, respectively,

$$\epsilon_2 = \inf_{|e,f\rangle} \langle e,f|W_1|e,f\rangle \langle e,f|P_2 + Q_2^|e,f\rangle,$$

and $W_2 \propto W_1 - \epsilon_2(p_{W_2} + Q_2^T)$. According to Lemma 2b we have that $W_2$ is nd–finer than $W_1$. Now we can define $p_{W_2}, p_{W_2^T}, P_3, Q_3$ and $W_3$ in the same way, and continue in this vein until for some $k$, $\epsilon_k = 0$. If $W_k$ is not yet optimal, we still have to find other projectors such that we can optimize as explained in the previous subsections.

In Section VII we illustrate this method with a family of edge PPTES from Ref. 13. In fact, as we will mention in that Section, we have checked that the optimization method typically works as well by starting with three random vectors, and following a similar procedure to the one indicated here. This means that in our construction method we do not need in practice to start from a “edge” PPTES.

**D. Sufficient condition for PPTES**

In this subsection we use the results derived in the previous one to construct a sufficient criterion for non–separability of PPTES. As shown in Ref. 20,21, given an operator $\rho \geq 0$, with $\rho^T \geq 0$, we can always decompose it in the form

$$\rho = \rho_s + \delta,$$

where $\rho_s$ is separable and $\delta$ is an “edge” PPTES. More details concerning this decomposition, and in particular its canonical optimal form are presented in Appendix B. In this section we use this decomposition together with the following

**Lemma 7:** Given a non–separable operator $\rho = \rho_s + \delta$, where $\rho_s \geq 0$ is separable then for all EW, $W$, such that $\langle \rho|W < 0$ we have that $\langle \delta|W < 0$.

**Proof:** Obvious from the definition of EW.

**Lemma 7** tells us that if $\rho$ is non–separable, then there must exist some EW that detect both $\delta$ and $\rho$. Actually, it is clear that there must exist an OEW with that property. In particular, if $\rho^T \geq 0$, it must be a nd–OEW. In the previous subsection we have shown how to build them out of “edge” PPTES. Thus, given $\rho$ we can always decompose it in the form (13), construct an OEW that detects $\delta$ and check whether it detects $\rho$. In that case, we will have that $\rho$ is non–separable. Thus, this provides a sufficient criterion for non–separability.
We stress the fact that for PPTES only a special class of states, namely the class of “edge” PPTES, is responsible for the entanglement properties. In fact, one should stress that very many of the examples of PPTES discussed so far in the literature belong to the class of “edge” PPTES: the $2 \otimes 4$ family from [13], the $n \otimes n$ states obtained via unextendible product basis construction [14], the $3 \otimes 3$ states obtained via the chess-board method [14] (b), and projections of continuous variable PPTES onto finite dimensional subspaces [15] (c).

VI. POSITIVE MAPS

It is known that PM allow for necessary and sufficient conditions for separability (or, equivalently, entanglement) of bipartite mixed states [11]. PM’s have been also applied in the context of distillation of entanglement [25] and information theoretic analysis of separability [36]. In this Section we will use the isomorphism between operators and linear maps to extend the properties derived for witnesses to PM [25]. We will first review some of the definitions and properties of linear maps.

Let us consider a linear map $\mathcal{E} : B(H_A) \to B(H_C)$. We say that $\mathcal{E}$ is positive if for all $Y \in B(H_A)$ positive, $\mathcal{E}(Y) \geq 0$. One can extend a linear map as follows. Given $\mathcal{E} : B(H_A) \to B(H_C)$, we define its extension $\mathcal{E} \otimes 1_B : B(H_A) \otimes B(H_B) \to B(H_C) \otimes B(H_B)$ according to $\mathcal{E} \otimes 1_C(\sum_i Y_i \otimes Z_i) = \sum_i \mathcal{E}(Y_i) \otimes Z_i$, where $Y_i \in B(H_A)$ and $Z_i \in B(H_B)$. A linear map is completely positive if all extensions are positive. The classification and characterization of positive (but not completely positive) maps is an open question (see, e.g. Ref. [28,29]).

An example of positive (but not completely positive) map is transposition (in a given basis $O_A$); that is, the map $\mathcal{E}_T$ such that $\mathcal{E}_T(Y) = Y^T$. The corresponding extension is the partial transposition [12]. A map $\mathcal{E}$ is called decomposable if it can be written as $\mathcal{E} = \mathcal{E}_1 + \mathcal{E}_2 \cdot \mathcal{E}_T$, where $\mathcal{E}_1, \mathcal{E}_2$ are completely positive.

One can relate linear maps with linear operators in the following way. We will assume $d_A \equiv \dim(H_A) \leq \dim(H_C)$, but one can otherwise exchange $H_A$ by $H_C$ in what follows. Given $X \in B(H_A \otimes H_C)$ and an orthonormal basis $O_A = \{|k\rangle\}_{k=1}^{d_A}$ in $H_A$, we define the linear map $\mathcal{E}_X : B(H_A) \to B(H_C)$ according to

$$\mathcal{E}(Y) = \text{tr}_A(X^{T_A}Y),$$

for all $Y \in B(H_A)$, where $\text{tr}_A$ denotes the trace in $H_A$ and the partial transpose is taken in the basis $O_A$. Similarly, given a linear map we can always find an operator $X$ such that (13) is fulfilled. For instance, if we choose $T = (|\Psi\rangle\langle\Psi|)^{T_A}$, where

$$|\Psi\rangle = \sum_{k=1}^{d_A} |k\rangle_A \otimes |k\rangle_C,$$
A. Family of “edge” PPTES

We consider $H_A = \mathbb{C}^2$ and $H_B = \mathbb{C}^4$, and denote by $\{ |k\rangle \}_{k=0}^{d_A}$ ($\alpha = A, B$) an orthonormal basis in these spaces, respectively. Most of the time we will write the operators in those bases; that is, as matrices. For operators acting in $H_A \otimes H_B$ we will always use the following order $\{ |0,0\rangle, |0,1\rangle, \ldots, |1,0\rangle, |1,1\rangle, \ldots \}$. On the other hand, all partial transposes will be taken with respect to $H_B$.

We consider the following family of positive operators

$$\rho_b = \frac{1}{7b + 1} \begin{pmatrix} b & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & b & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & b & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & b & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1+b}{2} & 0 & 0 & \frac{1-b}{2} \\ b & 0 & 0 & 0 & 0 & b & 0 & 0 \\ 0 & b & 0 & 0 & 0 & 0 & b & 0 \\ 0 & 0 & b & 0 & 0 & 0 & 0 & b \end{pmatrix}, \quad (23)$$

where $b \in [0, 1]$. For $b = 0, 1$ those states are separable, whereas for $0 < b < 1$, $\rho_b$ is an “edge” PPTES. This can be shown by checking directly that they violate the range criterion of Ref. [13], i.e. the definition given in Section IVC.

