A complete family of separability criteria

Andrew C. Doherty,[1] Pablo A. Parrilo,[2] and Federico M. Spedalieri[1]

[1]*Institute for Quantum Information, California Institute of Technology, Pasadena, CA 91125, USA*
[2]*Automatic Control Laboratory, ETH Zentrum, CH-8092 Zürich, Switzerland*

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We introduce a new family of separability criteria that are based on the existence of extensions of a bipartite quantum state ρ to a larger number of parties satisfying certain symmetry properties. It can be easily shown that all separable states have the required extensions, so the non-existence of such an extension for a particular state implies that the state is entangled. One of the main advantages of this approach is that searching for the extension can be cast as a convex optimization problem known as a semidefinite program (SDP). Whenever an extension does not exist, the dual optimization constructs an explicit entanglement witness for the particular state. These separability tests can be ordered in a hierarchical structure whose first step corresponds to the well-known Positive Partial Transpose (Peres-Horodecki) criterion, and each test in the hierarchy is at least as powerful as the preceding one. This hierarchy is complete, in the sense that any entangled state is guaranteed to fail a test at some finite point in the hierarchy, thus showing it is entangled. The entanglement witnesses corresponding to each step of the hierarchy have well-defined and very interesting algebraic properties that in turn allow for a characterization of the interior of the set of positive maps. Coupled with some recent results on the computational complexity of the separability problem, which has been shown to be NP-hard, this hierarchy of tests gives a complete and also computationally and theoretically appealing characterization of mixed bipartite entangled states.

I. INTRODUCTION

Entanglement is one of the most fascinating features of quantum mechanics. As Einstein, Podolsky and Rosen [1] pointed out, the quantum states of two physically separated systems that interacted in the past can defy our intuitions about the outcomes of local measurements. Entangled pure states have zero entropy but can appear to have maximal entropy when the experimenter only has access to one of the subsystems. On the other hand, Bell inequalities [2] quantify the extent to which local measurements on separated quantum systems can be correlated in ways that are forbidden in any local classical model. Violations of these inequalities require entanglement. Moreover, it has recently been recognized that entanglement is a very important resource in quantum information processing, allowing certain important tasks such as teleportation, quantum computation, quantum cryptography and quantum communication to name a few [3].

For the case of pure states, determining when a given state is entangled is very easy, since it is based on properties of the Schmidt decomposition or, equivalently, the rank of the reduced density matrices, which can be computed very efficiently. However, for the case of mixed bipartite states, no single practical procedure that can be guaranteed to detect the entanglement of every entangled state has been found. In the past few years, a considerable effort has been dedicated to this problem [4, 5, 6, 7]. Still only incomplete criteria have been proposed, that can detect some entangled states but not all of them or that work only for certain restricted dimensions. This is a somewhat uncomfortable situation, since all the quantum states generated in the laboratory for practical applications of quantum information processing are mixed

states. Hence the need, not only from the theoretical but also from the practical point of view, of having an efficient tool that would allow us to determine when a given state is entangled.

A bipartite mixed state is said to be separable [8] (not entangled) if it can be written as a convex combination of pure product states

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i|, \qquad (1)$$

where $|\psi_i\rangle$ and $|\phi_i\rangle$ are state-vectors on the spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ of subsystems A and B respectively, and $p_i > 0, \sum_i p_i = 1$. If a state admits such a decomposition, then it can be created by local operations (unitary transformations, measurements, etc.) and classical communication (LOCC) by the two parties, and hence it cannot be an entangled state. Despite the simplicity of (1), it has been shown recently by Gurvits [9] that deciding whether or not such a decomposition exists for a given density matrix is an NP-hard problem. This result destroys any hope of finding a computationally efficient tool to determine entanglement of mixed states as was the case for pure states, so long as the widely believed result $P \neq NP$ is actually true. But there are some instances of the separability problem that allow efficient algorithms to solve them. This is one of the basic ideas behind separability criteria.

A separability criterion is based on a simple property that can be shown to hold for every separable state. They provide necessary but not sufficient conditions for separability. If some state ρ does not satisfy the property, then it must be entangled. But if it does satisfy it, that does not imply that the state is separable. One of the first and most widely used of these criteria is the Positive Partial Transpose (PPT) criterion, introduced by Peres [10]. If ρ has matrix elements $\rho_{ik,jl} = \langle i| \otimes \langle k|\rho|j\rangle \otimes |l\rangle$ then the

partial transpose ρ^{T_A} is defined by

$$\rho^{T_A}_{ik,jl} = \rho_{jk,il}. \qquad (2)$$

If a state is separable, then it must have a positive partial transpose (PPT). To see this consider the decomposition (1) for ρ. Partial transposition takes $|\psi_i\rangle\langle\psi_i|$ to $|\psi_i^*\rangle\langle\psi_i^*|$, so the partial tranpose of ρ can be written as

$$\rho^{T_A} = \sum p_i |\psi_i^*\rangle\langle\psi_i^*| \otimes |\phi_i\rangle\langle\phi_i|. \qquad (3)$$

Clearly ρ^{T_A} is a valid quantum state and in particular it must be positive semidefinite. Thus any state for which ρ^{T_A} is not positive semidefinite is necessarily entangled. This criterion is computationally very easy to check. Furthermore, it was shown by the Horodeckis [11], based on previous work by Woronowicz [12], to be both necessary and sufficient for separability in $\mathcal{H}_2 \otimes \mathcal{H}_2$ and $\mathcal{H}_2 \otimes \mathcal{H}_3$. However, in higher dimensions, there are PPT states that are nonetheless entangled, as was first shown in [13], again based on [12]. These states are called bound entangled states because they have the peculiar property that no entanglement can be distilled from them by local operations [14].

A different useful separability criterion, that has been used to show entanglement of PPT states, is the range criterion [12, 13]. It is based on the fact that for every separable state ρ there exist a set of pure product states $\{|\psi_i\rangle|\phi_i\rangle\}$ that span the range of ρ while $\{|\psi_i^*\rangle|\phi_i\rangle\}$ span the range of ρ^{T_A}, as can be easily seen by looking at equations (1) and (3). This criterion is sometimes stronger than PPT, but in some cases it can be weaker (for example, when considering full rank non-PPT states).. Other criteria, that are in general weaker than PPT are the reduction criterion [15, 16] and the majorization criterion [17]. None of these criteria, nor a combination of them are sufficient to give a complete characterization of separable states.

Another approach to distinguishing separable and entangled states involves the so called *entanglement witnesses* (EW) [18]. An EW is an observable W whose expectation value is nonnegative on any separable state, but strictly negative on an entangled state ρ. We say in this case that W "witnesses" the entanglement of ρ. Besides giving another theoretical tool to detect entangled states, this idea addresses the question of whether there is an experimental way of distinguishing an entangled state from a separable one. By studying the geometrical structure of the set of quantum states, it can be shown that for every entangled state there exists an entanglement witness W [11, 12]. Thus, there is always an observable that can be measured that will show that the state is entangled.

There are two other important mathematical objects related to entanglement witnesses. Although these do not have the physical interpretation of observables they allow connections to other results in the mathematical and mathematical physics literature. In the first place,

there is a correspondence that relates entanglement witnesses to linear positive (but not completely positive) maps from operators on $\mathcal{H}_A$ to operators on $\mathcal{H}_B$ (or vice versa); see equation (89) and reference [19]. Applying such a map to one half of an entangled state does not necessarily result in a positive matrix. For this reason positive maps were rejected as possible physical evolutions of quantum states in favor of the completely positive maps. The PPT test has this structure where the transpose is the positive map. Any positive but not completely positive map results in an analogous separability criterion. The equivalence between entanglement witnesses and positive maps implies that if ρ is entangled there is always a positive map that will detect the entanglement in this way [11, 12]. The characterization of positive linear maps was in fact the original motivation for studying the separability question [12].

Finally, there is a well known mapping between positive linear maps and positive semidefinite biquadratic forms [20, 21]. This can be appreciated simply by writing the condition that W is positive on pure product states explicitly in terms of the elements of W and the state vectors for the two systems, as in equation (43) in Section VI. This suggests the use of results from real algebraic geometry (see for example [22] and the references therein) to attack the separability problem. Indeed, the semidefinite programming techniques we employ here were first developed in this general context [23].

The question of whether a given state ρ is separable may be phrased as quantified polynomial inequalities in a finite number of variables:

$$\forall W [\forall|\psi\rangle\forall|\phi\rangle \ \langle\psi|\langle\phi|W|\psi\rangle|\phi\rangle \geq 0 \implies \mathrm{Tr}[\rho W] \geq 0]. \qquad (4)$$

If this proposition is satisfied then ρ is separable. Since the inequalities may be expressed in terms of polynomials of the variables (the components of W, $|\psi\rangle$, $|\phi\rangle$) this is a semi-algebraic problem. Much is known about the general class of semi-algebraic problems, in particular the fact that they are *decidable*. The Tarski-Seidenberg decision procedure [22] can then be used to provide an explicit algorithm to solve the separability problem in all cases and therefore to decide whether ρ is entangled. A drawback of this approach is that most exact techniques in algebraic geometry scale very poorly with the number of variables (the Hilbert space dimensions in the separability problem). For this problem, these methods do not perform well in practice except for very small problem instances. This is in contrast to the PPT test which may be implemented very efficiently but does not always settle the question of separability of ρ. In this paper we discuss a set of separability criteria that also have this property; they all scale polynomially with the Hilbert space dimension and perform well in practice, any state ρ that is entangled is detected by one of the tests but no one test detects all entangled states. Since the separability problem is NP-Hard it is very unlikely that a procedure guaranteed to solve the problem in all instances can scale well with Hilbert space dimension. As a result our fam-

ily of separability tests is, in some sense, the best way of solving the problem from a practical point of view, in that simple tests will detect the easiest instances of the problem, while the more complicated instances genuinely require more computational resources.

The most important characteristic of the separability problem is the fact that the separable states form a convex set. The existence of entanglement witnesses, observables that are positive on separable states but negative on some entangled state, is a direct result of this convexity. There has been much work on the separability problem, particularly from the Innsbruck-Hannover group as reviewed in [5, 6], that emphasizes convexity and proceeds by characterizing entanglement witnesses in terms of their extreme points, the so-called optimal entanglement witnesses, and PPT entangled states in terms of their extreme points, the edge PPT entangled states [24, 25]. Convexity also plays a central role in our work which provides a computational means of constructing entanglement witnesses with certain properties. It is interesting that our construction will allow us to characterize the interior of the set of entanglement witnesses, but not its extreme points.

Beyond the separability problem, many problems of interest in quantum information have the structure of convex optimizations [26], a fact that has found increasing application in the field in recent years. One early example is the use of results about linear programming to find the optimal local entanglement concentration procedure for a pure bipartite state in [27]. Our work will involve convex optimizations known as semidefinite programs [26, 28], generalizations of linear programs that optimize a linear function of a positive matrix subject to linear constraints. Semidefinite programming arguments have also been used been used in the quantum information literature to address questions about quantum coin tossing, distillation and optimal state transformations [29, 30, 31, 32, 33].

In this paper we discuss in detail a family of separability criteria introduced in [34], that can be ordered into a hierarchy of tests that have the following two very important properties: i) the hierarchy is complete, i.e., any entangled state will be detected by some test in the hierarchy, ii) there are efficient computational algorithms to check each of the tests. This provides us with a very practical algorithmic way for testing entanglement of a given bipartite mixed states, that is guaranteed to detect any entangled state. Furthermore, the algorithm constructs an explicit proof of this fact in the form of an entanglement witness. This in turn helps us to develop a characterization of almost all positive maps that are not completely positive.

The paper is organized as follows. In Section II we introduce a new family of separability criteria; in Section III we introduce and discuss the properties of semidefinite programs (SDP), and show that each separability test in the family can be cast as a SDP, and briefly discuss the resources needed to implement them. In Section IV we discuss how to take advantage of the symmetries that each test requires to further reduce the computational resources needed. In Section V we present an explicit proof of the completeness of the hierarchy, translating previous results [35, 36] into the language of density matrices. Section VI shows how the duality of the SDP can be exploited to construct an entanglement witness that proves entanglement for a given state, and we discuss the algebraic properties of these witnesses. In Section VII we present examples of the application of the hierarchy. In section VIII we discuss how to construct an entangled state that is not detected by the second test of the hierarchy and present several important consequences of this result. Section IX shows how to use an SDP to test indecomposability of an entanglement witness and construct a bound entangled state detected by it. In Section X we discuss the connection betweeen entanglement witnesses and positive maps, and show how the properties of the witnesses obtained through our hierarchy of tests can be translated into a characterization of strictly positive maps. Finally, in Section XI, we summarize our results and present our conclusions.

II. PPT SYMMETRIC EXTENSIONS AND NEW SEPARABILITY CRITERIA

Any separable state ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$ can be written as in (1). Consider now the state $\tilde{\rho}$ in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A$, given by

$$\tilde{\rho} = \sum p_i |\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i| \otimes |\psi_i\rangle\langle\psi_i|. \qquad (5)$$

Then $\tilde{\rho}$ has the following properties: i) $\tilde{\rho}$ is an extension of ρ to three parties, in the sense that

$$\mathrm{Tr}_C[\tilde{\rho}] = \rho, \qquad (6)$$

where Tr_C means that we take the partial trace over the third party which we have taken to be equal to $\mathcal{H}_A$. ii) $\tilde{\rho}$ is symmetric under interchanges of the first and third parties, i.e., the two copies of party A. More precisely, if we define the swap operator P by

$$P|i\rangle \otimes |k\rangle \otimes |j\rangle = |j\rangle \otimes |k\rangle \otimes |i\rangle, \qquad (7)$$

the symmetry condition can be written as

$$\tilde{\rho} = P\tilde{\rho}P. \qquad (8)$$

iii) $\tilde{\rho}$ must remain positive under any partial transposition (since $\tilde{\rho}$ is also a separable state). Note that, due to the symmetry (8), taking partial transpose with respect to the third subsystem is equal to taking it with respect to the first one. Now, for an *arbitrary* state ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$, we will call $\tilde{\rho}$ a *PPT symmetric extension of ρ to two copies of $\mathcal{H}_A$*, if and only if, $\tilde{\rho}$ satisfies the three properties stated above. Since we have shown by construction that any separable state has a PPT symmetric

extension to two copies of $\mathcal{H}_A$, then we can use its existence as a separability criterion. If a given state does not have such an extension, then the state must necessarily be entangled.

