# Positive but not Completely Positive Maps

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Our research project focuses on linear positive maps and their application in quantum information theory. These maps –whose study is relevant to a range of other topics, from algebraic geometry to semidefinite programming– can be used as criteria for detecting quantum entanglement, and are interestingly related to another family of tools that are used for entanglement detection, namely entanglement witnesses.

The problem of recognizing quantum states that are not entangled has been proven to be an NP-hard problem. Nevertheless, the need for doing optimizations over this set arises often in quantum information theory. The aim of this project is to study positive but not completely positive maps in order to find better relaxations for these optimization problems. In this report, we present a literature survey on this topic, as well as the the proofs of the original results obtained during the project, and the relevant numerical results obtained from numerical simulations ran by the author.

#### I. INTRODUCTION

#### A. Quantum Mechanics: A Brief Recap

#### 1. A Dynamical System Formulation

Almost everyone is familiar with the myth of a falling apple, which inspired young Isaac Newton when it hit him on the head and spurred him to develop his theory, which attempts to explain the *Philosophiae Naturalis* mathematically. Regardless of whether this narrative is historically accurate, we begin this section by utilizing the falling fruit example to recap what (quantum) mechanics is all about.

Consider the previously physical system, namely a fruit that has fallen from a tree and is traveling towards the ground. Some of the physical qualities of this fruit change as it moves, whereas the others do not. For example, its height, velocity, kinetic, and potential energy all change as it moves, yet its mass remains constant. The first family of attributes is known as *dynamic* properties, whereas the second family is known as *static* properties.

Generally speaking, the goal of classical (quantum) mechanics is to study the dynamical properties of those macroscopic (microscopic) physical systems made up of moving parts. To achieve this, it seems natural to mathematically model these dynamical variables as continuoustime dynamical systems. Consequently, many physical problems could be formulated as mathematical problems in the theory of dynamical systems. Assume, in the falling fruit example, you're wondering about the relation between the fruit's original height and its velocity when it strikes the ground. This might be readily phrased in dynamical system, could one anticipate the state of the system at a specific moment?".

To formulate a dynamical system, it is essential to specify two components: the system's state space, and how the system's state evolves over time. In quantum mechanics, a general approach involves defining the state space using *density matrices* and characterizing the evolution of the system using *quantum channels*.

In accordance with one of the postulates of quantum mechanics, associated to every physical system is a complex Hilbert space. A density matrix over a Hilbert space  $\mathcal{H}$  is an operator  $\rho : \mathcal{H} \to \mathcal{H}$ , with the conditions that  $\operatorname{tr}(\rho) = 1$  and  $\rho$  is positive semidefinite (PSD), represented as  $\rho \geq 0$ . For a physical system with the associated Hilbert space  $\mathcal{H}$ , the state space of the system is the set of all density matrices over  $\mathcal{H}$ . If we have a composite system, with two subsystems A and  $\mathcal{H}_B$ , the Hilbert space associated to the whole composite system is  $\mathcal{H}_A \otimes \mathcal{H}_B$ , and the state space of the system consists of all density matrices over  $\mathcal{H}_A \otimes \mathcal{H}_B$ . Here,  $\otimes$  denotes the tensor product of two linear spaces.

Another postulate of quantum mechanics asserts that the evolution of the system's state can be described by a special type of maps, namely quantum channels. Suppose that  $\mathcal{H}_{\mathcal{A}}$  and  $\mathcal{H}_{\mathcal{B}}$  are two Hilbert spaces. A map  $\Phi$  :  $\mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ , is said to be a quantum channel if (1) it preserves the trace, i.e. for all  $\rho \in \mathcal{L}(\mathcal{H}_A)$ ,  $\operatorname{tr}(\rho) =$  $\operatorname{tr}(\Phi(\rho))$ , and if (2) it is completely positive, i.e. for any Hilbert space  $\mathcal{H}_C$  and for all  $\rho_{AC} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_C)$  with  $\rho_{AC} \geq 0$ ,  $(\Phi \otimes \mathcal{I}_C)(\rho_{AC}) \geq 0$ . Although the definition of a quantum channel may initially seem strange, the following theorem provides an efficient way for checking whether a map is a quantum channel.