If we take the partial transpose in the basis $\{ |k\rangle \}$, the density operators $\rho_b$ have the property that $\rho_b^T = U_B \rho_b U_B^T$, with $U_B = (\sigma_x)_{03} \oplus (\sigma_x)_{12}$. Here, the subscript $ij$ denotes the subspace, $\mathcal{H}_{Bij} \subset \mathcal{H}_B$ spanned by $\{ |i\rangle, |j\rangle \}$ and $\sigma_x$ is one of the Pauli-operators. Note that $U_B$ is a real unitary operator acting only on $H_B$. This immediately implies that

$$\tilde{\rho}^T_b = \tilde{\rho}_b,$$  \quad (24)

where $\tilde{\rho}_b = V_B \rho_b V_B^T$ and $V_B = 1 \sqrt{2} (1 + i \sigma_x)_{03} \oplus (1 + i \sigma_x)_{12}$. We will use the property (24) to simplify the problem of constructing the nd–OEW. Thus, we will concentrate from now on the operators $\rho_b$ [13]. Obviously, $\tilde{\rho}_b$ is an “edge” PPTES for $1 > b > 0$.

The projector onto the kernel of $\rho_b$, $P_1$, is invariant under the transformation $T_{AB} = T_A \otimes T_B$, where

$$T_A = \begin{pmatrix} 1 & 0 \\ 0 & e^{i 2 \pi / 3} \end{pmatrix}, \quad (25)$$

$$T_B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos (2 \pi / 3) & - \sin (2 \pi / 3) & 0 \\ 0 & \sin (2 \pi / 3) & \cos (2 \pi / 3) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$  \quad (26)

Note that $T_B$ is a real matrix. Later on we will need its eigenstates with real coefficients; they are $|0\rangle \pm |3\rangle$. Note also that $T_{AB}^3 = I$.

B. Construction of nd–EW’s

We use now the methods developed in Section V to obtain a nd–OEW starting from $\tilde{\rho}_b$. That is, we define $W_b = P_1 + P_1^T$, where $P_1$ is the projector onto $K(\tilde{\rho}_b) = K(\tilde{\rho}_b^T)$. Our procedure consists of first subtracting the identity to obtain $W_1 = W_b - e_1 1$. Then, we subtract $P_2 + Q_2^T$, $P_3 + Q_3^T$, etc. in the $n$–th step we will have

$$W_n = W_{n-1} - e_n (P_n + Q_n^T), \quad (27)$$

where $P_n$ ($Q_n$) is the projector orthogonal to the space spanned by $P_{W_{n-1}}$ ($P_{W_{n-1}}^T$). We will use the symmetries of $\tilde{\rho}_b$ to better understand the structure of $W_n$.

(a) $W_n = W_n^T$. We can prove this by induction. First, it is clear that $W_1 = W_1^T$. Let us now assume that $W_{n-1} = W_{n-1}^T$. Then we show that $W_n = W_n^T$. For that, we just have to show that the subspace spanned by $P_{W_{n-1}}$ is the same that the one spanned by $P_{W_{n-1}}^T$, so that $Q_n = P_n$. But this is clear since $W_{n-1} = W_{n-1}^T$.

(b) $T_{AB} W_n T_{AB}^† = W_n$. We prove this by induction. First, for $W_1 = P_1 + P_1^T$ we have that $T_{AB} W_1 T_{AB}^† = (P_1 T_1^† + P_1^T T_1^† - e_1 1 = W_1$, since $T_{AB} P_1 T_1^† T_{AB} = (T_{AB} P_1 T_{AB}) T_{AB}^†$ (given the fact that $T_B$ is real) and $P_1$ is invariant under $T_{AB}$. Then, let us assume that $T_{AB} W_{n-1} T_{AB}^† = W_{n-1}$. In order to show that $T_{AB} W_n T_{AB}^† = W_n$ we just have to show that $P_n$ is invariant under $T_{AB}$, or, equivalently, that the subspace spanned by $P_{W_{n-1}}$ is invariant under $T_{AB}$. But this follows immediately from the fact that $T_{AB} W_{n-1} T_{AB}^† = W_{n-1}$.

Starting the property (a) it follows that the vectors $|e, f\rangle \in P_{W_n}$ will have $|f\rangle$ real (unless we have degeneracies). This can be seen by noticing that those vectors minimize $\langle e | f \| W_n | e \rangle$: defining $W_n = \langle e | W_n | e \rangle$, we have that $W_n = W_n = W_n^T$ is symmetric, and therefore the eigenstate corresponding to its minimum eigenvalue can be chosen to be real. On the other hand, starting from the property (b) it follows that if $|e, f\rangle \in P_{W_n}$ then $T_{AB}^† |e, f\rangle, T_{AB}^† |e, f\rangle \in P_{W_n}$. According to that, we will typically have two kinds of product vectors in $P_{W_n}$:

(1) $|e, f\rangle$ is an eigenstate of $T_{AB}^†$ with $|f\rangle$ real: There are only 4 possible product vectors which fulfill these conditions: $\{ |0\rangle, |1\rangle \} \subseteq \{ |0\rangle + |3\rangle, |0\rangle - |3\rangle \}$.

(2) $|e, f\rangle$ is not an eigenstate of $T_{AB}^†$: Then, we will also have: $T_{AB}^† |e, f\rangle, (T_{AB}^†)^2 |e, f\rangle \in P_{W_n}$. We have carried out this procedure for $\tilde{\rho}_b$ and found nd–OEW for each $b$. We find that for the optimal EW we have two vectors of the kind (1) and six of the kind (2).
In total we find eight product vectors in \( P_W \), which span the whole Hilbert space and therefore the corresponding EW are optimal (see Corollary 2). This means that any operator of the form (2) with \( |e_k, f_k⟩ ∈ P_W \) the product vectors we have found, and \( p_k > 0 \) will be a full range separable density operator that lies on the boundary between separable and PPTES. Up to our knowledge, this constitutes the first example of those operators \( \ref{2} \). We have also created the PM corresponding to the nd–OEW, which are the first examples of non–decomposable PM with minimal “qubit” domain, or – equivalently – minimal hermitian conjugate codomain.

In Fig. 1 we show for which \( b' \) \( \hat{ρ}_b \) is still detected by the nd–OEW created out of \( \hat{ρ}_b \). We find that for a given \( b \), the optimal witness that we create detects all \( \hat{ρ}_b \) for \( b ≤ b' \). Thus, in the figure we plot \( b' \) as a function of \( b \). As explained above, the corresponding positive map detects more than the witness itself. In the figure one can also see how much is detected by the positive map.