We can take this idea of the existence of PPT symmetric extensions further by considering extending the state to an arbitrary number of copies of subsystem A. For any separable state in $\mathcal{H}_A \otimes \mathcal{H}_B$ given by (1), the state

$$\tilde{\rho} = \sum p_i |\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i| \otimes |\psi_i\rangle\langle\psi_i|^{\otimes n-1}, \quad (9)$$

is a state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A^{\otimes n-1}$ that, i) is symmetric under interchanges of any two copies of subsystem A, ii) yields the original state ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$ when we trace out any $n-1$ copies of subsystem A, and iii) remains positive under all possible partial transpositions. Again, for an arbitrary state ρ, we will call $\tilde{\rho}$ a *PPT symmetric extension of ρ to n copies of party A*, if and only if, $\tilde{\rho}$ satisfies properties i), ii) and iii). And as before, we can use the existence of this extension to n copies of subsystem A as a separability criterion. We have thus generated a countably infinite family of separability criteria. Note that the same idea can be generalized to the multipartite case: the existence of PPT symmetric extensions to any number of copies of the parties is a separability criterion.

For the bipartite case, these separability criteria are not completely independent of each other, but they actually have a hierarchical structure. We will now show that if a state has a PPT symmetric extension to n copies of A, call it $\tilde{\rho}_n$, then it must have a PPT symmetric extension to $n-1$ copies of A. Let $\tilde{\rho}_{n-1} = \mathrm{Tr}_A[\tilde{\rho}_n]$, where A represents one of the copies of A. It is easy to see that $\tilde{\rho}_{n-1}$ will inherit from $\tilde{\rho}_n$ the property of being symmetric under interchanges of copies of party A, since we have just removed one of the copies. It is also obvious that $\tilde{\rho}_{n-1}$ is an extension of ρ to $n-1$ copies of A. Let's assume that is not PPT. Then there is a subset $\mathcal{I}$ of the parties such that $\tilde{\rho}_{n-1}^{T_\mathcal{I}}$ has a negative eigenvalue, where $T_\mathcal{I}$ represents the partial transpose with respect to all the parties in subset $\mathcal{I}$. Let $|e\rangle$ be the corresponding eigenvector and let $\{|i\rangle\}$ be a basis of the system A over which the partial trace was performed. Since $\tilde{\rho}_n$ is PPT, then $\langle e|\langle i|\tilde{\rho}_n^{T_\mathcal{I}}|e\rangle|i\rangle \geq 0$, for all i. Then

$$\sum_i \langle e|\langle i|\tilde{\rho}_n^{T_\mathcal{I}}|e\rangle|i\rangle = \langle e|\mathrm{Tr}_A[\tilde{\rho}_n^{T_\mathcal{I}}]|e\rangle \geq 0. \quad (10)$$

Since we performed the partial trace over a party that is not included in $\mathcal{I}$, we can commute the trace and the partial transpose, and using $\tilde{\rho}_{n-1} = \mathrm{Tr}_A[\tilde{\rho}_n]$, we have $\langle e|\tilde{\rho}_{n-1}^{T_\mathcal{I}}|e\rangle \geq 0$, which contradicts the fact that $|e\rangle$ is an eigenvector of $\tilde{\rho}_{n-1}^{T_\mathcal{I}}$ with negative eigenvalue.

We have then constructed a family of separability criteria with a natural hierarchical structure. If we take the usual PPT criterion as the first step of the hierarchy, the existence of a PPT extension to two copies of A as the second step, and so on, we see that the tests are ordered in such a way that each test is at least as powerful as the previous one, in the sense that if a state was shown to be entangled by one of them, it will be also shown to be entangled by all the tests that are higher in the hierarchy. This family of tests has several very important and useful properties. It can be shown that each test can be cast as a semidefinite program (SDP), which is a class of convex optimization problems for which efficient algorithms exist. The duality structure of the SDP allows us to construct an explicit entanglement witness whenever a state fails one of the tests. And finally, it can be proven that the hierarchy is *complete*, i.e., every entangled state is guaranteed to fail the test at some finite point in the hierarchy.

III. SEMIDEFINITE PROGRAMS AND SEARCHING FOR PPT SYMMETRIC EXTENSIONS

In this section we will introduce and discuss the structure of a semidefinite program and we will show explicitly how to apply it to the problem of searching for a PPT symmetric extension.

A. Semidefinite programs

A semidefinite program (SDP) is a particular type of convex optimization problem [26, 28]. An SDP corresponds to the optimization of a linear function subject to a linear matrix inequality (LMI). A typical SDP has the form

$$\begin{aligned} \text{minimize} \quad & c^T\mathbf{x} \\ \text{subject to} \quad & F(\mathbf{x}) \geq 0, \end{aligned} \quad (11)$$

where c is a given vector, $\mathbf{x} = (x_1, \ldots, x_n)$, and $F(\mathbf{x}) = F_0 + \sum_i x_i F_i$, for some fixed hermitian matrices F_i. The inequality in the second line means that the matrix $F(\mathbf{x})$ must be positive semidefinite. The minimization is performed over the vector $\mathbf{x}$, whose components are the variables of the problem. The set of feasible solutions, i.e., the set of $\mathbf{x}$ that satisfy the LMI, is a convex set. In the particular case in which $c = 0$, there is no function to minimize and the problem reduces to whether or not the LMI can be satisfied for some value of the vector $\mathbf{x}$. In this case, the SDP is refered to as a *feasibility problem*. The convexity of the SDP has made it possible to develop sophisticated and reliable analytical and numerical methods to solve them [28].

A very important property of a SDP, both from the theoretical and applied points of view, is its *duality structure*. To any SDP of the form (11), which is usually called the *primal problem*, there is associated another SDP, called the *dual problem*, that can be stated as

$$\begin{aligned} \text{maximize} \quad & -\mathrm{Tr}[F_0 Z] \\ \text{subject to} \quad & Z \geq 0 \\ & \mathrm{Tr}[F_i Z] = c_i, \end{aligned} \quad (12)$$

where the matrix Z is hermitian and is the variable over which the maximization is performed. This corresponds to the maximization of a linear functional, subject to linear constraints and a LMI. Let $\mathbf{x}$ and Z be any two feasible solutions of the primal and dual problems respectively. Then we have the following relationship

$$c^T \mathbf{x} + \text{Tr}[F_0 Z] = \text{Tr}[F(\mathbf{x})Z] \geq 0, \qquad (13)$$

where the last inequality follows from from the fact that both $F(\mathbf{x})$ and Z are positive semidefinite. From (11) and (12) we can see that the left hand side of (13) is just the difference between to objective functions of the primal and dual problem. The inequality in (13) tells us that the value of the primal objective function evaluated on any feasible vector $\mathbf{x}$, is always greater or equal than the value of the dual objective function evaluated on any feasible matrix Z. This property is known as *weak duality*. Thus, we can use any feasible $\mathbf{x}$ to compute an upper bound for the optimum of $-\text{Tr}[F_0 Z]$, and we can also use any feasible Z to compute a lower bound for the optimum of $c^T \mathbf{x}$.

If the feasibility constraints on both the primal and dual problems are satisfied for some $Z > 0$ and $\mathbf{x}$ such that $F(\mathbf{x}) > 0$, the problems are termed *strictly feasible*, and the optimum values of the primal and dual formulations are equal. This property is called *strong duality*. Furthermore, there is a feasible pair $(\mathbf{x}_{\text{opt}}, Z_{\text{opt}})$ achieving the optimum. In this case, as can be seen from equation (13), we have $\text{Tr}[F(\mathbf{x}_{\text{opt}})Z_{\text{opt}}] = 0$, and thus $F(\mathbf{x}_{\text{opt}})Z_{\text{opt}} = 0$, so the hermitian matrices $F(\mathbf{x}_{\text{opt}})$ and Z_{opt} have orthogonal ranges. This is known as the *complementary slackness* condition [28].

Equation (13) has another important application. Consider the particular case of a feasibility problem (i.e., $c = 0$). Then, equation (13) will read

$$\text{Tr}[F_0 Z] \geq 0, \qquad (14)$$

and this must hold for *any feasible solution* of the dual problem. This property can be used to give a *certificate of infeasibility* for the primal problem: *if there exists Z such that $Z \geq 0$ and $\text{Tr}[F_i Z] = 0$, that satisfies $\text{Tr}[F_0 Z] < 0$, then the primal problem must be infeasible.* We will show later that for the particular case of our hierarchy of separability tests, whenever a PPT symmetric extension of ρ cannot be found (primal problem is infeasible), the certificate provided by the dual problem is nothing but an entanglement witness for the state ρ.

B. Separability tests as semidefinite programs

Each test in the hierarchy of separability criteria introduced in Section II can be written as a semidefinite program. We will show in detail how the SDP is setup for the second test in the hierarchy, which corresponds to searching for PPT symmetric extensions of ρ to two copies of subsystem A. The general case, of extensions to n copies of party A, can be constructed in a similar way.

Let $\{\sigma_i^A\}_{i=1}^{d_A^2}, \{\sigma_j^B\}_{j=1}^{d_B^2}$ be bases for the space of hermitian matrices that operate on $\mathcal{H}_A$ and $\mathcal{H}_B$, of dimensions d_A and d_B respectively, such that they satisfy

$$\text{Tr}[\sigma_i^X \sigma_j^X] = \alpha_X \delta_{ij} \quad \text{and} \quad \text{Tr}[\sigma_i^X] = \delta_{i1}, \qquad (15)$$

where X stands for A or B, and α_X is some constant—the generators of SU(n) could be used to form such a basis. Then we can expand ρ in the basis $\{\sigma_i^A \otimes \sigma_j^B\}$, and write $\rho = \sum_{ij} \rho_{ij} \sigma_i^A \otimes \sigma_j^B$, with $\rho_{ij} = \alpha_A^{-1} \alpha_B^{-1} \text{Tr}[\rho\, \sigma_i^A \otimes \sigma_j^B]$. In the same way, we can expand the extension $\tilde{\rho}$ in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A$ as

$$\tilde{\rho} = \sum_{\substack{ijk \\ i<k}} \tilde{\rho}_{ijk} \{\sigma_i^A \otimes \sigma_j^B \otimes \sigma_k^A + \sigma_k^A \otimes \sigma_j^B \otimes \sigma_i^A\} +$$
$$+ \sum_{kj} \tilde{\rho}_{kjk}\, \sigma_k^A \otimes \sigma_j^B \otimes \sigma_k^A, \qquad (16)$$

where we made explicit use of the swapping symmetry between the first and third parties, that we require from $\tilde{\rho}$. To satisfy the condition that $\tilde{\rho}$ is an extension of ρ, we need to impose

$$\text{Tr}_C[\tilde{\rho}] = \rho, \qquad (17)$$

where Tr_C means tracing out the third party. Using (15) and the fact that $\{\sigma_i^A \otimes \sigma_j^B\}$ form a basis of $\mathcal{H}_A \otimes \mathcal{H}_B$, equation (17) reduces to

$$\tilde{\rho}_{ij1} = \rho_{ij}. \qquad (18)$$

This fixes some of the components of $\tilde{\rho}$. The remaining ones will play the role of the variables in the SDP. The LMIs come from requiring that the extension $\tilde{\rho}$ and all its partial tranposes are positive semidefinite. If we define

$$G_0 = \sum_j \rho_{1j}\, \sigma_1^A \otimes \sigma_j^B \otimes \sigma_1^A +$$
$$+ \sum_{i=2, j=1} \rho_{ij} \{\sigma_i^A \otimes \sigma_j^B \otimes \sigma_1^A + \sigma_1^A \otimes \sigma_j^B \otimes \sigma_i^A\}$$
$$G_{iji} = \sigma_i^A \otimes \sigma_j^B \otimes \sigma_i^A \qquad\qquad i \geq 2,$$
$$G_{ijk} = (\sigma_i^A \otimes \sigma_j^B \otimes \sigma_k^A + \sigma_k^A \otimes \sigma_j^B \otimes \sigma_i^A) \quad k > i \geq 2, \qquad (19)$$

we can write the PSD condition $\tilde{\rho} \geq 0$ as

$$G(\mathbf{x}) = G_0 + \sum_J x_J G_J \geq 0, \qquad (20)$$

where we have collected all the subindices in (19) into one subindex J. Equation (20) has exactly the form that appears in (11). The role of the variable $\mathbf{x}$ is played by the coefficients $\tilde{\rho}_{ijk}(k \neq 1, k \geq i)$, which can vary freely without affecting the extension condition (17). The number of free variables is $m = (d_A^4 d_B^2 - d_A^2 d_B^2)/2$, and each matrix G_J has dimension $n = d_A^2 d_B$. Since $\tilde{\rho}$ is symmetric under swaps of the first and third parties, there are

only two independent partial transpositions that can be applied to it, which we can take as partial transposes with respect to the first and second parties (one of the copies of A, and subsystem B). The requirement that these two partial transposes are positive leads to two more LMIs, given by

$$\tilde{\rho}^{T_A} \geq 0 \quad \text{and} \quad \tilde{\rho}^{T_B} \geq 0, \tag{21}$$

where the G_J matrices for these two inequalities are related to the matrices given in (19) by the appropriate partial transposes, namely $G_J^{T_A}$ and $G_J^{T_B}$. We can actually combine the three LMIs into one, by defining the matrix

$$F = \tilde{\rho} \oplus \tilde{\rho}^{T_A} \oplus \tilde{\rho}^{T_B}, \tag{22}$$

and using the fact that a block-diagonal matrix $C = A \oplus B$ is positive semidefinite, if and only if, both A and B are positive semidefinite.