**Theorem 1** (Kraus-Choi representation (Choi, 1975a; Kraus *et al.*, 1983)). Let  $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$  be a linear map. The following are equivalent:

- 1.  $\Phi$  is a quantum channel.
- 2. There exist linear operators  $K_i : \mathcal{H}_A \to \mathcal{H}_B$  with  $\sum_i K_i^{\dagger} K_i = \mathbb{I}_A$  such that

$$\Phi(X) = \sum_{i} K_i X K_i^{\dagger}.$$
 (1)

The  $K_i s$  are called Kraus operators.

3. Define the Choi matrix  $C_{\Phi} : \mathcal{H}_A \otimes \mathcal{H}_B \to \mathcal{H}_A \otimes \mathcal{H}_B$ of the map  $\Phi$  as:

$$C_{\Phi} = (\mathcal{I}_A \otimes \Phi) |\Omega\rangle \langle \Omega|,$$
  
where  $|\Omega\rangle = \sum_i |ii\rangle$ . Then  $\operatorname{tr}_B(C_{\Phi}) = \mathbb{I}_A$  and  
 $C_{\Phi} \ge 0.$  (2)

In the above theorem, one can see that the complete positivity condition and relations (1) and (2) are equivalent.

A linear map  $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$  is said to be positive, if for any  $\rho \in \mathcal{L}(\mathcal{H}_A)$  with  $\rho \ge 0$ ,  $\Phi(\rho) \ge 0$ . It is clear that every completely positive map is also positive, but the converse does not necessarily hold.

# 2. Entanglement: The Distinctive Essence of Quantum Mechanics

Following the formalism provided above, one immediately notices that interesting phenomena may arise. Suppose that we have a composite bipartite system, consisting of two subsystems A and B, with the associated Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively. A state  $\rho_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$  of this composite system is called *separable* if it can be written as

$$\rho_{AB} = \sum_{i} p_i \sigma_i \otimes \tau_i,$$

where  $\sigma_i \in \mathcal{L}(\mathcal{H}_A)$  and  $\tau_i \in \mathcal{L}(\mathcal{H}_B)$  are density matrices for all *i*'s, and  $p_i$ 's are positive real numbers with the condition that  $\sum_i p_i = 1$ . A state that is not separable, is called *entangled*.

Entanglement plays an important role in quantum physics, and as Schrödinger addresses in his key paper (Schrödinger and Born, 1935), it is "the characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought". Several significant consequences of the existence of entangled quantum states have been discovered, and the study is currently ongoing. In particular, it is known that quantum entanglement is a crucial resource for quantum algorithms to have an exponential speed-up over classical computing (Jozsa and Linden, 2003). There are also several other computer science related applications of quantum entanglement, e.g. quantum teleportation, quantum superdense coding and entanglement-based quantum key distribution protocols.

For a bipartite system consisting of two subsystems A and B, with the associated Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , we denote the set of all density matrices over  $\mathcal{H}_A \otimes \mathcal{H}_B$  by  $\mathsf{D}(n, m)$ , and the set of all separable states by  $\mathsf{SEP}(n, m)$ , where n and m are the dimensions of  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively. Unless it causes confusion, we

typically replace D(n, m) and SEP(n, m) with D and SEP, respectively, and omit specifying the local dimensions.

With the introduction of the set of entangled and separable states, one might ask if it is possible to efficiently determine if a given state is separable or not. The following theorem states that recognising SEP is not an easy problem.

**Theorem 2.** It is NP-hard to determine whether an arbitrary quantum state within an inverse polynomial distance from SEP is entangled (*Gharibian*, 2010).

#### B. Motivation of the Work

Theorem 2 shows that determining whether a given state is separable, is an asymptotically difficult problem. Nonetheless, there exist scenarios in quantum information theory that we are interested in solving an optimisation problem over the set of separable states.

As an example, suppose that we are interested in finding a way to measure the amount of entanglement for a bipartite system. This is a fundamental problem in quantum theory, which has led to the emergence of various measures of entanglement. One of these measures, which was proposed in (Vedral and Plenio, 1998), is known as the *relative entropy of entanglement*, and is defined as

$$E_{R}\left(\rho_{AB}\right) := \min_{\sigma_{AB} \in \mathsf{SEP}} S\left(\rho_{AB} \| \sigma_{AB}\right),$$

where  $S(\rho_{AB} || \sigma_{AB})$ , which is called the *relative entropy* of the states  $\rho_{AB}$  and  $\sigma_{AB}$  is defined as  $S(\rho_{AB} || \sigma_{AB}) :=$  $\operatorname{tr}(\rho_{AB} \log \rho_{AB}) - \operatorname{tr}(\rho_{AB} \log \sigma_{AB})$ . Other examples of such optimization problems can be found in (Tavakoli *et al.*, 2023).