Finally, let us note that we have observed using numerical calculations that if one starts with a random projector, \( P \) of rank 3, and optimizes the decomposable operator \( W ≡ P + P^T ρ_b \) in the same way as the one described here, then one will end up with a nd–OEW \( W_b \), where \( p_W \) is complete. This means that in order to create nd–OEW one does not need to know in practice an edge PPTES. In another words, optimization itself is a way to reach nondecomposableness.

C. Analytical procedure

In this subsection we will present an analytical way to create nd–EW’s. Furthermore we will given an example of such a witness, which detects \( ρ \) for all \( b ∈ (0, 1) \). From Fig. 1 we see that the witness which detects most is the one we created out of \( \hat{ρ}_b \), where \( b \) is very close to 1. We will work with the original \( \hat{ρ}_b \).

We consider two hermitian operators \( A \) and \( B \), with \( A \) positive on product vectors, i.e., \( ⟨ e, f | A | e, f ⟩ ≥ 0 \), whereas \( B \) does not have to. As before we denote by \( P_A \) (\( P_B \)) the (not necessarily complete) set of product vectors on which \( A \) (\( B \)) vanishes. We require that for all \( | e, f ⟩ ∈ P_A \), \( ⟨ e, f | B | e, f ⟩ ≥ 0 \). Then we define \( W(x) ≡ \frac{1}{2}(A + xB) \) for any real \( x \). So we have the following

**Lemma 9:** If \( \lim_{x→0} ⟨ e, f | W(x) | e, f ⟩ < 0 \) then \( ρ \) is entangled.

**Proof:** We prove that \( \lim_{x→0} ⟨ e, f | W(x) | e, f ⟩ ≥ 0 \). This implies that if \( ρ \) is separable, then \( \lim_{x→0} ⟨ e, f | W(x) | e, f ⟩ ≥ 0 \). Let us therefore distinguish two cases: (i) if \( | e, f ⟩ ∈ P_A \) then we have that \( \lim_{x→0} ⟨ e, f | W(x) | e, f ⟩ = ⟨ e, f | B | e, f ⟩ \), which is, per assumption, positive. (ii) \( | e, f ⟩ ∉ P_A \) then we have \( \lim_{x→0} ⟨ e, f | W(x) | e, f ⟩ = \lim_{x→0} \frac{a}{2} + b \), where \( a = ⟨ e, f | A | e, f ⟩ > 0 \) and \( b = ⟨ e, f | B | e, f ⟩ \). Thus this limit tends to infinity, which proves the statement.

Note that \( W(x) \) is not an EW since it is not necessarily

FIG. 1. Values of \( b' \) for which \( b ≤ b' \), \( \hat{ρ}_b \) is detected by the witness and the positive map created starting from \( \hat{ρ}_b \).

FIG. 2. Maximum \( λ \) such that \( \hat{ρ}_b + λ1 \) is still detected by the witness and the positive map created starting from \( \hat{ρ}_b \).
positive on product vectors. However, one can make it positive by adding the identity operator to convert it into an EW.

**Corollary 6:** Given any \( x_0 > 0 \), then \( W(x_0) = \frac{1}{x_0}(A + x_0 B) + \lambda_x \mathbb{1} \), with \( \lambda_x = -\min_{e,f} \langle e,f \rangle \langle e,f \rangle_0 (A + x_0 B) \) is an EW.

Let us now illustrate how we can use Lemma 9 to detect all the states \( \rho_b \). We define

\[
A = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
-2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
\end{pmatrix}, \quad (27)
\]

\[
B = \begin{pmatrix}
1 & 0 & 0 & 1 & 0 & -2 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & -2 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & -2 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 \\
\end{pmatrix}. \quad (28)
\]

One can easily show that \( A = |\psi\rangle\langle\psi| + (|\phi\rangle\langle\phi|)^T_B \), where \( |\psi\rangle = |01\rangle - |12\rangle \) and \( |\phi\rangle = |02\rangle - |11\rangle \). Thus this operator is positive on product vectors, since it is decomposable. Let us now use unnormalized states in order to present the set of product vectors on which \( A \) vanishes, i.e. \( P_A \). \( P_A = P_{A_1} \cup P_{A_2} \), where \( P_{A_1} = \{(00) + (01)\} \otimes (x0) + y(3)\} \forall \alpha, x, y \) and \( P_{A_2} = \{(00) + (01)\} \otimes (x0) + y(3) + z(11) + e^{-i\Phi}|2| + e^{-i\Phi}|3\} \forall \phi \). The operator \( B \) has to be positive on those product vectors, i.e., \( \forall e,f \in P_{A_1} \) \( \langle e,f \rangle B(e,f) \geq 0 \). In order to show that this is indeed the case, we use that \( \forall e,f \in P_{A_2} \). In the first case we have that

\[
\langle e|B|e \rangle = \begin{pmatrix}
1 + |\alpha|^2 & -2\alpha & 0 & 1 - |\alpha|^2 \\
-2\alpha^* & 1 + |\alpha|^2 & 0 & 0 \\
0 & 0 & 1 + |\alpha|^2 & -2\alpha \\
1 - |\alpha|^2 & 0 & -2\alpha^* & 1 + |\alpha|^2 \\
\end{pmatrix}
\]

and so \( \langle e,f \rangle B(e,f) = |x + y|^2 + |\alpha|^2|x - y|^2 \geq 0 \). If \( e,f \in P_{A_2} \) then

\[
\langle e|B|e \rangle = \begin{pmatrix}
2 & -2e^{i\Phi} & 0 & 0 \\
-2e^{-i\Phi} & 2 & 0 & 0 \\
0 & 0 & 2 & -2e^{i\Phi} \\
0 & 0 & -2e^{-i\Phi} & 2 \\
\end{pmatrix} \quad (30)
\]

which is a positive operator and so \( \langle e,f \rangle B(e,f) \geq 0 \). So those two operators \( A \) and \( B \) fulfill all the required properties. Furthermore one can show that \( \langle \rho_b | A = 0 \) and \( \langle \rho_b | B < 0 \) for all \( 0 < b < 1 \). Thus we have that \( \lim_{x \to 0} (W(x) \rho_b) < 0 \) for all \( 0 < b < 1 \), where we defined \( W(x) = \frac{1}{x}(A + x B) \).