We have then stated the search of a PPT symmetric extension of ρ as an SDP, in which the objective function is zero ($c = 0$), so it corresponds to a feasibility problem, and the LMI condition reads $F = \tilde{\rho} \oplus \tilde{\rho}^{T_A} \oplus \tilde{\rho}^{T_B} \geq 0$, which encodes the requirement of the extension and its partial transposes being positive semidefinite. The SDP will then take the form

$$\begin{aligned} \text{minimize} \quad & 0 \\ \text{subject to} \quad & F \geq 0. \end{aligned} \tag{23}$$

In appendix A, we discuss a slightly modified version of the SDP that has the advantage of performing better numerically, but we will keep the form (23) for all the analytical discussions, since its dual form is more clearly related to the construction of entanglement witnesses, which is another one of the main results of this paper.

The SDP for other tests of the hierarchy (extensions to more copies of party A), can be constructed in the same way, by generating the matrices G_J with the appropriate symmetry, and constructing the block-diagonal matrix F, whose blocks correspond to all the independent partial transposes that can be applied to the extension $\tilde{\rho}$.

C. Resources needed to implement the tests

As we mentioned before, there are very efficient algorithms to solve semidefinite programs, and we can use their properties to discuss the computational resources required to implement a general step in our hierarchy of tests. Assume that we are searching for a PPT symmetric extension of a state ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$ to k copies of subsystem A, with d_A and d_B the dimensions of $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively. Then, the corresponding semidefinite program will have $m = \left[\binom{d_A^2+k-1}{k} - d_A^2 \right] d_B^2$ variables and a matrix G with $(k+1)$ blocks of dimension $d_A^{2k}d_B^2$. Numerical SDP solvers are described in detail in [28].

Typically they involve the solution of a series of least squares problems each requiring a number of operations scaling with problem size as $O(m^2n^2)$, where $F(\mathbf{x})$ is an $n \times n$ matrix. For SDPs with a block structure these break into independent parts each with a value of n determined by the block size. The number of iterations required is known to scale no worse than $O(n^{1/2})$. Thus for any fixed value of k the computation involved in checking our criteria scales no worse than $O(d_A^{13k/2})$ which is polynomial in the system size. On the other hand, for d_A and d_B fixed, the size of the matrix $F(\mathbf{x})$ scales exponentially with the number of copies k. There is, however, a significant improvement that can be accomplished by exploiting the swapping symmetry to its fullest. In the next section we will show that we can impose a stronger restriction on the extension that brings the scaling of resources down to polynomial in the number of copies of subsystem A, for fixed d_A, d_B. It is important to point out that the resources required to solve the separability problem have been proven to scale super polynomially only when the dimensions of *both* systems are allowed to vary. These two results are consistent, although the complexity result implies that there is no value of k such that the kth test detects all entangled states for all values of d_A, d_B.

IV. EXPLOITING THE SYMMETRY

Each test for separability searches for an extension of a state ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$ of dimension $d_A d_B$, to the space $\mathcal{H}_A^{\otimes k} \otimes \mathcal{H}_B$, that has dimension $d_A^k d_B$ (where, without loss of generality, we have interchanged the order of $\mathcal{H}_B$ and all copies of A for convenience). We see that the dimension of the extended space increases exponentially with the number of copies of party A. We have shown that we can impose further restrictions on the extension, and in particular we require it to be invariant under swaps of the copies of subsystem A. This reduces the size of the space over which we search for the extension, but the scaling with the number of copies remains exponential, which is not desirable of a practical tool for deciding separability of a state. However, we can actually impose a stronger constraint on the form of the extension, that reduces the scaling of its size from exponential to polynomial in the number of copies.

As we pointed out before, any separable state in $\mathcal{H}_A \otimes \mathcal{H}_B$ of the form (1) has a PPT symmetric extension to $\mathcal{H}_A^{\otimes k} \otimes \mathcal{H}_B$, that we can explicitly write as

$$\tilde{\rho} = \sum p_i |\psi_i\rangle\langle\psi_i|^{\otimes k} \otimes |\phi_i\rangle\langle\phi_i|. \tag{24}$$

This extension is obviously invariant under swaps of copies of A, and we used this property to restrict the form of the matrices F_J in the LMI of our SDP. But $\tilde{\rho}$ has a more constraining property: *its support and range are contained in the symmetric subspace of $\mathcal{H}_A^{\otimes k} \otimes \mathcal{H}_B$* (where the symmetry is understood to apply only to the copies of A). For the case of the extension to two copies

of system A, we can write the projector into this symmetric subspace as $\pi = \frac{1}{2}(\mathbb{1} + P)$, with P the swap operator defined in (7). Then, the symmetry requirement on the extension takes the form $\tilde{\rho} = \pi\tilde{\rho}\pi$.

For an arbitrary ρ, we can now restrict our search to extensions that satisfy this property. If $\{S_i^A\}$ is a basis of hermitian matrices having support and range in the symmetric subspace of $\mathcal{H}_A^{\otimes k}$, this restriction is equivalent to only considering matrices G in (20) of the form $G = S_i^A \otimes \sigma_j^B$. Since the dimension of the symmetric subspace in $\mathcal{H}_A^{\otimes k}$ is

$$d_{S_k} = \binom{d_A + k - 1}{k}, \qquad (25)$$

with d_A the dimension of $\mathcal{H}_A$, the number of matrices of this form is $d_{S_k}^2 d_B^2$. The number of variables in the SDP is this number minus the number of constraints given by equation (17), which is $m = (d_{S_k}^2 - d_A^2)d_B^2$. By using (25), we get $m = O(k^{(d_A-1)})$, which for a fixed size of A is only polynomial in the number of copies. Since the matrices G_J have range and support only on this symmetric subspace, we know that by a suitable change of basis they can be simultaneously block-diagonalized, with the only nonzero block having size $n = d_{S_k}^2 d_B^2$.

The SDP that searches for the PPT extension also requires to check positivity of a certain number of partial transposes of the extension $\tilde{\rho}$. These checks translate into a bigger LMI, although we will now show that this does not change the scaling properties of its size. Consider the case in which we apply the partial transpose to the first l copies of A, which we will denote $\tilde{\rho}^{T_A \otimes l}$. Since the matrices G_J have support and range only on the symmetric subspace of $\mathcal{H}_A^{\otimes k}$, it is not difficult to show that the matrices $G_J^{T_A \otimes l}$ must have support *only on the tensor product of a subspace isomorphic to the symmetric subspace of $\mathcal{H}_A^{\otimes l}$ and the symmetric subspace of $\mathcal{H}_A^{\otimes (k-l)}$*. The dimension of this tensor product is just the product of the dimensions of the two subspaces. If we perform a change of coordinates by rotating to a basis that contains a basis of this tensor product of symetric subspaces, we can see that the size of the matrices $G^{T_A \otimes l}$ can be taken as $d_{S_l}^2 d_{S_{(k-l)}}^2$. This scales at most as $O(k^{2(d_A-1)})$. Since the number of independent partial tranposes is $(k+1)$, as a result of the symmetry requirements, the size n of the matrices in the LMI scales not worse than $O(k^{2d_A-1})$. Combining this with the scaling of the number of variables m shown above and the scaling properties of solving the SDP, which is given by $O(m^2n^2)$, we can see that for fixed d_A, the tests in the hierarchy scale as $O(k^{(6d_A-4)})$, which is polynomial on the number of copies of party A for a fixed d_A.

V. COMPLETENESS OF THE HIERARCHY OF TESTS

One of the main results of this paper is the *completeness* of the hierarchy of separability tests. This result allows us to give an algorithm that will show if a state is entangled in a finite number of steps (although this number may be high for some states). Even though the hierarchy of tests is a new result, the proof of its completeness is identical to the proof of certain properties of the possible equilibrium states of a system that interacts with a thermal bath. These results, which were proved by Raggio *et al.* [36], and Fannes *et al.* [35], have been in the literature for quite some time.

It was noted in [37] that this result [35, 36] could be interpreted as a characterization of bipartite quantum states, that requires that the only states that can have symmetric extensions to any number of copies of one of its subsystyems, are the *separable states.* The same idea was independently conjectured recently by Schumacher [38].

We will present a proof of the completeness of the hierarchy, which is basically the proof found in [35], applied to the case of bipartite mixed states on finite dimensional spaces. Our discussion has the same level of mathematical rigor and is based on the techniques presented in the discussion of the Quantum de Finetti Theorem in [39]. The theorem we will prove is stronger than our hierarchy, since it requires the existence of symmetric extensions without any requirements on the partial transposes. The completeness of our hierarchy can be deduced from this result as a corollary.

Theorem 1 (Completeness) *Let ρ be a bipartite mixed state in $\mathcal{H}_A \otimes \mathcal{H}_B$. Then ρ has a symmetric extension to k copies of subsystem A for any k, if and only if, ρ is separable.*

Proof: One of the implications is trivial. Assume ρ is separable. Then we can write

$$\rho = \sum p_i |\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i|. \qquad (26)$$

¿From this expression, we can write down explicitly a symmetric extension $\tilde{\rho}$ for any value of k, namely

$$\tilde{\rho} = \sum p_i |\psi_i\rangle\langle\psi_i|^{\otimes k-1} \otimes |\phi_i\rangle\langle\phi_i|, \qquad (27)$$

and this completes the first part of the proof.

To prove the other implication, the idea is to use the existence of the extensions to construct a set of states in $\mathcal{H}_A^{\otimes n}$ that can be shown to be separable by using the Quantum de Finetti Theorem, and then show that this result implies that the extensions themselves have to be separable. Let ρ be a state in $\mathcal{H}_A \otimes \mathcal{H}_B$ such that for any n, there is a symmetric extension of ρ in $\mathcal{H}_A^{\otimes n} \otimes \mathcal{H}_B$, which we will call $\tilde{\rho}_n$. Let us pick a fixed value k for the number of copies of party A. Let the set $\{b_i\}_{i=1}^{d_B^2}$ be a basis for the set of hermitian operators in $\mathcal{H}_B$, such

that $b_i > 0$ for all i (i.e., all these operators are positive definite [40]), and in particular let us choose $b_1 = \mathbb{1}_B$, the identity in $\mathcal{H}_B$. Now we define the operator

$$\bar{\rho}_{b_i,k} = \text{Tr}_B\left[(\mathbb{1}_A^{\otimes k} \otimes b_i)\tilde{\rho}_k\right], \qquad (28)$$

where $\mathbb{1}_A$ is the identity on subsystem A. The operator $\bar{\rho}_{b_i,k}$ is positive semidefinite (PSD) and non zero since all the operators b_i were taken to be strictly positive. Then $\bar{\rho}_{b_i,k}$ is proportional to a state in $\mathcal{H}_A^{\otimes k}$, since it is hermitian and PSD. We can choose the operators b_i such that $\text{Tr}[\bar{\rho}_{b_i,k}] = 1$ for all k, so that (28) is actually a normalized state in $\mathcal{H}_A^{\otimes k}$.

We will now prove that the existence of symmetric extensions $\tilde{\rho}_k$ of ρ for all k, imply that we can choose the states $\bar{\rho}_{b_i,k}$ to be *exchangeable* [39]. Recalling the definition of exchangeability we need to show that, for any $l > 0$, there are states $\bar{\rho}_{b_i,(k+l)}$ that are symmetric and satisfy

$$\bar{\rho}_{b_i,k} = \text{Tr}_{A_{k+1}\dots A_{k+l}}[\bar{\rho}_{b_i,(k+l)}]. \qquad (29)$$

Let us fix k and assume that there is not an extension $\tilde{\rho}_k$ such that the state $\bar{\rho}_{b_i,k}$ given by (28) is exchangeable. That means that there has to be a value l_1 for which equation (29) is not satisfied for any $\bar{\rho}_{b_i,k}$ and $\bar{\rho}_{b_i,(k+l_1)}$. But since ρ has symmetric extensions for all k, we can just choose an extension to $(k+l_1)$ copies $\tilde{\rho}_{(k+l_1)}$, and we have that $\text{Tr}_{A_{k+1}\dots A_{k+l_1}}[\tilde{\rho}_{(k+l_1)}]$ is a symmetric extension of ρ to k copies, and

$$\begin{aligned}
\bar{\rho}_{b_i,k} &= \text{Tr}_B\left[(\mathbb{1}_A^{\otimes k} \otimes b_i)\text{Tr}_{A_{k+1}\dots A_{k+l_1}}[\tilde{\rho}_{(k+l_1)}]\right] \\
&= \text{Tr}_{A_{k+1}\dots A_{k+l_1}}\left[\text{Tr}_B[(\mathbb{1}_A^{\otimes k+l_1} \otimes b_i)\tilde{\rho}_{(k+l_1)}]\right] \\
&= \text{Tr}_{A_{k+1}\dots A_{k+l_1}}\left[\bar{\rho}_{b_i,(k+l_1)}\right]. \qquad (30)
\end{aligned}$$

This is a contradiction, so we can conclude that we can always choose the states $\bar{\rho}_{b_i,k}$ to be exchangeable.

The state $\bar{\rho}_{b_i,k}$ satisfies then the hypothesis of the Quantum de Finetti Theorem [39], and so we know there is a *unique* probability measure function $P_{b_i}(\varrho) \geq 0$, such that

$$\bar{\rho}_{b_i,k} = \int_D \varrho^{\otimes k} P_{b_i}(\varrho) d\varrho, \qquad (31)$$

where D represents the space of states in $\mathcal{H}_A$ (i.e., the set of hermitian, positive semidefinite operators of trace one).