As mentioned above we can use now \( W(x) \) in order to create other PPTES just by adding product vectors on which \( W(x) \) vanishes. To find the product vectors we can add, we need all we need to do is to determine the intersection between \( P_A \) and \( P_B \). Since \( P_B = \{(00) + (01)\} \otimes (|0\rangle + e^{-i\Phi}|1\} + b(2) + e^{-i\Phi}|3\} \forall \phi, a, b \) we have that \( S = P_A \cap P_B = \{(00) + (01)\} \otimes (|0\rangle + e^{-i\Phi}|1\} + e^{-i\Phi}(2) + e^{-i\Phi}|3\} \forall \phi \). Note that \( S \) spans a 5 dimensional subspace and that the orthogonal subspace is spanned by the vectors \( \{|02\rangle + |13\rangle, -|01\rangle + |12\rangle, -|00\rangle + |11\rangle \} \).

**VIII. CONCLUSIONS**

Entanglement witnesses allow us to study the separability properties of density operators. We have defined OEW, which are those that detect entanglement in an optimal way. We have given necessary and sufficient conditions for an EW to be optimal, and we have shown a way to construct them. We have also concentrated on nd-EW, which are those that detect PPTES. We have extended the definitions of optimality and the optimization procedure to those EW. It turns out that one can optimize nd–EW by subtracting decomposable operators. We have also given an explicit method to construct nd–EW starting from “edge” PPTES. We have also mentioned that this method works by starting out from random operators. We have extended our techniques to PM, and therefore given a method to systematically construct non–decomposable positive maps. We have illustrated our methods with a family of “edge” PPTES acting on \( \mathbb{C}^2 \otimes \mathbb{C}^2 \). The corresponding PM constitute the first examples of PM with minimal “qubit” domain, or – equivalently – minimal hermitian conjugate codomain. We have also constructed the first examples of separable states of full range that lie on the boundary between separable and PPTES. These states can be used for experimental realization of PPTES [3].

In this paper we have also introduced the “edge” PPTES, which violate the range criterion of separability. As shown in Appendix B, the “edge” PPTES allow us to construct a canonical form of PPTES in Hilbert spaces of arbitrary dimensions. They also allow us to give a novel sufficient condition for non–separability which applies to operators with positive partial transpose. It is based on the fact that among all PM (or EW) only the subset \( \{A_{\text{edge}}\} \) of those PM that detect edge PPTES are needed to study the separability of PPTES. This opens many interesting questions. Is it possible that in the set \( \{A_{\text{edge}}\} \) there is some map that is globally finer than the transposition? In another words, is there a map detecting the entanglement of all the states with non–positive partial transpose? What is the minimal subset of \( \{A_{\text{edge}}\} \) providing such condition? Is it finite?
Finally, let us consider the implications of the our results for the very interesting problem of locality of PPTES. There is a conjecture [20] that those states can be local in the sense that they admit a local hidden variable (LHV) model for any set of possible local measurements. The problem is not trivial given the fact that it may be important to take into account the role of sequential measurements and the possible existence of many copies. Quite recently it has been shown that PPTES satisfy Bell-type of inequalities introduced by Mermin [21]. There have been no examples of LHV models for states of low rank, so far. Thus, perhaps completely new techniques will be needed to study this problem. In this Appendix we study necessary and sufficient conditions under which an operator cannot be subtracted from an EW. This will give us automatically a criterion to determine when W is optimal.

In all this appendix we will use that given an EW, W, and an operator $P \geq 0$ we say that $P$ cannot be subtracted from W if for all $\lambda > 0$, $W - \lambda P$ does not fulfill (I). In other words, there exist $|e(\lambda)\rangle \in H_A$ and $|f(\lambda)\rangle \in H_B$ such that

$$\langle e(\lambda), f(\lambda)|(W - \lambda P)|e(\lambda), f(\lambda)\rangle < 0.$$  \hspace{1cm} (A1)

Note that $\langle e(\lambda), f(\lambda)|P|e(\lambda), f(\lambda)\rangle$ must be strictly positive, so that (A1) can be expressed as

$$\lim_{\lambda \rightarrow 0} \frac{\langle e(\lambda), f(\lambda)|(W|e(\lambda), f(\lambda)\rangle}{\langle e(\lambda), f(\lambda)|P|e(\lambda), f(\lambda)\rangle} = 0.$$  \hspace{1cm} (A2)

In the first subsection we will introduce some definitions and notation. In the second one we give a method to determine the set of product vectors $P_W$, on which W vanishes. In the third subsection we find a necessary and sufficient condition under which an operator cannot be subtracted from an EW. We will see that there must exist a vector $|e_0, f_0\rangle \in P_W$, some other vectors $|e_1\rangle$ and $|f_1\rangle$, and certain phases $\phi_e, f$ and $\theta$ such that some quantity is zero. In the next subsection we will see that the problem can be reduced to finding only the vectors $|e_0, f_0\rangle$ and $|f_0, e_0\rangle$. Finally, we will show that if $\dim(H_A) = 2$ we just have to find $|e_0\rangle$ and $|f_0\rangle$, which is very simple.

1. Definitions and notation

In order to prove the results of this appendix in a compact and readable form we have made an extensive numbers of definitions.

We will always denote by $|e_0, f_0\rangle$ a product vector in $P_W$, and by $|e_1\rangle \in H_A$ and $|f_1\rangle \in H_B$ two vectors orthogonal to $|e_0\rangle$ and $|f_0\rangle$, respectively. We will use the following notation:

$$W^k_l \equiv \langle e_i, f_j|W|e_k, f_l\rangle, \hspace{0.5cm} (i, j, k, l = 0, 1). \hspace{1cm} (A3)$$

and we will write

$$W^{0,1}_{1,0} = |W^{0,1}_{1,0}|e^{i\phi_0} \hspace{1cm} (A4a)$$

$$W^{1,1}_{0,0} = |W^{1,1}_{0,0}|e^{i\phi_1}. \hspace{1cm} (A4b)$$

We will also define the following operators:

$$w^e_{i,j} \equiv \langle e_i|W|e_j\rangle, \hspace{1cm} (A5a)$$

$$w^f_{i,j} \equiv \langle f_i|W|f_j\rangle. \hspace{1cm} (A5b)$$

The following vectors will be used in the context of Eq. (A3):

$$|e(\epsilon)\rangle = \frac{1}{\sqrt{1 + |\cos(\theta)\epsilon|^2}}(|e_0\rangle + \epsilon \cos(\theta) e^{i\phi_0} |e_1\rangle), \hspace{1cm} (A6a)$$

$$|f(\epsilon)\rangle = \frac{1}{\sqrt{1 + |\sin(\theta)\epsilon|^2}}(|f_0\rangle + \epsilon \sin(\theta) e^{i\phi_1} |f_1\rangle), \hspace{1cm} (A6b)$$
where \( \epsilon \) is a real number, and \( \phi, f \in [0, \pi] \) and \( \theta \in [0, \pi/2] \) are certain constants. Given a product vector \(|e(e), f(e)\rangle\) and an operator, \( W \), we will expand \(|e(e), f(e)|W|e(e), f(e)\rangle\) by collecting terms with the same powers in \( \epsilon \); that is, except for a normalization constant,

\[
\langle e(e), f(e)|W|e(e), f(e)\rangle \propto \sum_{i=1}^{4} \epsilon^i A_i(W), \quad (A7)
\]

where

\[
A_0(W) = W_{0,0}^{0,0}, \quad (A8a)
\]

\[
A_1(W) = 2\text{Re} \left[ \cos(\theta) e^{i\phi_e} W_{1,0}^{0,1} + \sin(\theta) e^{i\phi_f} W_{0,0}^{0,1} \right], \quad (A8b)
\]

\[
A_2(W) = \cos^2(\theta) W_{1,0}^{1,0} + \sin^2(\theta) W_{0,1}^{1,0} + 2\sin(\theta) \cos(\theta) \left[ e^{-i(\phi_e + \phi_f)} W_{1,0}^{0,1} + e^{i(\phi_e + \phi_f)} W_{0,0}^{0,1} \right], \quad (A8c)
\]

\[
A_3(W) = 2\sin(\theta) \cos(\theta) \left[ \cos(\theta) e^{i\phi_e} W_{1,1}^{1,1} + \sin(\theta) e^{i\phi_f} W_{0,1}^{1,1} \right], \quad (A8d)
\]

\[
A_4(W) = \sin^2(\theta) \cos^2(\theta) W_{1,1}^{1,1}. \quad (A8e)
\]

On the other hand, we will define

\[
|\Psi_{0,1}\rangle \equiv \sin(\theta) e^{i\phi_f} |e_0, f_1\rangle + \cos(\theta) e^{i\phi_e} |e_1, f_0\rangle. \quad (A9)
\]

Finally, the following quantity will play an important role in determining whether there exist vectors and parameters for which (A2):

\[
X(W) \equiv W_{1,0}^{1,0} W_{0,1}^{0,1} - (|W_{1,0}^{0,1}| + |W_{0,1}^{0,1}|)^2. \quad (A10)
\]

2. Determining \( P_W \)

As stated in Lemma 3, not every positive operator \( P \) can be subtracted from an EW, \( W \); it must vanish on \( P_W \). Thus, in order to choose \( P \) one has to know the set \( P_W \). In this subsection we give a method to determine it.

We start by characterizing the vectors in \( P_W \):

Lemma A1: Given an operator \( W \) satisfying (I), then \(|e_0, f_0\rangle \in P_W \) iff

\[
\langle e_0|W|e_0\rangle|f_0\rangle = 0, \quad (A11a)
\]

\[
|f_0\rangle|W|e_0\rangle|e_0\rangle = 0, \quad (A11b)
\]

Proof: (If) We just apply \(|f_0\rangle\) to Eq. (A11a). (Only if) Since \( W \) fulfills (I) then \( W_{e_0} = \langle e_0|W|e_0\rangle \) must be positive. Thus, \( \langle f_0|W|e_0\rangle|f_0\rangle = 0 \) implies Eq. (A11b). In the same way we obtain Eq. (A11b). □

In practice, for a given \( W \) the set \( P_W \) can be found as follows. Due to the fact that \( W \) is an EW we have that for any \(|e\rangle \in H_A, W_e \equiv \langle e|W|e\rangle \) must be a positive operator (i.e. \( \langle f|W_e|f\rangle \geq 0 \) for all \(|f\rangle \in H_B \)). Thus, the determinant \( \text{det}(W_e) \geq 0 \). According to Lemma A1, this determinant is zero iff there exists some \(|f_0\rangle \in H_B \) such that \( \langle f_0|W_{e_0}|f_0\rangle = 0 \), i.e., if \(|e_0, f_0\rangle \in P_W \). That is, the determinant as a function of \(|e\rangle \) has a minimum (which is zero) at \(|e_0\rangle \). We can use this fact to find \(|e_0\rangle \). Then, we can easily obtain \(|f_0\rangle \) via Eq. (A11a). We can expand an unnormalized state \(|e\rangle \) in an orthonormal basis \( \{|k\rangle\} \) as

\[
|e\rangle = \sum_{k=1}^{\dim(H_A)} c_k |k\rangle, \quad (A12)
\]

and impose that the corresponding determinant is zero. This gives us a polynomial equation for the coefficients \( c_k \), i.e.

\[
P(c_k, c_k^*) = 0. \quad (A13)
\]

We also impose that, given the fact that the determinant is a minimum,

\[
\frac{\partial}{\partial c_k} P(c_k, c_k^*) = \frac{\partial}{\partial c_k^*} P(c_k, c_k^*) = 0, \quad (A14)
\]

which also give a set of polynomial equations. These equations can be solved using the method mentioned in Ref. [20].

3. Necessary and sufficient conditions for subtracting an operator

In this subsection we give a necessary and sufficient condition for an operator \( P \) to be subtractable from an EW. We start out by giving some properties of the coefficients \( A(W) \) defined above (A8).

Lemma A2: Given \( W \) satisfying (I) and \(|e_0, f_0\rangle \in P_W \), then for all \(|e_1\rangle \in H_A \) and \(|f_1\rangle \in H_B \) we have

(i) \( A_0(W) = A_1(W) = 0 \).

(ii) \( A_2(W) \geq 0 \).

(iii) If \( A_2(W) = 0 \) then \( A_3(W) = 0 \).

Proof: (i) It is a direct consequence from Lemma A1. In order to prove (ii–iii) we use the fact that \( W \) satisfies (I). We define \(|e(e)\rangle\) and \(|f(e)\rangle\) as in (A6). We impose that \( \langle e(e), f(e)|W|e(e), f(e)\rangle \geq 0 \). Using the expansion (A7) and taking into account (i), we have \( A(e) \equiv A_2(W) + \epsilon A_3(W) + \epsilon^2 A_4(W) \geq 0 \) for all \( \epsilon \). This automatically implies (ii), since otherwise for sufficiently small \( \epsilon \) we would have \( A(e) < 0 \). It also implies (iii), since if \( A_3(W) < 0 \) \( A_3(W) > 0 \) then for sufficiently small \( \epsilon > 0 \) \( \epsilon < 0 \) we would have \( A(e) < 0 \). □

Now, we are at the position of giving a necessary and sufficient condition under which an operator cannot be subtracted from an EW:
Lemma A3: Given $P$ fulfilling $PP_W = 0$, it cannot be subtracted from $W$ iff there exists $(e_0, f_0) \in P_W$, $(e_1) \perp (e_0)$, $(f_1) \perp |f_0\rangle$, $\phi_{e,f}$, and $\theta$ such that $A_2(W) = 0$ but $A_2(P) \neq 0$.