For each ϱ, we can think of $P_{b_i}(\varrho)$ as a functional applied to the operators b_i, which we will note F_ϱ, defined as $F_\varrho(b_i) = P_{b_i}(\varrho)$. This functional is *linear* on convex combinations of positive operators. To see this, let $\mu > 0$. Then $F_\varrho(\mu b_i + (1-\mu)b_j) = P_{\mu b_i + (1-\mu)b_j}(\varrho)$, where $P_{\mu b_i + (1-\mu)b_j}$ is the unique probability density that satis-

fies

$$\begin{aligned}
\bar{\rho}_{(\mu b_i + (1-\mu)b_j),k} &= \int_D \varrho^{\otimes k} P_{\mu b_i + (1-\mu)b_j}(\varrho) d\varrho \\
&= \text{Tr}_B\left[(\mathbb{1}_A^{\otimes k} \otimes (\mu b_i + (1-\mu)b_j))\tilde{\rho}_k\right] \\
&= \mu\text{Tr}_B\left[(\mathbb{1}_A^{\otimes k} \otimes b_i)\tilde{\rho}_k\right] + \\
&\quad + (1-\mu)\text{Tr}_B\left[(\mathbb{1}_A^{\otimes k} \otimes b_j)\tilde{\rho}_k\right] \\
&= \int_D \left(\mu P_{b_i}(\varrho) + (1-\mu)P_{b_j}(\varrho)\right) \varrho^{\otimes k} d\varrho.
\end{aligned}$$
$$(32)$$

The second equality in (32) holds because we are considering a convex combination of the operators b_i, which guarantees that $\text{Tr}_B[(\mathbb{1}_A^{\otimes k} \otimes (\mu b_i + (1-\mu)b_j))\tilde{\rho}_k]$ is normalized. Then, by the uniqueness of the probability density in the Quantum de Finetti Theorem, we have

$$P_{\mu b_i + (1-\mu)b_j}(\varrho) = \mu P_{b_i}(\varrho) + (1-\mu)P_{b_j}(\varrho), \qquad (33)$$

which translates into

$$F_\varrho(\mu b_i + (1-\mu)b_j) = \mu F_\varrho(b_i) + (1-\mu)F_\varrho(b_j). \qquad (34)$$

Then F_ϱ is a linear functional on convex combinations of positive states in $\mathcal{H}_B$.

Since F_ϱ is defined on a basis, there is a unique way of extending this functional linearly to the whole space of operators in $\mathcal{H}_B$. So we have a linear, positive and continuous functional on a finite dimensional Hilbert space, and it is a well-known result that any such functional can be written as

$$F_\varrho(b) = \text{Tr}_B[\bar{\sigma}_\varrho b] \quad \forall b, \qquad (35)$$

for some *unique* positive semidefinite operator $\bar{\sigma}_\varrho$ in $\mathcal{H}_B$. This operator might not be a state in $\mathcal{H}_B$ since it need not be normalized. We can then define a function

$$P(\varrho) = \text{Tr}[\bar{\sigma}_\varrho], \qquad (36)$$

that is nonnegative. If $P(\varrho)$ is nonzero, we can define $\sigma_\varrho = \bar{\sigma}_\varrho/P(\varrho)$. Then (35) takes the form

$$P_b(\varrho) = F_\varrho(b) = \text{Tr}_B[\sigma_\varrho b]P(\varrho) \quad \forall b. \qquad (37)$$

Note that since σ_ϱ is normalized, $P(\varrho) = P_{\mathbb{1}_B}(\varrho)$, which shows that $P(\varrho)$ is a probability density. Using (37) in (31), we get

$$\begin{aligned}
\bar{\rho}_{b_i,k} &= \int_D \varrho^{\otimes k} \text{Tr}_B[\sigma_\varrho b_i] P(\varrho) d\varrho \\
&= \text{Tr}_B\left[(\mathbb{1}_A^{\otimes k} \otimes b_i) \int_D \varrho^{\otimes k} \otimes \sigma_\varrho P(\varrho) d\varrho\right].
\end{aligned}$$
$$(38)$$

If $P(\varrho) = 0$ for some ϱ, we can define σ_ϱ arbitrarily, since it would not contribute to the integral in (38). Since (38) is valid for all the elements b_i of a basis of hermitian matrices in $\mathcal{H}_B$, by comparing the expression in the second line with (28), we can deduce that

$$\tilde{\rho}_k = \int_D \varrho^{\otimes k} \otimes \sigma_\varrho P(\varrho) d\varrho. \qquad (39)$$

This means that $\tilde{\rho}_k$ is a separable state, since (39) is an explicit decomposition as a convex combination of product states. Furthermore, since $\tilde{\rho}_k$ is an extension of our original state ρ, we have

$$
\begin{aligned}
\rho &= \mathrm{Tr}_{A_2\ldots A_k}[\tilde{\rho}_k] \\
&= \int_D \varrho \otimes \sigma_\varrho \, P(\varrho) d\varrho, \quad (40)
\end{aligned}
$$

which shows that ρ has to be a separable state. This concludes the proof of the theorem. □

It is clear that this theorem implies the completeness of the hierarchy of separability tests introduced in Section II, since a state that has PPT symmetric extensions to k copies of party A for all values of k obviously has *symmetric extensions for all values of k*, which according to the theorem implies that the state must be separable. However, it is interesting to note that the PPT requirement is not essential for the completeness of the hierarchy. Searching just for symmetric extensions is also a complete family of separability criteria and one that requires less resources.

In [41] local hidden variable (LHV) theories were also constructed for quantum states possessing so-called symmetric quasi-extensions, where rather than requiring that the extension be positive as a matrix it is only required that it is positive on product states. The number of extensions corresponds to the number of independent local measurement settings that the theory is able to describe. In fact our argument that only separable states have an arbitrary number of symmetric extensions generalizes to this case. Essentially all that is needed is a version of the Quantum de Finetti theorem that holds for entanglement witnesses as well as states but it is straightforward to check that the argument of [39] holds in this case also since only POVMs that act as tensor products on each subsystem are used in the proof. Hence although the use of quasi-extensions is strictly stronger for a small number of local measurement settings, if the LHV is required to work for an arbitrary number of local measurement settings, the construction will only work for separable states.

We could generate more families of criteria, by searching for symmetric extensions that have to satisfy some other constraint, and this family of tests would still be complete although it would in general require more resources. If the constraint can be written in terms of linear equalities and LMIs, we could still use an SDP to implement the tests. Choosing between these many possibilities is a matter of how well they perform in actual examples. It becomes a trade-off between how much more powerful the tests become when more constraints are placed on the extensions, and how much this increases the resources needed. Including the PPT requirement on the extension has the advantage that it guarantees that the second and higher tests in the hierarchy are stronger than the PPT criterion, and we have found this to be a good trade-off in practice.

VI. CONSTRUCTION OF ENTANGLEMENT WITNESSES

An entanglement witness (EW) for a state ρ is a hermitian operator W that satisfies

$$
\mathrm{Tr}[\rho W] < 0 \quad \text{and} \quad \mathrm{Tr}[\rho_{sep} W] \geq 0, \quad (41)
$$

where ρ_{sep} is any separable state [11, 18]. It is clear that if (41) is satisfied, then ρ cannot be separable, and W gives a proof of that fact. This property has a very nice geometric interpretation. Since the set of separable states is convex, any point that does not belong to it (like any entangled state), can be separated from the set by an hyperplane. In our case, the operator W defines the hyperplane. This result is known as the Hahn-Banach theorem [42]. In practice, finding a W satisfying $\mathrm{Tr}[\rho W] < 0$ is not difficult, but proving $\mathrm{Tr}[\rho_{sep} W] \geq 0$ might be very hard. To understand the reason for this, let us recall that any separable state can be written as a convex combination of projectors into pure product states

$$
\rho_{sep} = \sum_i p_i |x\rangle\langle x| \otimes |y\rangle\langle y|, \quad (42)
$$

where $|x\rangle = \sum_i x_i |i\rangle$, $|y\rangle = \sum_j y_j |j\rangle$, for some bases $\{|i\rangle\}$ and $\{|j\rangle\}$ of $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. Then, $\mathrm{Tr}[\rho_{sep} W] \geq 0$ for any separable state ρ_{sep}, if and only if, $\mathrm{Tr}[|x\rangle\langle x| \otimes |y\rangle\langle y| W] \geq 0$ for any product state $|x\rangle\langle x| \otimes |y\rangle\langle y|$. Then we have

$$
\begin{aligned}
E_W(x,y) = \langle xy|W|xy\rangle &= \mathrm{Tr}[|x\rangle\langle x| \otimes |y\rangle\langle y| W] \\
&= \sum_{ijkl} W_{ijkl} x_i^* y_j^* x_k y_l. \quad (43)
\end{aligned}
$$

We can the interpret then the requirement that $\mathrm{Tr}[\rho_{sep} W] \geq 0$ as a positivity condition on the bihermitian form $E_W(x,y)$ associated with the entanglement witness W, where bihermitian means that the form is hermitian with respect to x and hermitian with respect to y. It is a well-known result that checking positivity of an arbitrary real form is an NP-hard problem, and the result in [9] implies the same is true for bihermitian forms. This is the reason why constructing entanglement witnesses is not easy in general.

As we mentioned in Section III, any primal SDP has an associated dual problem that is also a SDP, and in particular, whenever the primal problem is infeasible, the dual problem provides a certificate of this infeasibility. We will show that in the case of our separability tests, this infeasibility certificate generated by the dual problem is actually an entanglement witness.

Consider the SDP (23), and let us focus on the second test of the hierarchy, i.e., searching for PPT symmetric extensions to two copies of party A. In this case, the dual problem takes the form

$$
\begin{aligned}
\text{maximize} \quad & -\mathrm{Tr}[F_0 Z] \\
\text{subject to} \quad & Z \geq 0, \\
& \mathrm{Tr}[F_i Z] = 0, \quad (44)
\end{aligned}
$$

where F_0 has three blocks that encode the extension and its two independent partial transposes, and from (22) we can see that it has the form

$$F_0 = G_0 \oplus G_0^{T_A} \oplus G_0^{T_B}. \qquad (45)$$

Due to this block structure, we can restrict the search over Z in the dual program, to Z that have the same structure, so we can take

$$Z = Z_0 \oplus Z_1^{T_A} \oplus Z_2^{T_B}, \qquad (46)$$

where the Z_i are operators in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A$. The positivity condition on Z in (44), translates into a positivity requirements for each of the blocks in (46). Using this structure we can write

$$\mathrm{Tr}[F_0 Z] = \mathrm{Tr}[G_0(Z_0 + Z_1 + Z_2)], \qquad (47)$$

since $\mathrm{Tr}[G_0^{T_X} Z_i^{T_X}] = \mathrm{Tr}[G_0 Z_i]$, for $i = 1, 2$ and $X = A, B$. We defined G_0 in equation (19) as a linear function of ρ, so we can write $G_0 = \Lambda(\rho)$, where Λ is a linear map from operators on $\mathcal{H}_A \otimes \mathcal{H}_B$ to operators on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A$, whose action on an arbitrary operator Y on $\mathcal{H}_A \otimes \mathcal{H}_B$ is given by

$$\Lambda(Y) = Y \otimes \mathbb{1}_A/d_A + P(Y \otimes \mathbb{1}_A)P/d_A \\ - \mathbb{1}_A \otimes \mathrm{Tr}_A[Y] \otimes \mathbb{1}_A/d_A^2, \qquad (48)$$

where P is the swap operator defined by $P|i\rangle \otimes |k\rangle \otimes |j\rangle = |j\rangle \otimes |k\rangle \otimes |i\rangle$. We can now define an operator $\tilde{Z}$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ given by $\tilde{Z} = \Lambda^*(Z_0 + Z_1 + Z_2)$, where Λ^* is the adjoint map of Λ and is defined as the map that satisfies $\mathrm{Tr}[\Lambda(X)Y] = \mathrm{Tr}[X\Lambda^*(Y)]$ for any hermitian operators X, Y. For our particular case, this map takes the form

$$\Lambda^*(V) = \mathrm{Tr}_C[V]/d_A + \mathrm{Tr}_C[PVP]/d_A \\ - \mathbb{1}_A \otimes \mathrm{Tr}_{AC}[V]/d_A^2. \qquad (49)$$

Then we have

$$\mathrm{Tr}[\rho\tilde{Z}] = \mathrm{Tr}[\Lambda(\rho)(Z_0 + Z_1 + Z_2)] = \mathrm{Tr}[F_0 Z]. \qquad (50)$$

Let ρ_{sep} be any separable state. Then we know that there is a PPT symmetric extension of ρ_{sep}, or equivalently, the primal problem (23) is feasible. Then from (13), and using the fact that $c = 0$, we have that $\mathrm{Tr}[F_0 Z] \geq 0$ for all dual feasible Z and so from (50) we have

$$\mathrm{Tr}[\rho_{sep}\tilde{Z}] \geq 0, \qquad (51)$$

for any $\tilde{Z}$ obtained from a feasible dual solution Z. This means that any operator $\tilde{Z}$ constructed in this way, satisfies one of the two properties required in (41), and is therefore a candidate for an entanglement witness.

Now consider the case in which the primal problem is not feasible for a given state ρ. This can only occur if this state is entangled. We can then use the arguments presented in appendix B to affirm that there must be a feasible dual solution Z_{EW} that satisfies $\mathrm{Tr}[F_0 Z_{EW}] < 0$. Using (50) and (51) we can see that the corresponding hermitian operator $\tilde{Z}_{EW}$ satisfies the two conditions

$$\mathrm{Tr}[\rho\tilde{Z}_{EW}] < 0 \quad \text{and} \quad \mathrm{Tr}[\rho_{sep}\tilde{Z}_{EW}] \geq 0, \qquad (52)$$

which means that $\tilde{Z}_{EW}$ is an entanglement witness for the state ρ.

Even though we have shown the calculation explicitly only for the second test of the hierarchy, similar reasoning can be applied to all tests to show that if the primal problem is infeasible, there is a dual feasible solution that can be used to construct an entanglement witness for the state ρ. The EWs obtained for each of the tests have very well-defined and interesting algebraic properties, that can also be used to interpret each step in the hierarchy as a search for EWs of a particular form.

A. Algebraic properties of the entanglement witnesses

For any EW there is an associated bihermitian form given by (43). We have shown that the requirement that an entanglement witness W is positive on all separable states, is equivalent to requiring the associated form $E(x, y)$ to be positive.