Proof: (If) We define $|e(\lambda)\rangle$ and $|f(\lambda)\rangle$ as in (A4). Using Lemma A2(i) we have $A_2(W) = A_0(P) = A_1(W) = A_1(P) = 0$. Using Lemma A2(iii) we have that $A_3(W) = 0$. Thus, we can write the limit (A3) as

$$\lim_{\lambda \to 0} \frac{\lambda^2 A_4(W)}{A_2(P) + \lambda A_3(P) + \lambda^2 A_4(P)} = 0, \quad (\text{A15})$$

which obviously tends to zero given that $A_2(P) \neq 0$. (Only if) There exist two normalized vectors $|\tilde{e}(\lambda)\rangle$ and $|\tilde{f}(\lambda)\rangle$ (continuous functions of $\lambda$) fulfilling (A2). Taking the limit $\lambda \to 0$ in this expression we have that $\langle e(0), f(0)|W|\tilde{e}(0), \tilde{f}(0)\rangle = 0$, and therefore $|e_0, f_0\rangle \equiv |\tilde{e}(0), \tilde{f}(0)\rangle \in P_W$. This means that we can always choose $|\tilde{e}(\lambda)\rangle = |e(\lambda)\rangle$ and $|\tilde{f}(\lambda)\rangle = |f(\lambda)\rangle$ given in (A3), where $|e_1\rangle \perp |e_0\rangle$ and $|f_1\rangle \perp |f_0\rangle$ are two normalized vectors, $\lim_{\lambda \to 0} e(\lambda) = 0$, and $|e(\lambda), f(\lambda)\rangle \in P_W$.

We use (A6) to expand the numerator and denominator of (A3) as in (A7). According to Lemma A2(i) we have that $A_0(W) = A_0(P) = A_1(W) = A_1(P) = 0$. Thus, we must have

$$\lim_{\epsilon \to 0} \frac{A_2(W) + \epsilon A_3(W) + \epsilon^2 A_4(W)}{A_2(P) + \epsilon A_3(P) + \epsilon^2 A_4(P)} = 0. \quad (\text{A16})$$

This implies $A_2(W) = 0$ and $A_2(P) \neq 0$. Note that if both $A_2(W) = A_2(P) = 0$ then, according to Lemma A2(ii) we have that $A_3(W) = A_3(P) = 0$, so that $A_4(W)/A_4(P) = 0$. This can only be true because $A_4(W) = 0$ would imply that $|e(\lambda), f(\lambda)\rangle \in P_W$. Therefore $|e(\lambda), f(\lambda)\rangle \in P_W$.

Finally, we show in the next lemma that condition $A_2(W) = 0$ is equivalent to having certain vector in the kernel of $P$. We will use the vector $|\Psi_{0,1}\rangle$ defined in (A6).

Lemma A4: Given a positive operator $P$ and a set of vectors $|e_0, f_0\rangle \in K(P), |e_1\rangle \perp |e_0\rangle, |f_1\rangle \perp |f_0\rangle$, and parameters $\phi_{e,f}$, and $\theta$ then $A_2(P) = 0$ iff $|\Psi_{0,1}\rangle \in K(P)$.

Proof: Since $P \geq 0$ and $|e_0, f_0\rangle \in K(P)$ we have $P|e_0, f_0\rangle = 0$. Then, we can write $A_2(P) = \langle \Psi_{0,1}|P|\Psi_{0,1}\rangle$, with $|\Psi\rangle$ is defined in (A3), from which it is obvious that $A_2(P) = 0$ iff $|\Psi_{0,1}\rangle \in K(P)$.

4. Necessary and sufficient conditions for $A_2(W) = 0$

The previous lemmas tell us that we cannot subtract a given operator $P$ provided we can find some vectors and parameters such that $A_2(W) = 0$. The task of finding these vectors is difficult, in general. Here we will give a way to check whether these vectors exist. As before, we will denote by $|e_0, f_0\rangle$ a vector in $P_W$, and by $|e_1\rangle$ and $|f_1\rangle$ two vectors orthogonal to the first two. The quantity $X(W)$ defined in (A10) will play an important role in determining whether there exist vectors and parameters for which $A_2(W) = 0$. In this subsection, we will always have to choose the phases $\phi_{e,f}$ that minimize $A_2(W)$.

That is

$$e^{-i(\phi_e - \phi_f - \phi_0)} = -1, \quad e^{i(\phi_e + \phi_f + \phi_0)} = -1. \quad (\text{A17})$$

We will denote $\hat{A}_2(W)$ the value of $A_2(W)$ for this particular choice of phases. We have

$$\hat{A}_2(W) = \cos^2(\theta)W_{1,0}^1 + \sin^2(\theta)W_{0,1}^0 - 2\sin(\theta)\cos(\theta)\sqrt{W_{1,0}^0W_{0,1}^1} - X(W),$$

where we have used (A10).

Let us start showing that $X(W)$ is positive. We will use this property later on to reexpress the condition $A_2(W) = 0$ in terms of one that is simpler to check.

Lemma A5: $X(W) \geq 0$.

Proof: This follows from the fact that $A_2(W) \geq 0$ for all values of $\phi_{e,f}$. In particular, $A_2(W) \geq 0$, which according to (A18) implies $X(W) \geq 0$. □

The next lemma shows that we just have to check whether $X(W) = 0$ if we want to see if there exist parameters $\phi_{e,f}$ and $\theta$ such that $A_2(W) = 0$. This first condition is therefore much more useful than the last one.

Lemma A6: $X(W) = 0$ iff there exist $\phi_{e,f}$ and $\theta$ such that $A_2(W) = 0$.

Proof: (If) Given the phase $\theta = \theta_0$ we have that $0 = A_2(W) \geq \hat{A}_2(W)$. Thus, $\hat{A}_2(W) = 0$. According to (A18) we can have two cases: (a) $\theta_0 \neq 0, \pi/2$. In that case it is obvious that $X(W) = 0$. (b) $\theta_0 = 0, \pi/2$. In the first (second) case we must have $W_{1,0}^1 = 0$ ($W_{0,1}^0 = 0$). But this implies that $W_{1,0}^1 = W_{0,1}^0 = 0$, since otherwise we could always find some other value of $\theta$ such that $A_2(W) < 0$. Thus, $X(W) = 0$. (Only if) We choose $\phi_{e,f}$ as in (A17). For this value, according to (A18) we have

$$\hat{A}_2(W) = \left[\cos(\theta)\sqrt{W_{1,0}^1} - \sin(\theta)\sqrt{W_{0,1}^0}\right]^2,$$

which can always be zero for some particular value of $\theta$. □

Note that according to the proof of Lemma A6, if $W_{1,0}^1 = 0$ then $A_2(W) = 0$ only for $\theta = 0$. But in that case one can easily check that the vector $|e(\lambda), f(\lambda)\rangle \in P_W$, see (A5) which cannot be. Similarly, we conclude that $W_{1,0}^1 \neq 0$ if we want $A_2(W) = 0$. Thus, from now one we will assume that both $W_{1,0}^1$ and $W_{1,0}^0$ are not zero.