Let us consider an EW obtained form the first test in the hierarchy, which corresponds to the usual PPT criterion. It is a well-known result that all states that fail this criterion, can be shown to be entangled by an entanglement witness of the form

$$W = P + Q^{T_A}, \qquad (53)$$

where both P and Q are positive semidefinite operators. Entanglement witnesses that have this form are called *decomposable*. If we note by $|\psi_p\rangle$ the eigenvectors of P and by $|\phi_p\rangle$ the eigenvectors of Q, we can write

$$P = \sum_p \kappa_p |\psi_p\rangle\langle\psi_p|,$$
$$Q = \sum_p \lambda_p |\phi_p\rangle\langle\phi_p|,$$

where the eigenvalues κ_p and λ_p are nonnegative, since both P and Q are PSD. If we study the associated form $E_W(x, y)$, we have

$$E_W(x,y) \;=\; \langle xy|(P+Q^{T_A})|xy\rangle = \sum_p |\sqrt{\kappa_p}\langle\psi_p|xy\rangle|^2 + \sum_p |\sqrt{\lambda_p}\langle\phi_p|x^*y\rangle|^2$$

$$=\; \sum_p |\sqrt{\kappa_p}\sum_{ij}\psi_{ij}^p x_i y_j|^2 + \sum_p |\sqrt{\lambda_p}\sum_{ij}\phi_{ij}^p x_i^* y_j|^2, \tag{54}$$

with $|\psi_p\rangle = \sum_{ij}\psi_{ij}^p|ij\rangle$ and $|\phi_p\rangle = \sum_{ij}\phi_{ij}^p|ij\rangle$. The last equality in (54) shows that $E_W(x,y)$ can be written as a *sum of squared magnitudes* (SOS), which proves its positivity. This property is an alternative description of decomposable entanglement witnesses.

Now imagine that we have a state ρ that is PPT entangled, whose entanglement is detected by the second test of the hierarchy (i.e., ρ does not have a PPT symmetric extension to two copies of party A). Then we know that the dual SDP will provide us with an entanglement witness $\tilde{Z}_{EW}$ for this state. Let us concentrate on the properties of this $\tilde{Z}_{EW}$. First, it is clear that it cannot be decomposable, since decomposable EWs can only detect states that are not PPT. By setting $\rho_{sep} = |xy\rangle\langle xy|$ in (51), we have that

$$\begin{aligned}\mathrm{Tr}[|xy\rangle\langle xy|\tilde{Z}_{EW}] &= \langle xy|\tilde{Z}_{EW}|xy\rangle \\ &= E_{\tilde{Z}_{EW}}(x,y) \geq 0.\end{aligned} \tag{55}$$

According to equation (50), we have

$$\mathrm{Tr}[|xy\rangle\langle xy|\tilde{Z}_{EW}] = \mathrm{Tr}[\Lambda(|xy\rangle\langle xy|)(Z_0 + Z_1 + Z_2)]. \tag{56}$$

The operator Λ maps a state ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$ into an operator in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A$ that is invariant under swaps of the two copies of A and yields the original state ρ when one of the copies of A is traced out, but is in general not positive semidefinite. Now consider the state $|xyx\rangle\langle xyx|$. This state is invariant under swaps of copies of system A and also satisfies $\mathrm{Tr}_C[|xyx\rangle\langle xyx|] = |xy\rangle\langle xy|$. Then we know that there must exist some coefficients a_J such

that

$$|xyx\rangle\langle xyx| = \Lambda(|xy\rangle\langle xy|) + \sum_J a_J G_J, \tag{57}$$

since the G_J form a basis of the space of matrices M satisfying the swapping symmetry and $\mathrm{Tr}_C[M] = 0$. According to (44) we have $\mathrm{Tr}[G_J Z_i] = 0$, and hence we can rewrite (56) as

$$\mathrm{Tr}[|xy\rangle\langle xy|\tilde{Z}_{EW}] = \mathrm{Tr}[|xyx\rangle\langle xyx|(Z_0 + Z_1 + Z_2)]. \tag{58}$$

Combining (55) and (58), we have

$$\langle xy|\tilde{Z}_{EW}|xy\rangle = \langle xyx|(Z_0 + Z_1 + Z_2)|xyx\rangle. \tag{59}$$

Since we are working with normalized states, we know that $\langle x|x\rangle = 1$, so we can multiply the left-hand side of (59) by this factor without changing the equality, obtaining

$$E_{\tilde{Z}_{EW}}(x,y)\langle x|x\rangle = \langle xyx|(Z_0 + Z_1 + Z_2)|xyx\rangle. \tag{60}$$

This equation is, in principle, only valid when the variables x_i and y_i correspond to a normalized state, i.e., when $\sum_i |x_i|^2 = 1$ and $\sum_i |y_i|^2 = 1$. However, since both sides of (60) are homogeneous functions of fourth degree on the x_i, and of second degree on the y_i, we can extend this equality to all values of the variables, and interpret (60) as an equality between two forms *that is satisfied everywhere*. But we can now rewrite the right-hand side of (60) as

$$\langle xyx|(Z_0 + Z_1 + Z_2)|xyx\rangle = \langle xyx|Z_0|xyx\rangle + \langle x^*yx|Z_1^{T_A}|x^*yx\rangle + \langle xy^*x|Z_2^{T_B}|xy^*x\rangle. \tag{61}$$

Since $Z_0, Z_1^{T_A}$ and $Z_2^{T_B}$ are positive by construction, equation (61) gives an explicit sum of squares (SOS) decomposition of the right-hand side of (60). We can conclude then that even though the form $E_{\tilde{Z}_{EW}}(x,y)$ is not a SOS, *it becomes a SOS when multiplied by the strictly positive SOS form* $\langle x|x\rangle = \sum_i |x_i|^2$. This property holds for *any* EW obtained from the second test.

This result generalizes to all steps of the hierarchy: *the bihermitian form associated with an EW obtained from the $(k+1)^{th}$ test of the hierarchy, can be written as a SOS*

when multiplied by the SOS form $\langle x|x\rangle^k = (\sum_i |x_i|^2)^k$. We will say then that these EW are *k-SOS*. Then for example, an entanglement witness that is 0-*SOS* is decomposable, since its associated form can be written as a SOS (we will use SOS instead of 0-*SOS* for this particular case). It is clear that if an EW is *k-SOS*, it is also *l-SOS* for all $l \geq k$. Note that for $k \geq 1$, all *k-SOS* entanglement witnesses are *indecomposable*.

As we discussed in Section V, searching for symmetric extensions with no PPT requirement generates another

complete family of separability criteria. For this family, equation (60) takes the form

$$E_{\tilde{Z}_{EW}}(x,y)\langle x|x\rangle = \langle xyx|Z_0|xyx\rangle, \tag{62}$$

since now the LMI has only one block, corresponding to the positivity requirement on the extension. Since Z_0 is PSD, the right-hand side of (92) still is a SOS, so we will still say that $\tilde{Z}_{EW}$ is 1-SOS (or k-SOS if we replace $\langle x|x\rangle$ by $\langle x|x\rangle^k$ in (62)). The main difference between (62) and (61) is in the type of terms that appear in the sum of squares decomposition. Note that (62) involves only squares of polynomials in the variables (x_i, y_j) while the second and third terms in the right-hand side of (61) correspond to squares of polynomials in the (x_i^*, y_j, x_k) and (x_i, y_j^*) variables respectively. This situation extends to all the steps of the hierarchy. The SOS decomposition generated by the PPT family involves the squared magnitudes of all possible polynomials in the variables (x_i, y_j) *and their conjugates* that are compatible with the symmetry requirements, while the SOS decomposition obtained from the non-PPT family involves squared magnitudes of polynomials involving *only* the variables (x_i, y_j). The completeness theorem tells us that for any EW obtained from any of the two families, we could make the associated bihermitian form into a SOS by multiplying by a certain power of the SOS form $(\sum_i |x_i|^2)$. However, the value of the power needed in the non-PPT case will be in general higher than for the PPT case.

We presented our family of separability criteria as the search for an extension of the original state ρ that satisfied certain symmetries and had positive partial transposes, and showed that this search could be put in the primal form of a SDP. From the discussion above, we can see that by looking at the dual SDP, we can interpret this hierarchy as a search over possible entanglement witnesses for the state ρ that are k-SOS for some k. Note that this interpretation also applies to the non-PPT family of criteria, the only change being the type of terms allowed in the SOS decomposition. The completeness result proved in Section V tells us that the set of all entanglement witnesses that are k-SOS for some k, is *sufficient* for proving entanglement of any state. This raises a very interesting question: *are all EW k-SOS for some k?* We will now show that most EW are, and the only ones that may not be are those that are extremal in the sense that their associated hyperplane touches the set of separable states. These are the *optimal* EWs from [6].

Let us first introduce some definitions regarding convex sets. A set K is said to be a *convex cone* if it is convex and closed under linear combinations with non-negative coefficients, i.e., if $x, y \in K$ and $a, b \geq 0$, then $ax + by \in K$. The *dual cone* of K is defined as $K^* = \{z : \langle z, x\rangle \geq 0, \forall x \in K\}$, where $\langle,\rangle$ represents some inner product (note that K^* will be different for different inner products). It is easy to show that K^* is actually a closed convex cone even if K is not closed. An important property is that [42]

$$(K^*)^* = \mathrm{cl}(K), \tag{63}$$

where $\mathrm{cl}(K)$ represents the closure of K.

Let S be the set of all unnormalized separable states. S is a closed convex cone. Its dual cone is $S^* = \{Z : \mathrm{Tr}[Z\rho_{sep}] \geq 0, \forall \rho_{sep} \in S\}$, which contains the set of all entanglement witnesses. If $(S^*)^o$ notes the *interior* of S^*, we have $(S^*)^o = \{Z : \mathrm{Tr}[Z\rho_{sep}] > 0, \forall \rho_{sep} \in S\}$.

Theorem 2 *Let W be an entanglement witness such that $W \in (S^*)^o$. Then W is k-SOS for some k, i.e., $\exists k$ such that $E_W(x,y)(\sum_i |x_i|^2)^k$ is a SOS.*

Proof: Let $O_k = \{Z : E_Z(x,y)(\sum_i |x_i|^2)^k$ is a SOS$\}$. This is just the set of entanglement witnesses that are k-SOS. Clearly, $O_k \subset O_{k+1}$ and $O_k \subset S^*$. Now we define the set

$$O = \bigcup_{k=0}^{\infty} O_k. \tag{64}$$

O is a convex cone, although it may not be closed. We will now show that the dual of this cone is the set S. Let $\rho_{sep} \in S$. For any $Z \in O$, $\exists k$ such that $Z \in O_k$. But $Z \in S^*$, so $\mathrm{Tr}[Z\rho_{sep}] \geq 0$, which means that $\rho_{sep} \in O^*$, so we have

$$S \subset O^*. \tag{65}$$

Now, let $\rho \in O^*$ and assume $\rho \notin S$; then ρ is an entangled state. By the completeness of the hierarchy of separability tests, we know that there is a value of k for which $\mathrm{Tr}[Z\rho] < 0$ for some $Z \in O_k \subset O$, and then we must have $\rho \notin O^*$, which is a contradiction. Then

$$O^* \subset S. \tag{66}$$

¿From (65) and (66), we have $S = O^*$. Then we can use (63) to state that $S^* = \mathrm{cl}(O)$, which means

$$(S^*)^o \subset O. \tag{67}$$

If $W \in (S^*)^o$ then by (64) there exists k such that $W \in O_k$, and hence it is k-SOS. $\square$

This theorem has a very nice geometric interpretation. It says that the sequence of convex cones O_k approximates the convex cone of all entanglement witnesses S^* from the inside, giving a complete characterization of its interior in terms the k-SOS property. On the other hand, the entanglement witnesses on the boundary of S^* may not be k-SOS for any k. They satisfy $\mathrm{Tr}[Z\rho_{sep}] = 0$ for some separable state ρ_{sep}, and correspond to the *optimal* entanglement witnesses discussed in [6].

As we briefly mentioned in Section II, the separability criteria based on searching for certain extensions of a state can easily be generalized to the study of multipartite entanglement. The dual formulation of searching for an EW with certain algebraic properties also clearly applies to the multipartite case. It is known that multipartite entanglement cannot be characterized in terms of bipartite entanglement alone [43, 44]. However, our approach can be generalized to the multipartite case in order to construct another sequence of tests that is also *complete*. These results will be reported elsewhere [45].

VII. EXAMPLES

We present now some examples for which we applied our techniques to prove entanglement of certain PPT entangled states, and to construct the appropriate entanglement witnesses. For all these examples, the second test of the hierarchy (searching for PPT symmetric extensions to two copies of party A) was sufficient to show entanglement. We used MATLAB to code the corresponding SDP, and used the package SEDUMI [46] to solve it. The code is available at http://www.iqi.caltech.edu/publications.html.