5. Optimality test

Thus, we can now state the steps to check whether an EW, $W$, can be optimized or not. (1) For each $|e_0, f_0\rangle \in P_W$ we must check whether there exist $|e_1\rangle \perp |e_0\rangle$ and $|f_1\rangle \perp |f_0\rangle$ such that $X(W) = 0$. Let us denote by $|e_0^{(i)}\rangle$
and $|f_1^{(i)}\rangle$ the set of vectors fulfilling that. (2) For each of these vectors, we have to find the corresponding values of $\phi_{e,f}$ by using (A17) and of $\theta^{(i)}$ by imposing that $A_2(W) = 0$ in (A19). (3) Construct $|\Psi^{(i)}\rangle$ according to (A18). (4) See whether the space spanned by $P_W$ and $\{|\Psi^{(i)}\rangle\}$ is equal to $H_A \otimes H_B$. If it is, then $W$ is optimal. If it is not, we can always find some $|\psi\rangle$ orthogonal to that subspace that can be subtracted from $W$.

6. Necessary and sufficient conditions for $X(W) = 0$

The hard part of the procedure outlined before to see whether and $EW$ is optimal is the step (1), namely to find $|e_1\rangle$ and $|f_1\rangle$ such that $X(W) = 0$. We start out by giving a necessary and sufficient condition for $X(W) = 0$.

Lemma A7: Given $|e_0, f_0\rangle \in P_W$, and $|e_1\rangle \perp |e_0\rangle$ and $|f_1\rangle \perp |f_0\rangle$, then $X(W) = 0$ iff

$$w_{0,0}^0|f_1\rangle = -\sqrt{W_{0,1}^1 W_{1,0}^0} e^{-i\phi_e} (e^{-i\phi_w} W^e_{1,0} + e^{i\phi_w} W^w_{0,1})|f_0\rangle,$$

(A20a)

$$w_{0,0}^f|e_1\rangle = -\sqrt{W_{0,1}^1 W_{1,0}^0} e^{-i\phi_f} (e^{-i\phi_w} W^f_{1,0} + e^{i\phi_w} W^w_{0,1})|e_0\rangle,$$

(A20b)

where $\phi_{e,f}$ are given in (A17).

Proof: (If) We multiply by $|f_1\rangle$ Eq. (A20a) and take the square of the absolute value of the result. We obtain

$$W_{1,0}^1 W_{0,1}^0 = |e^{-i(\phi_e+\phi_f)} W_{0,0}^0 + e^{i(\phi_e-\phi_f)} W_{1,0}^0|^2 \leq (|W_{0,0}^1| + |W_{1,0}^0|)^2.$$

(A21)

Using Lemma A5 we conclude that $X(W) = 0$. (Only if) Since $X(W) = 0$ and according to Lemma A5 $X(W) \geq 0$, then $X(W)$ must be a minimum with respect to $|e_1\rangle$ and $|f_1\rangle$. Taking the derivatives of $X(W)$ with respect to these two vectors and imposing that they vanish, one obtains (A20). □

Equations (A20) are particularly useful if the dimension of one of the Hilbert spaces is 2. Without loss of generality, let us assume that $\text{dim}(H_A) = 2$. In that case we can choose $|e_1\rangle$ as the one that is orthogonal to $|e_0\rangle$ (with an arbitrary choice of the global phase). The determination of $\phi_e$ can be done as follows. Using (A22) we write

$$\sqrt{W_{1,0}^1 W_{0,1}^0} e^{i\phi_f} |f_1\rangle = -\frac{1}{w_{0,0}^e} (e^{-i\phi_w} W^e_{1,0} + e^{i\phi_w} W^w_{0,1})|f_0\rangle,$$

(A22)

where $1/w_{0,0}^e$ denotes the pseudo–inverse [33]. We can use this expression to impose

$$W_{1,0}^1 e^{-i(\phi_e-\phi_f)}, W_{0,1}^0 e^{i(\phi_e+\phi_f)} < 0,$$

(A23)

i.e. they are negative real numbers. We obtain that

$$e^{-i2\phi_e} \langle f_0|w^e_{1,0} \frac{1}{w_{0,0}^e} w^w_{0,1}|f_0\rangle < 0,$$

(A24)

so that we determine $\phi_e$. With these results, we can prove the following necessary and sufficient condition for $X(W) = 0$ when $\text{dim}(H_A) = 2$.

Lemma A8: If $\text{dim}(H_A) = 2$, given $|e_0, f_0\rangle \in P_W$, then there exists $|e_1, f_1\rangle$ such that $X(W) = 0$ iff

$$\langle f_0| \left[ w^e_{1,1} - w^w_{0,1} \frac{1}{w_{0,0}^w} w^w_{1,0} - w^e_{1,0} \frac{1}{w_{0,0}^e} w^e_{0,1} \right] |f_0\rangle = 2 \left| \langle f_0|w^e_{0,1} \frac{1}{w_{0,0}^e} w^e_{0,1}|f_0\rangle \right|.$$

(A25)

Proof: (If) We define

$$|f_1\rangle = -\frac{1}{w_{0,0}^e} (e^{-i\phi_w} W^e_{1,0} + e^{i\phi_w} W^w_{0,1})|f_0\rangle$$

(A26)

where $\phi_e$ is determined by the condition (A24). Using this expression to calculate $X(W)$ one finds that indeed $X(W) = 0$. (Only if) Using Lemma A7 we can write $|f_1\rangle$ as in (A22) so that the phases $\phi_{e,f}$ ensure that (A23) is fulfilled. Substituting $|f_1\rangle$ in the equation $X(W) = 0$ one finds (A25). □

In summary, for a given $|e_0, f_0\rangle \in P_W$, in order to find whether there exist $|e_1, f_1\rangle$ such that $X(W) = 0$ we just have to check the condition (A25). If it is fulfilled, we can easily find $|f_1\rangle$ and the phases $\phi_{e,f}$ using (A23) and (A24).