A. $3 \otimes 3$ state.

We consider the following state,described in [7], given by

$$\rho_\alpha = \frac{2}{7}|\psi_+\rangle\langle\psi_+| + \frac{\alpha}{7}\sigma_+ + \frac{5-\alpha}{7}V\sigma_+V, \quad (68)$$

with $0 \le \alpha \le 5$, $|\psi_+\rangle = \frac{1}{\sqrt{3}}\sum_{i=0}^{2}|ii\rangle$, $\sigma_+ = \frac{1}{3}(|01\rangle\langle01| + |12\rangle\langle12| + |20\rangle\langle20|)$ and V the operator that swaps the two systems (note they are both the same space). Notice that ρ_α is invariant under the simultaneous change of $\alpha \to 5 - \alpha$ and interchange of the parties. The state is separable for $2 \le \alpha \le 3$ and not PPT for $\alpha > 4$ and $\alpha < 1$, which was proved in [7] by using a positive map that is not completely positive due to Choi [20]. Our code solves the SDP for this state in about 5 seconds on a desktop computer. From this solution, numerical entanglement witnesses can be constructed for ρ_α in the range $3 + \epsilon < \alpha \le 4$ (and $1 \le \alpha < 2 - \epsilon$) with $\epsilon \ge 10^{-8}$. A witness for $\alpha > 3$ can be extracted from these by inspection:

$$\tilde{Z}_{EW} = 2\left(|00\rangle\langle00| + |11\rangle\langle11| + |22\rangle\langle22|\right) + |02\rangle\langle02| + |10\rangle\langle10| + |21\rangle\langle21| - 3|\psi_+\rangle\langle\psi_+|. \quad (69)$$

¿From this entanglement witness, the Choi form [20] can be recovered. This observable is nonnegative on separable states:

$$
\begin{aligned}
4\langle xy|\tilde{Z}_{EW}|xy\rangle\langle x|x\rangle &= 3\,|x_2x_0y_1^* - x_1x_2y_0^*|^2 + 3\,|x_1x_1^*y_0 - x_2x_0^*y_2|^2 + 3\,|x_2x_2^*y_2 - x_0x_2^*y_0|^2 + 3\,|x_2x_1^*y_2 - x_1x_1^*y_1|^2 \\
&\quad + |2x_0x_0^*y_2 - 2x_1x_2^*y_1 + x_2x_2^*y_2 - x_0x_2^*y_0|^2 + |2x_0x_1^*y_0 - 2x_2x_2^*y_1 + x_2x_1^*y_2 - x_1x_1^*y_1|^2 \\
&\quad + |2\,x_0x_1y_2^* - x_2x_0y_1^* - x_1x_2y_0^*|^2 + |2x_0x_0^*y_0 - 2x_1x_0^*y_1 + x_1x_1^*y_0 - x_2x_0^*y_2|^2 \ge 0.
\end{aligned}
$$

The expected value on the original state is $\mathrm{Tr}[\tilde{Z}_{EW}\rho_\alpha] = \frac{1}{7}(3-\alpha)$, demonstrating entanglement for all $\alpha > 3$. Applying the non-PPT tests to this state fails to show entanglement for $\alpha \lesssim 3.84$, even if we apply the 6th test, showing that this hierarchy can be considerably weaker than the PPT hierarchy.

B. $4 \otimes 4$ state

We consider next the $4 \otimes 4$ state given by [47]:

$$\rho_\alpha = \frac{1}{2+\alpha}(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| + \alpha\cdot\sigma), \quad \alpha \ge 0,$$

where

$$
\begin{aligned}
\psi_1 &= \frac{1}{2}(|00\rangle + |11\rangle + \sqrt{2}\,|22\rangle), \\
\psi_2 &= \frac{1}{2}(|01\rangle + |10\rangle + \sqrt{2}\,|33\rangle), \\
\sigma &= \frac{1}{8}(|02\rangle\langle02| + |03\rangle\langle03| + |12\rangle\langle12| + |13\rangle\langle13| + \\
&\quad + |20\rangle\langle20| + |21\rangle\langle21| + |30\rangle\langle30| + |31\rangle\langle31|).
\end{aligned}
$$

Applying the PPT criterion yields provable entanglement only for those states with $\alpha < 2\sqrt{2} \approx 2.82843$. It was suspected [47] that the state was actually entangled for all nonnegative values of α. Using our new criteria, we show that this is indeed the case, and provide an explicit entanglement witness and its decomposition. Again, only the second level of our hierarchy is needed. Using essentially the same approach as in the example above, from the dual solution of the semidefinite program we identify a particular witness:

$$W = (|22\rangle - |00\rangle)(\langle 22| - \langle 00|) + (|22\rangle - |11\rangle)(\langle 22| - \langle 11|) + (|33\rangle - |01\rangle)(\langle 33| - \langle 01|) + (|33\rangle - |10\rangle)(\langle 33| - \langle 10|) +$$
$$+ |23\rangle\langle 23| + |32\rangle\langle 32| - |22\rangle\langle 22| - |33\rangle\langle 33|.$$

This witness is nonnegative on all product states, as the following identity certifies:

$$\langle xy|W|xy\rangle\langle x|x\rangle = |x_0 x_0^* y_0 + x_1 x_1^* y_0 - x_2 x_0^* y_2 - x_3 x_1^* y_3|^2 + |x_0 x_0^* y_1 + x_1 x_1^* y_1 - x_2 x_1^* y_2 - x_3 x_0^* y_3|^2 +$$
$$|x_2 x_2^* y_2 + x_3 x_3^* y_2 - x_0 x_2^* y_0 - x_1 x_2^* y_1|^2 + |x_2 x_2^* y_3 + x_3 x_3^* y_3 - x_1 x_3^* y_0 - x_0 x_3^* y_1|^2 +$$
$$|x_1 x_3 y_2^* - x_0 x_2 y_3^*|^2 + |x_0 x_3 y_2^* - x_1 x_2 y_3^*|^2 + |x_1 x_2 y_0^* - x_0 x_2 y_1^*|^2 + |x_0 x_3 y_0^* - x_1 x_3 y_1^*|^2 \geq 0.$$

Applying the witness W to the state, we obtain $\mathrm{Tr}[W\rho_\alpha] = -\frac{2(\sqrt{2}-1)}{2+\alpha} < 0$, therefore certifying entanglement for *all* values of α in the allowable range.

We have applied the second test of the hierarchy to many bound entangled states found in the literature of dimensions up to 6 by 6 . In all cases, this test has been *sufficient* to demonstrate entanglement and construct numerical (and in some cases analytical) entanglement witnesses. However, we know from complexity arguments that there must be states that pass the second test in the hierarchy but are nonetheless entangled as we will discuss in the next section.

VIII. PROPERTIES OF THE SETS OF ENTANGLED STATES WITH PPT SYMMETRIC EXTENSIONS

For every k, let us consider the set of states that are not detected by the kth test of the hierarchy, which can also be characterized as the states having PPT symmetric extensions to k copies of party A. They generate a sequence of nested sets, each one containing the set of separable states. The completeness theorem tells us that this sequence actually converges to the set of separable states. It is natural then to try to understand the properties of these particular sets. First of all, it is not difficult to see that these sets are all convex and compact. But there are other interesting questions we can ask about them. Are they nonempty? Is this sequence infinite or does it collapse to a finite number of steps for certain cases? What is the volume of the subset of entangled states contained in each set? Are these sets invariant under LOCC? In this section we will address some of these questions by explicitly constructing states with PPT symmetric extensions and studying the implications of their existence.

A. Constructing entangled states with PPT symmetric extensions

We will now show explicitly how to construct an entangled state that passes the second test in the hierarchy, which means it has a PPT symmetric extension to two copies of system A. We will proceed by studying the

properties of an EW obtained from the second test under a particular scaling and then use duality arguments to infer the existence of the required entangled state. The procedure is based on a scaling technique developed recently by Reznick [48].

Let ρ be a PPT entangled state that is detected by the second test of the hierarchy. Then we know that there is an entanglement witness Z that satisfies $\mathrm{Tr}[\rho Z] < 0$ and

$$\langle xy|Z|xy\rangle\langle x|x\rangle \text{ is a } SOS, \tag{70}$$

which implies that $\mathrm{Tr}[Z\rho_{sep}] \geq 0$ for any separable state ρ_{sep}. Since ρ is PPT, we know that the bihermitian form $\langle xy|Z|xy\rangle$ cannot be a SOS, otherwise Z can easily be shown to be decomposable and hence unable to detect a PPT entangled state, which would be a contradicition. Now, let us consider the following hermitian operator

$$Z_\gamma = (A^{-1})^\dagger \otimes \mathbb{1}_B \, Z \, A^{-1} \otimes \mathbb{1}_B, \tag{71}$$

with $A = diag(1, \gamma, \ldots, \gamma)$, $\gamma > 0$. This operator satisfies

$$\langle xy|Z_\gamma|xy\rangle = \langle (A^{-1}x)y| \, Z \, |(A^{-1}x)y\rangle \geq 0, \tag{72}$$

since Z is positive on product states. Now consider the state

$$\rho_\gamma = \frac{1}{N}(A \otimes \mathbb{1}_B)\,\rho\,(A^\dagger \otimes \mathbb{1}_B), \tag{73}$$

with N a positive normalization constant. The state ρ_γ is entangled for all $\gamma > 0$, because

$$\mathrm{Tr}[\rho_\gamma Z_\gamma] = \frac{1}{N}\mathrm{Tr}[\rho Z] < 0. \tag{74}$$

This, together with (72), proves that Z_γ is actually an entanglement witness. Now, let us assume that Z_γ is *1-SOS* for all $\gamma > 0$, that is

$$\langle xy|Z_\gamma|xy\rangle\langle x|x\rangle \text{ is a } SOS. \tag{75}$$

By using (71) and introducing the variables $\tilde{x} = A^{-1}x$, we obtain

$$\langle \tilde{x}y|Z|\tilde{x}y\rangle\langle A\tilde{x}|A\tilde{x}\rangle \text{ is a } SOS, \tag{76}$$

where the SOS structure is preserved due to the linearity of the transformation from x to $\tilde{x}$. Specializing for A in (76) we get

$$\langle \tilde{x}y|Z|\tilde{x}y\rangle((\tilde{x}_1^2 + \gamma^2(\tilde{x}_2^2 + \ldots + \tilde{x}_{d_A}^2)) \text{ is a } SOS. \quad (77)$$

Since the set of forms that can be written as a SOS is a closed set, the assertion in (77) must be valid also for $\gamma = 0$, and in that case we must have that

$$\langle \tilde{x}y|Z|\tilde{x}y\rangle \tilde{x}_1^2 \text{ is a } SOS. \quad (78)$$

But this implies that the form $\langle \tilde{x}y|Z|\tilde{x}y\rangle$ is itself a SOS, which contradicts our assumption. Then we conclude that there must be a value $\gamma^* > 0$ such that for all $\gamma < \gamma^*$, the entanglement witness Z_γ has the property that

$$\langle xy|Z_\gamma|xy\rangle\langle x|x\rangle \text{ is not a } SOS. \quad (79)$$

Note that this argument is only based in the fact that there is a PPT entangled state detected by the second test of the hierarchy. Whenever this happens, we know that we can construct an EW that satisfies (79), regardless of the dimensionality of the subsystems.

We can now very easily show that the existence of an EW satisfying (79) implies the existence of an entangled state that is not detected by the second test. We just need a very simple lemma of convex analysis.

Lemma 1 *Let K_1 and K_2 be two closed convex cones such that $K_1 \subset K_2$, where $\subset$ represents strict inclusion. Then the dual cones satisfy $K_2^* \subset K_1^*$.*

Proof: Recall the definition of the dual of a cone K, $K^* = \{z | \langle z, x\rangle \geq 0, \forall x \in K\}$. Let $z \in K_2^*$, then $\langle z, x\rangle \geq 0, \forall x \in K_2$. Since $K_1 \subset K_2$, $\langle z, x\rangle \geq 0, \forall x \in K_1$, so $z \in K_1^*$ and hence $K_2^* \subseteq K_1^*$. Now, let $\tilde{x} \in K_2$ such that $\tilde{x} \notin K_1$. Assume that $K_2^* = K_1^*$. Let $z \in K_1^*$; then we also have $z \in K_2^*$ and so $\langle z, \tilde{x}\rangle \geq 0$. But since this is true $\forall z \in K_1^*$, this means that $\tilde{x} \in K_1^{**} = K_1$, since K_1 is closed, and this is a contradiction. Then we must have $K_2^* \subset K_1^*$. □

In our case we have the closed convex cones $O_k = \{Z : \langle xy|Z|xy\rangle(\sum_i |x_i|^2)^k \text{ is a } SOS\}$, $k = 0, 1, \ldots$, that we have already defined for the proof of Theorem 2. In this section we have shown that if there is an entangled state that is detected by an EW in O_1 that is not in O_0, then O_1 is *strictly contained* in O_2. According to the lemma above this means that O_2^*, which is the set of states that *are not* detected by the third test of the hierarchy, is strictly contained in O_1^*, the set of states that *are not* detected by the second test. Thus, that there has to be a state that *is not* detected by an EW in O_1, because it belongs to O_1^* (equivalently, it passes the second test), but *is* detected by an EW in O_2, (because it does not belong to O_2^*) and hence is entangled.

The discussion above shows that there has to be an entangled state that passes the second test, but it does not give an explicit construction. But since we know that Z_γ ceases to be in O_1 for some small value of γ, and since

we have shown that it detects the entanglement of ρ_γ for all $\gamma > 0$, we could be tempted to say that then ρ_γ has to be a state that passes the second test for small enough γ. The problem is that even though Z_γ is an EW for ρ_γ, it is not clear that there is not another EW in O_1 that detects the entanglement of ρ_γ. However, even if we are not assured that it would be the case, we can still check whether ρ_γ actually passes the second test for small γ. We did this numerically using our code for the case of the Choi state (68) with $\alpha = 3.0001$, and we found that indeed there is a value $\gamma^* \simeq 0.4901$ of the parameter such that for all $\gamma < \gamma^*$, the state ρ_γ is entangled but cannot be detected by the second test of the hierarchy.

B. Properties of the hierarchy

¿From an algebraic point of view, the result of the previous subsection is related to the fact that the fixed multiplier approach to proving nonnegativity by finding a SOS decomposition does not behave well under linear transformations. A solution to this problem may be allowing the multiplier $\langle x|x\rangle$ to vary as well, although it appears that this approach to checking for entanglement cannot be stated as a SDP.

¿From a physical point of view, this result has a very interesting interpretation. The transformation represented by Equation (73) corresponds to applying an element of a POVM that acts locally on system A and leaves system B alone. Such a transformation can be implemented by local operations with some finite probability. We see then that by SLOCC (stochastic local operations and classical communication), we can transform a state that is detected by the second test into a state that is not. Moreover, since the matrix A in (73) is invertible, the reverse transformation is *also possible under SLOCC*. Then we could start with the state ρ', whose entanglement is not detected by the second test, and by LOCC operations obtain, with some probability, a state ρ that *is* detected by the second test. This shows clearly that, unlike the PPT class of states, the classes of states derived from the second and higher tests of the hierarchy *are not invariant under LOCC*.

This scaling behavior of both states and entanglement witnesses is very general and has very important consequences on the hierarchy of tests. First, note that if we assume that Z_γ is k-SOS (for any fixed k) for all $\gamma > 0$, this will be equivalent to replacing $\langle x|x\rangle$ by $\langle x|x\rangle^k$ in (75). We can then follow the exact same steps discussed after (75) and arrive to the same contradiction (i.e., that $\langle \tilde{x}y|Z|\tilde{x}y\rangle$ is a SOS). Then for γ small enough, $\langle xy|Z_\gamma|xy\rangle\langle x|x\rangle^k$ must cease to be a SOS for *any* fixed value of k. By applying Lemma 1 again, we can conclude that *if there exists a PPT-entangled state ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$, then for any value of k, there must be an entangled state ρ_k that is not detected by the kth test of the hierarchy.* Note that this result depends only on the existence of at least one bound entangled state, and not on the dimen-

sions of the system. Since there are explicit examples of bound entangled states in $3 \otimes 3$ (like Equation (68)) and $2 \otimes 4$ (see [13]), and we can (by embedding) use them to construct bound entangled states in $N \otimes M$, $N \times M > 6$, we can conclude that *there are always entangled states in $\mathcal{H}_A \otimes \mathcal{H}_B$, $d_A \times d_B > 6$, that pass the first k tests in the hierarchy, for any fixed k.* In other words, the hierarchy *never collapses to a finite number of steps, even for fixed dimensions* (except in the already known cases of $2 \otimes 2$ and $2 \otimes 3$).

A very interesting question has to do with what is actually the volume of the set of entangled states that are detected by the kth test, but are not detected by the $(k-1)^{th}$ test (or equivalently, the set of states that have PPT symmetric extensions to $(k-1)$ copies of A, but not to k copies). Even though we cannot give any estimate on the value of this volume, we can assert that this volume is *finite*, i.e., the set in question has *nonzero measure* when we consider the measure on the set of states introduced in [49]. This is true for all values of k for which this set is nonempty. The proof of this fact is a straightforward translation of the result presented in Lemma 7 of [49]. This lemma proves that if a convex set C_1 strictly contains a compact convex set C_2 that itself contains a nonempty ball, then C_1 contains a nonempty ball that does not intersect C_2. In our case we can take C_1 to be the set of states with PPT symmetric extensions to $(k-1)$ but not to k copies of A, and C_2 the ones with extensions to k copies. Since both C_1 and C_2 are convex and compact, and C_2 contains the set of separable states that contains a nonempty ball, the lemma proves that there is a nonempty ball of states that have PPT symmetric extensions to $(k-1)$ copies of A, but not to k copies.

IX. CONSTRUCTING BOUND ENTANGLED STATES FROM INDECOMPOSABLE ENTANGLEMENT WITNESSES

In previous sections we have discussed how to use semidefinite programs to implement separability criteria, and in particular we showed how to exploit the duality of the SDP to generate an indecomposable entanglement witness from a bound entangled state. In this section we will show that we can also use a SDP to test whether a given entanglement witness is decomposable. If the EW is indecomposable, the dual program constructs a bound entangled state that is detected by the witness. The results of this section were reported in [50] which we follow closely.

As discussed above, a sufficient but not necessary condition for any hermitian matrix Z to be an entanglement witness is for it not to be positive but rather decomposable as $Z = P + Q^{T_A}$, where $P \geq 0, Q \geq 0$. Such entanglement witnesses are obtained whenever a state fails the first test of the hierarchy, which is just the PPT criterion. These entanglement witnesses can only detect entangled states that have a non-positive partial transpose. As it was shown in (54), the bihermitian forms associated with them can be written as a SOS.

If we know only the matrix elements of Z it may not be clear how to determine whether Z is decomposable or not. Consider the following semidefinite program in the dual form

$$\begin{aligned}
\text{maximize} \quad & -\text{Tr}\,[P + Q^{T_A}]/d_A d_B \\
\text{subject to} \quad & P \geq 0, \quad Q \geq 0 \\
& H(P + Q^{T_A}) = H(Z), \quad (80)
\end{aligned}$$

where $H(Y) = Y - (\text{Tr}[Y])\mathbb{1}/d_A d_B$ is a linear map that outputs the traceless part of Y. We can make (80) take the more familiar form (12) if we introduce the matrix variable X, defined by $X = P \oplus Q$ (X will play the role of Z in (12)). The final equality constraint may be enforced by a finite number ($d_A^2 d_B^2 - 1$) of trace constraints that define the matrices F_i and the coefficients c_i. F_0 is then proportional to the identity. By adding a sufficiently large multiple of the identity to any matrix satisfying the trace constraints, it is always possible to construct an $X = P \oplus Q > 0$ also satisfying the constraints. This means that the optimization is strictly feasible. Let η be the optimum value of the objective function $-\text{Tr}\,[P + Q^{T_A}]/d_A d_B$, and P_{opt}, Q_{opt} be the values of P and Q that achieve this optimum. If

$$\eta \geq -\text{Tr}\,[Z/d_A d_B], \quad (81)$$

then for $\epsilon \equiv \text{Tr}[Z/d_A d_B] + \eta \geq 0$ it is clear that we can write

$$Z = (P_{\text{opt}} + \epsilon \mathbb{1}_{AB}) + Q_{\text{opt}}^{T_A}, \quad (82)$$

which shows that Z is decomposable.

We have stated the semidefinite program in its dual form. The primal form is worth considering since in the case where Z is nondecomposable, it constructs bound entangled states that are detected by Z. Using the formulae (11),(12) and (80), the primal form may be shown to be

$$\begin{aligned}
\text{minimize} \quad & \text{Tr}\,[Z\rho] - \text{Tr}\,[Z/d_A d_B] \\
\text{subject to} \quad & \rho \geq 0, \quad \rho^{T_A} \geq 0 \\
& \text{Tr}\,[\rho] = 1, \quad (83)
\end{aligned}$$

where now the variables are the components of the state ρ in some basis. The completely mixed state is strictly positive and is a feasible solution of (83). Thus, because of the strict feasibility of both the primal and dual problems the optima of these two programs are equal [28] and there are matrices $\rho_{\text{opt}}, P_{\text{opt}}, Q_{\text{opt}}$ achieving the optimum. By complementary slackness the range of P_{opt} is orthogonal to the range of ρ_{opt} and the range of Q_{opt} is orthogonal to the range of $\rho_{\text{opt}}^{T_A}$.

Suppose now that the optimum η satisfies $\eta < -\text{Tr}[Z/d_A d_B]$. This, together with $\eta = \text{Tr}[Z\rho_{\text{opt}}] - \text{Tr}[Z/d_A d_B]$, means that

$$\text{Tr}\,[Z\rho_{\text{opt}}] < 0. \quad (84)$$

Since we know that Z is an EW, then (84) means that the state ρ_{opt} is entangled. Furthermore, since this state is a feasible solution of (83), it must satisfy $\rho_{\text{opt}}^{T_A} \geq 0$, so this state is bound entangled. For any $P \geq 0$, $Q \geq 0$ we have

$$\text{Tr}\left[(P + Q^{T_A})\rho_{\text{opt}}\right] = \text{Tr}\left[P\rho_{\text{opt}}\right] + \text{Tr}\left[Q\rho_{\text{opt}}^{T_A}\right] \geq 0, \quad (85)$$

so Z cannot be decomposable, since it satisfies (84).

We will now show that ρ_{opt} is the so-called edge PPT entangled state. Since ρ_{opt} is a PPT entangled state, we can write $\rho_{\text{opt}} = (1-p)\rho_{sep} + p\delta$, where ρ_{sep} is separable, δ is a so-called edge PPT entangled state and $p > 0$ is the minimum value for which such a decomposition is possible [25]. An edge PPT entangled state δ has the property that for any pure product state $|x, y\rangle$ and $\epsilon > 0$, $\delta - \epsilon|x, y\rangle\langle x, y|$ is either not positive or not PPT. Since $\text{Tr}\left[Z\rho_{sep}\right] \geq 0$ (because Z is an EW), if $p < 1$ then

$$\text{Tr}\left[Z\rho_{\text{opt}}\right] > \text{Tr}\left[Z\delta\right]. \quad (86)$$

But (86) contradicts the optimality of ρ_{opt}, unless ρ_{opt} is itself an edge PPT entangled state.

This SDP finds the canonical decomposition of an indecomposable EW discussed in [25]. Defining $\epsilon = -\text{Tr}[Z\rho_{\text{opt}}] > 0$, we have

$$Z = P_{\text{opt}} + Q_{\text{opt}}^{T_A} - \epsilon \mathbb{1}_{AB}, \quad (87)$$

and as a result of the original dual form of the optimization, ϵ is the smallest value for which such an expression holds with $P \geq 0$, $Q \geq 0$. The range properties of $P_{\text{opt}}, Q_{\text{opt}}$ and ρ_{opt} mean that this is the canonical form for Z introduced by Lewenstein *et al.*[25].

X. CHARACTERIZATION OF POSITIVE MAPS

It has been known for quite some time that there is a close relationship between entanglement witnesses, positive bihermitian forms and positive maps [12, 20]. In particular, this relationship was exploited in [11] to give a complete characterization of the separability problem in terms of positive maps. We will now show how to translate the properties of the entanglement witnesses generated by our hierarchy of separability tests into a characterization of the set of strictly positive maps.

Let us denote by $\mathcal{A}_A$ and $\mathcal{A}_B$ the set of linear operators acting on $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively. We will call $\mathcal{L}(\mathcal{A}_A, \mathcal{A}_B)$, the set of linear maps from $\mathcal{A}_A$ to $\mathcal{A}_B$. We say that a map $\Lambda \in \mathcal{L}(\mathcal{A}_A, \mathcal{A}_B)$ is *positive*, if for any operator $L \in \mathcal{A}_A$, $L \geq 0$, then $\Lambda(L) \geq 0$. A *completely positive* (CP) map, is a map Λ such that the induced map

$$\Lambda_n = \Lambda \otimes \mathbb{1}_n : \mathcal{A}_A \otimes \mathcal{M}_n \to \mathcal{A}_B \otimes \mathcal{M}_n, \quad (88)$$

is positive for all n, with $\mathcal{M}_n$ being the space of operators in a Hilbert space of dimension n and $\mathbb{1}_n$ the identity

map in that space. CP maps have very important applications in characterizing the set of physically meaningful evolutions of a quantum state.

It is clear that any CP map is also a positive map. However, there are positive maps that are not CP. This has very important consequences on the study of entanglement of quantum states. In particular, there is a one to one correspondence [11] between entanglement witnesses and positive non-CP maps. Since the hierarchy of separability tests offers a characterization of the interior of the set of entanglement witnesses, it is not difficult to translate this characterization to the set of positive non-CP maps. To do this, we use the fact that for any linear operator $L \in \mathcal{A}_A \otimes \mathcal{A}_B$, we can define a map $\Lambda \in \mathcal{L}(\mathcal{A}_A, \mathcal{A}_B)$ by

$$\langle k|\Lambda(|i\rangle\langle j|)|l\rangle = \langle i| \otimes \langle k|L|j\rangle \otimes |l\rangle. \quad (89)$$

Conversely, equation (89) can be used to uniquely construct the operator L from the map Λ. Equivalently, we can write [19]

$$\Lambda(\rho) = \text{Tr}_A\left[L(\rho^T \otimes \mathbb{1}_B)\right], \quad (90)$$

were ρ is an operator in $\mathcal{A}_A$. Note that the same operator $L \in \mathcal{A}_A \otimes \mathcal{A}_B$ can be used to define two different maps in $\mathcal{L}(\mathcal{A}_A, \mathcal{A}_B)$ and in $\mathcal{L}(\mathcal{A}_B, \mathcal{A}_A)$. It was shown [19] that this relationship gives in fact a one to one correspondence between entanglement witnesses, i.e., hermitian operators that are positive on separable states but have a negative eigenvalue, and positive non-CP maps. By using (90) it is not dificult to see that the interior of the set of entanglement witnesses, which correspond to those Z that satisfy $\text{Tr}[Z\rho_{sep}] > 0$ for any separable state ρ_{sep}, is mapped onto the set of positive maps that map any nonzero positive semidefinite operator into a *positive definite* operator. Our characterization of entanglement witnesses will translate into a characterization of this subset of positive maps. The maps that are left out are those that send at least one PSD operator into a another PSD operator that is not positive definite.

In Section VI we showed that any Z in the interior of the cone of all entanglement witnesses is *k-SOS* for some k. Since they correspond to strictly positive maps (the ones that map any nonzero PSD operator into a positive definite operator), we can characterize these maps by associating a bihermitian form directly to the map, using equation (89). Then we can state that a map is strictly positive only if the form

$$\begin{aligned} E_\Lambda(x, y) &= \langle y|\Lambda(|x^*\rangle\langle x^*|)|y\rangle \\ &= \sum_{ijkl}(\langle k|\Lambda(|i\rangle\langle j|)|l\rangle)x_i^* y_k^* x_j y_l, \quad (91) \end{aligned}$$

is *k-SOS* for some value of k.

We can also give an interpretation of this characterization in a language that only involves statements about maps. To do this we need to analyze in more detail some of the properties of the EW generated by the SDP. Let us

consider the family of separability criteria that searches for symmetric extensions of a certain state, but does not require positive partial transposes. It is not difficult to see that the entanglement witnesses generated by the second test will satisfy

$$\langle xyx|(Z_{EW} \otimes \mathbb{1}_A)|xyx\rangle = \langle xyx|Z_0|xyx\rangle, \qquad (92)$$

for all states $|x\rangle$ and $|y\rangle$, with $Z_0 \geq 0$. This is the analogue to equation (60). It is not difficult to show that this equality implies that the operators $Z_{EW} \otimes \mathbb{1}_A$ and Z_0 actually *coincide* when they are restricted to the symmetric subspace of the copies of system A. Furthermore, this is true for any number of copies of system A. If we denote by π_k the projector onto the symmetric subspace of $\mathcal{H}_A^{\otimes k}$ (which we will denote by $\mathcal{H}_A^{\vee k}$), we have

$$\pi_k \otimes \mathbb{1}_B (Z_{EW} \otimes \mathbb{1}_{A^{\otimes(k-1)}}) \pi_k \otimes \mathbb{1}_B = (\pi_k \otimes \mathbb{1}_B) Z_0 (\pi_k \otimes \mathbb{1}_B). \qquad (93)$$

Since Z_0 is PSD on the space $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A^{\otimes(k-1)}$, its restriction to the tensor product of $\mathcal{H}_A^{\vee k}$ and $\mathcal{H}_B$ remains PSD, which is the right-hand side of (93). The completeness theorem of Section V then tells us that if Z_{EW} is a strictly positive entanglement witness, then there must exist a finite k for which equation (93) is true.