APPENDIX B: CANONICAL FORM OF PPTES

The concept of “edge” PPTES seems to play a very special role in the characterization of PPTES. In particular, in view of the criterion given in Section VD, which is based on the fact that any density operator $\rho$ can be decomposed into a separable part and an “edge” PPTES [1]. Among all the possible decompositions there might be one for which the trace of the separable part is maximal. When it exists, such a decomposition was termed positive partial transpose best separable approximation (PPT BSA) to $\rho$ [21]. It extended the idea of BSA introduced in Refs. [22,23] to the case of PPTES, which were based on the method of diminishing the range of $\rho$ by subtracting product vectors from its range, while keeping the remainder and, at the same time, its partial transpose, positive [22,23,20,21]. In this Appendix we formalize the results regarding the existence and properties of the PPT BSA. In particular, the proofs presented in the quoted papers were restricted to the case in which there exist a finite, or at most, countable number of projectors on product vectors that can be subtracted from $\rho$. We will extend them below to continuous families of product
vectors. The Appendix is written in a self-contained way, and can be read independently of the body of the paper.

We denote by $\Gamma_\rho$ the set of projectors on product vectors $\{|e_\alpha,f_\alpha\rangle|e_\alpha,f_\alpha\rangle\}$ such that $|e_\alpha,f_\alpha\rangle \in R(\rho)$ and $|e_\alpha,f_\alpha\rangle^* \in R(\rho^T)$. In Ref. [21] we showed that if $\Gamma_\rho$ is finite then there exist an optimal decomposition (PPT BSA) $\rho = (1 - p)\rho_{sep} + p\delta$ where $\delta$ is an “edge” PPTES, and $\rho$ is minimal. Note that PPT BSA involves the state $\rho$ way, i.e. with the additional requirement that $\Gamma_\rho$ is a finite set. It can happen that there is an uncountable dimensional space. The Appendix is written in a self-contained way, with the additional requirement that $\Gamma_\rho$ is a finite set. It can happen that there is an uncountable family of product vectors depending on continuous parameter that can be used for subtracting projectors. In the following we will show that in such case the above result is valid.

In order to consider the case of continuous families of product vectors we first prove the following:

**Lemma B1:** Let $\rho$ will be a PPTES defined on a Hilbert space $\mathcal{H}$, dim$\mathcal{H} < \infty$. Then the set of product vectors $\Gamma_\rho$ is compact.

**Proof:** Obviously $\Gamma_\rho$ is a bounded set in finite-dimensional space, so it is enough to show that it is closed. Consider any sequence $|g_n,h_n\rangle \rightarrow |\phi\rangle$, $|g_n,h_n\rangle \in R(\rho)$, $|g_n,h_n\rangle \in R(\rho^T)$. The limit vector must: (i) they respect the condition of orthogonality to $K(\rho)$ [i. e. they must belong to $K(\rho)$], (ii) belong to the sphere (i. e. set of all vectors $|\phi\rangle$ with $||\phi|| = 1$), (iii) finally, it must be a product state, because if it was entangled then its distance from the compact set of product pure states $\Gamma_\rho$ defined as min$_{|e,f\rangle}$ $||\phi - |e,f\rangle||$ would be nonzero, which is obviously impossible. We conclude thus $|\phi\rangle = |g,h\rangle \in R(\rho)$ for some $|g\rangle,|h\rangle$, which implies (up to irrelevant absolute value factors) that $|g_n\rangle \rightarrow |g\rangle$ and $|h_n\rangle \rightarrow |h\rangle$. We have (again up to irrelevant absolute value factors) $|g_n,h_n^*\rangle \rightarrow |g,h^*\rangle$. The latter must belong to $R(\rho^T)$, as any element of the corresponding sequence is orthogonal to $K(\rho^T)$. □

Let us now prove the following general lemma, which is a generalization of one theorem from Ref. [22]:

**Lemma B2:** Let the PPTES $\rho$ be defined on a finite dimensional Hilbert space. Consider the set $\Sigma_\rho$ consisting of the trivial zero operator plus all unnormalized states $\tilde{\rho}$ (tr$\tilde{\rho} \leq 1$) such that $\tilde{\rho} \equiv \rho - \tilde{\rho}$ is positive and has positive partial transpose. Then, one can find $\tilde{\rho} \in \Sigma_\rho$ such that $\text{tr}(\tilde{\rho}) \leq 1$ is optimal in the sense that:

(i) The trace of $\tilde{\rho} \equiv \rho - \tilde{\rho}$ is minimal with respect to all separable $\tilde{\rho}$’s leading to positive partial transpose $\tilde{\rho}$’s.

(ii) The state $\delta = \tilde{\rho}/\text{tr}(\tilde{\rho})$ is an “edge” PPTES.

**Proof:** To prove the existence of $\tilde{\rho} \in \Sigma_\rho$ we just have to show that $\Sigma_\rho$ is compact. This can be done by showing that $\Sigma_\rho$ is a closed subset of another compact set, namely $C = \text{conv}\{\Gamma_\rho \cup 0\}$. The latter set $C$ is compact as it is a convex hull of the compact set $\{\Gamma_\rho \cup 0\}$ in a finite dimensional space.

Note first that $\Sigma_\rho \subset C$. Indeed, by virtue of $\tilde{\rho} \geq 0$ any nonzero $\tilde{\rho}$ cannot have any vector in its range not belonging to $R(\rho)$. Analogously $R(\tilde{\rho}) \subset R(\rho)$.

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Given an operator $X$ and an orthonormal basis $\{|k\rangle\}_{k=1}^{N} \in H_B$, one defines the partial transposed of $X$ with respect to $B$ in that basis as follows:

$$X^{T_B} = \sum_{k,k'=1}^{N} |k'\rangle_B \langle k|X|k'\rangle_B \langle k|.$$  \hspace{1cm} (B2)

One can analogously define the partial transposed of $X$ with respect to $A$ in a given basis, $X^{T_A}$. Partial transposition fulfills the following useful property

$$\text{tr}(X^{T_A}Y) = \text{tr}(XY^{T_B}).$$  \hspace{1cm} (B3)

We say that positive operator has a positive partial transposition if $\rho^{T_A} \geq 0$. Note that this property is basis independent, and that $\rho^{T_A} \geq 0$ iff $\rho^{T_B} \geq 0$. The relation between separable and positive partial transpose operators was established in Refs. [10,11]. All separable operators have positive partial transposition. The converse is, however, not true in general. That is, there are positive partial transpose operators which are nonseparable.

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Note that if we define a basis in $H_B$ as $\{V_B^k|k\}$ we have that $\rho_B^k = \rho_b$, where the partial transposition is taken in that basis.

These states can be prepared locally and, can be used to construct the PPTES by mixing them “weakly” with entangled states. This provides an interesting possibility of experimental realization of PPTES. This suggestion has been formulated by A. Weinfurter.

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