We can now use the isomorphism defined by (89) to restate (93) in terms of properties of maps. First we use the fact that this isomorphism gives a one to one correspondence between PSD operators $L \in \mathcal{A}_A \otimes \mathcal{A}_B$ and CP maps $\Lambda \in \mathcal{L}(\mathcal{A}_B, \mathcal{A}_A)$. Let $\Lambda : \mathcal{A}_B \to \mathcal{A}_A$ be the positive non-CP map associated with Z_{EW}, and let $\bar{\Lambda}_k : \mathcal{A}_A \to \mathcal{A}_{\mathcal{H}_A^{\vee k}}$ be defined by $\bar{\Lambda}_k(\rho) = \pi_k(\rho \otimes \mathbb{1}_{A^{\otimes(k-1)}})\pi_k$. Equation (90) can be used to check that the map associated with the operator $\pi_k \otimes \mathbb{1}_B (Z_{EW} \otimes \mathbb{1}_{A^{\otimes(k-1)}}) \pi_k \otimes \mathbb{1}_B$ is given by

$$\left(\bar{\Lambda}_k \circ \Lambda\right) : \mathcal{A}_B \to \mathcal{A}_{\mathcal{H}_A^{\vee k}}. \qquad (94)$$

But since the right-hand side of (93) is PSD, this map has to be *completely positive*.

On the other hand, if Λ is not a positive map, then the map $\left(\bar{\Lambda}_k \circ \Lambda\right)$ cannot be completely positive for any k. This is true because the map $\bar{\Lambda}_k$ always maps a non-PSD matrix into a non-PSD matrix, as we can easily show. Let $|i\rangle$ be an eigenvector of a non-PSD operator σ in $\mathcal{H}_A$, with negative eigenvalue. Then $\langle i|\sigma|i\rangle < 0$. For any k the vector $|i\rangle^{\otimes k}$ belongs to the symmetric subspace $\mathcal{H}_A^{\vee k}$ and satisfies $\pi_k|i\rangle^{\otimes k} = |i\rangle^{\otimes k}$. Then we have

$$
\begin{aligned}
\left(\langle i|^{\otimes k}\right) \bar{\Lambda}_k(\sigma) \left(|i\rangle^{\otimes k}\right) &= \left(\langle i|^{\otimes k}\right) \pi_k(\sigma \otimes \mathbb{1}_A^{\otimes k-1})\pi_k \left(|i\rangle^{\otimes k}\right) \\
&= \left(\langle i|^{\otimes k}\right)(\sigma \otimes \mathbb{1}_A^{\otimes k-1})\left(|i\rangle^{\otimes k}\right) \\
&= \langle i|\sigma|i\rangle < 0, \qquad (95)
\end{aligned}
$$

and so $\bar{\Lambda}_k(\sigma)$ cannot be PSD. Thus, we have the following result:

Theorem 3 *If the map $\Lambda : \mathcal{A}_B \to \mathcal{A}_A$ is strictly positive, then there is a finite k such that the map $\left(\bar{\Lambda}_k \circ \Lambda\right) : \mathcal{A}_B \to \mathcal{A}_{\mathcal{H}_A^{\vee k}}$ is completely positive. If for some k the map $\left(\bar{\Lambda}_k \circ \Lambda\right)$ is completely positive, then Λ is a positive map.*

k	α
1	0.4
2	0.58769
3	0.68556
4	0.72727
5	0.77663
6	0.80766
7	0.823529
8	0.846137

TABLE I: Number of extensions and optimal value of α.

Since this characterization of positive maps does not require solving a SDP, because we only need to check positivity of a matrix, it is interesting to study how efficient this approach is in actually proving positivity of a map. To answer this question we consider the following example based on the case of the $3 \otimes 3$ state considered in Section VII A. Let the map Λ_0 be defined as $\Lambda_0(\rho) = \frac{1}{n}\text{Tr}[\rho]\mathbb{1}_3$, where $\mathbb{1}_3$ stands for the identity map in $\mathcal{H}_3$. The map Λ_0 lies in the interior of the cone of positive maps. Consider now a convex combination of Λ_0 and the positive map $\Lambda_{\tilde{Z}_{EW}}$ induced by the witness in equation (69), i.e.,

$$\Lambda_\alpha = (1-\alpha)\Lambda_0 + \alpha\Lambda_{\tilde{Z}_{EW}}, \quad 0 \leq \alpha \leq 1.$$

The map $\Lambda_{\tilde{Z}_{EW}}$ is in the boundary of the cone of positive maps. We have normalized the maps so that $\Lambda_\alpha(\mathbb{1}_3) = \mathbb{1}_3$. Since for $\alpha = 0$ we have $\Lambda_\alpha = \Lambda_0$ and for $\alpha = 1$ we have $\Lambda_\alpha = \Lambda_{\tilde{Z}_{EW}}$, the maps Λ_α are contained in a line segment with endpoints near the center and in the boundary of the cone of positive maps, respectively. This implies that Λ_α is a strictly positive map for $\alpha < 1$.

A natural question in this case is to determine the ranges of α for which we can effectively recognize positivity by applying the result of Theorem 3. For this, as explained, we have to form the tensor product of the given map with $k-1$ copies of the identity, project on the symmetric subspace, and check whether the resulting matrix is positive semidefinite. The computation of the optimal α can be done in this case by solving a simple generalized eigenvalue problem.

We have solved this numerically, for values of k up to 8 (this involves matrices of size $3 \cdot \binom{3+k-1}{k}$, i.e., 135×135). The obtained extreme values are shown in Table I, where k is the number of extensions. The results are consistent with the expected behavior $\lim_{k\to\infty} \alpha_k = 1$.

Notice that the convergence appears to be relatively slow, of order $1/k$; in contrast, the SDP tests presented earlier based on the PPT hierarchy can get all the way to the boundary $\alpha = 1$ in just one step.

It is interesting to note that Jamiołkowski also studied the problem of checking positivity of maps [21]. His approach was related to ours in the sense that he showed that checking positivity of a given map was equivalent

to the nonnegativity of a certain associated real polynomial. He then applied a general technique for checking positivity of polynomials. As discussed in the introduction there are several such algebraic methods and they all scale badly with the problem size. In our case the specific problem of checking positivity of a linear map between matrix algebras has been reduced to a series of tests of matrix positivity, but none of them succeeds uniformly for all maps. However, it is still the case that for many instances, the positivity of a given linear map can be determined and certified efficiently.

XI. CONCLUSIONS AND DISCUSSION

In this paper we have discussed a new family of separability criteria for bipartite mixed states. Each criteria consists in searching for an extension of a given state in a bigger space formed by adding a number of copies of one of the subsystems, and requiring this extension to be symmetric under exchanges of the copies and to remain positive under any partial transpose. A failure to find such an extension proves entanglement of the state, since it can be explicitly shown that separable states have the required extensions. If an extension is found, the test is inconclusive. This family of tests can be arranged in a hierarchical structure, with each test being at least as powerful as all the previous ones, and with the first test corresponding to the well-known Peres-Horodecki PPT criterion.

This hierarchy of tests has two main properties that make it useful and appealing. First, the hierarchy is complete: any entangled state will fail one of the tests at some finite point in the sequence. Second, each test can be cast as a semidefinite program, which can be efficiently solved. Furthermore, by exploiting the dual structure of semidefinite programs, whenever a state is proven to be entangled by failing one of the tests, an entanglement witness for that state can be explicitly constructed. This duality can also help us to interpret the hierarchy as trying to prove entanglement of a state by searching for entanglement witnesses with a particular algebraic property that states that the bihermitian form associated with the entanglement witness can be written as a sum of squares when multiplied by a fixed sum of squares to a certain power. The completeness of the hierarchy can then be used to show that this algebraic property characterizes all the elements in the interior of the cone of entanglement witnesses.

We analyzed the computational resources needed to implement these tests. We found that for a fixed test in the hierarchy, they scale polynomially in the dimensions of the state. When we keep the size of the state fixed, the resources also scale polynomially with the number of copies added, or equivalently, with the order of the test in the hierarchy. This behavior is very interesting in light of recent results on the worst case complexity of the separability problem. It has been shown that checking separability of a state is an NP-hard problem when we study the scaling with respect to the dimensions of both parties, so computational resources to solve it cannot scale polynomially in this general case. In our family of tests this non-polynomial behavior is reflected in how high up the hierarchy we need to go to detect all entangled states. Even though each test is efficiently implementable, there are states for which we need to go arbitrarily high in the hierarchy to show that they are entangled.

The dual formulation of the hierarchy can also be understood as the construction of a sequence of cones, each one containing the previous ones, that approximate the dual of the cone of separable states (which contains the entanglement witnesses) from the inside, giving a complete characterization of its interior.

We can also interpret the primal formulation as the construction of a sequence of nested cones that approximate the cone of separable states from the outside. It is worth comparing this point of view with the results in [51], where a semidefinite program was used to approximate the cone of separable states from the inside. This result however, only applies when one of the subsystems has dimension 2, and gives a complete characterization of separability only in this particular case, while our hierarchy works for arbitrary dimensions of the subsystems.

The hierarchy of tests allows us to divide the set of entangled states into different classes, according to whether they have PPT symmetric extensions to k copies of one of the parties or not. This generates a nested sequence of subsets of entangled states. This sequence can be shown to be infinite for all dimensions of the subsystems, except for $2 \otimes 2$ and $2 \otimes 3$ where it is well-known that the PPT criterion is enough to characterize entanglement (in these two special cases, the hierarchy collapses to the first step). Furthermore, if the set of states with PPT symmetric extensions to $(k-1)$ copies of A but not to k copies is nonempty, then it can be shown to have nonzero measure. These classes of states however, are not closed under LOCC operations, since we can transform a state that is not detected by the second test into a state that is, with finite probability and by applying only local operations.

XII. ACKNOWLEDGEMENTS

APPENDIX A: IMPROVED SDP FOR IMPLEMENTING THE TESTS

We will now introduce a slight modification of the SDP given in (23), that has the advantage of performing better numerically. With F given by (22), let us consider the following SDP

$$
\begin{aligned}
\text{minimize} \quad & t \\
\text{subject to} \quad & t\mathbb{1}_{ABA} + F(\mathbf{x}) \geq 0, \quad\quad \text{(A1)}
\end{aligned}
$$

where $\mathbb{1}_{ABA}$ is the identity matrix on the space $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A$. It is clear that we can always choose t such that the LMI on the second line of (A1) is satisfied. If the minimum of t is negative or zero, then there exists a value of $\mathbf{x}$ such that $F(\mathbf{x}) \geq 0$, which is equivalent to say that (23) is feasible. On the other hand, if the minimum of t is strictly positive, then we know that $F(\mathbf{x})$ cannot be PSD. Thus we see that feasibility of (23) is equivalent to whether the minimum of (A1) is strictly positive or not. So we can use (A1) to detect entangled states. This approach has the property that the SDP (A1) is *always feasible*. This property makes the SDP solver to behave better numerically (because it uses an interior point algorithm). This is in fact the SDP that our code is solving when applying the tests to a given quantum state.

APPENDIX B: STRONG DUALITY AND SDP INFEASIBILITY

We want to obtain infeasibility witnesses for the SDP

$$
F_0 + \sum_{i=1}^{m} x_i F_i \geq 0.
$$

Clearly, *if* we can find a $W \geq 0$ such that

$$
\text{Tr}[F_i W] = 0, \quad \text{Tr}[F_0 W] < 0,
$$

then the SDP is necessarily infeasible, as follows by the argument given after equation (14). Under what conditions does such a W exist? As we mentioned earlier, we need some form of strong duality to hold.

Consider the set $\mathcal{S} := \text{range}\,\mathcal{F} + K$, where K is the PSD cone, $\mathcal{F} : \mathbb{R}^m \to \mathbb{S}^n$ is the linear map defined by $\mathcal{F}(x) := \sum_{i=1}^{m} x_i F_i$, and $A + B = \{y | y = a + b, a \in A, b \in B\}$. Feasibility of the SDP is equivalent to $F_0 \in \mathcal{S}$. The set $\mathcal{S}$ is obviously convex. Now, *if* $\mathcal{S}$ is also closed, then we can apply the separating hyperplane theorem, and conclude the existence of a W as above.

The difficulty, of course, is than in general the sum of two closed sets may not be closed. In particular, in SDP things can go wrong. For instance, for

$$
\begin{bmatrix} x & 1 \\ 1 & 0 \end{bmatrix} \geq 0
$$

which is obviously infeasible, it is not hard to see that *no witness* $W \geq 0$ as above can exist. This can be traced back to the fact that $\mathcal{S}$ in this case is not closed.

So, what conditions can be required to guarantee that $\mathcal{S}$ be closed? An often-used criterion is the so-called *Slater condition* [42], which in our case is the following:

If $\ker \mathcal{F}^* \cap \text{ri}\, K^* \neq \emptyset$, then $\text{range}\,\mathcal{F} + K$ is closed.

Here, $\mathcal{F}^*$ is the adjoint map of $\mathcal{F}$, K^* is the dual cone (equal to K, in this case), and ri denotes the relative interior of a set.

In other words, to guarantee the existence of infeasibility witnesses of the form we described (for any possible F_0), it is sufficient to show a $Z > 0$, that satisfies $\text{Tr}[F_i Z] = 0$, for all $i = 1, \ldots, m$. Notice that this *almost* looks like the certificate W we are after, except that F_0 does not appear in the expression (otherwise, the condition would be useless). In general, checking whether the Slater condition is satisfied in concrete problems is not too difficult.

For our SDPs in (23) and (44), it is immediate to show that the criterion is indeed satisfied, as all the matrices F_i are traceless, so we can just take $Z = \mathbb{1} > 0$.

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