In these scenarios, it is common to relax the original optimization by finding efficiently computable partial conditions on the solutions, that lead us to bounds on the best solution. This is where *entanglement criteria* come into play.

#### 1. Entanglement Criteria Based on Positive Maps

Suppose that we have a bipartite system consisting of two subsystems A and B, with the associated Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$ . Let  $\Phi : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$  be a positive but not completely positive map. We define the set of all states that are positive under partial application of  $\Phi$  by

$$\mathsf{PP}\Phi := \{\rho_{AB} \in \mathsf{D} : (\mathcal{I}_A \otimes \Phi)\rho_{AB} \ge 0\}.$$

One can see that the above set is a proper subset of D (as we will prove in Proposition 14). Moreover, for any

separable state  $\rho = \sum_{i} p_i \sigma_i \otimes \tau_i$ ,

$$(\mathcal{I}_A \otimes \Phi) \rho = \sum_i p_i \sigma_i \otimes \Phi(\tau_i) \ge 0,$$

which implies that SEP is contained in PP $\Phi$ . Thus, these sets serve as criteria for entanglement: for any positive but not completely positive map  $\Phi$ , all the states that are not in PP $\Phi$  are necessarily entangled. In other words, each PP $\Phi$  provides a necessary condition for separability. We say that a state  $\rho$  satisfies the PP $\Phi$  criterion if  $\rho \in$ PP $\Phi$ . Notably, checking whether a state is in PP $\Phi$  can be efficiently done, unlike checking the separability of a state.

A well-known example of a map that is positive but not completely positive is the transposition map, and the associated PP $\Phi$  set of states is known as PPT. In many optimization scenarios, it's common to relax the original optimization over SEP to an optimization over PPT. In low dimensions, it turns out that PPT = SEP, while they are provably not equal in other dimensions (Fawzi, 2021; Woronowicz, 1976). Our main motivation for the study of positive but not completely positive maps is to explore whether the widespread use of PPT as an approximation of SEP is merely a convention or if the transposition map possesses properties that make it, in a sense, fundamental, and PPT is the best choice for these relaxation.

#### 2. Entanglement Criteria based on Entanglement Witnesses

Another family of entanglement criteria that plays an important role in the study of quantum entanglement, especially from a physical viewpoint, are entanglement witnesses.

**Definition** A Hermitian operator  $W \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$  is called an entanglement witness if

- 1. W is not a positive operator,
- 2. for all product states  $|\psi_A\rangle \langle \psi_A| \otimes |\psi_B\rangle \langle \psi_B|$ ,

$$\operatorname{tr}(W |\psi_A\rangle \langle \psi_A | \otimes |\psi_B\rangle \langle \psi_B |) \ge 0.$$

Using the spectral decomposition theorem, one can see that entanglement witnesses can be used for detecting entanglement, meaning that for any witness  $W \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$  and any state  $\rho_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ , if  $tr(W\rho) < 0$ , then  $\rho$  is entangled.

The physical importance of entanglement witnesses lies in their Hermitian nature, rendering them as observables that can be measured in a laboratory. Thus, by experimentally measuring W, we can determine whether a state  $\rho$  has the property that  $tr(W\rho) < 0$ , and hence potentially conclude that the state is entangled. (Horodecki *et al.*, 2009). Another motivation for this project is the study of relationships between positive but not completely positive map and entanglement witnesses, and using them to improve our relaxations for the aforementioned optimization problems.

#### C. Author's Contributions and the Structure of the Report

My contributions in this project can be classified in three categories:

- A significant part of this project was dedicated to reviewing and understanding the existing literature, by personally proving the results. In particular, for almost every result that is mentioned in this report, except for those stated without proof, I have written my own proof.
- I ran numerical simulations (in python) to implement most of the fundamental concepts that will be discussed throughout this report, to help us better understand the entanglement criteria and their properties. The results of these simulations had a significant influence on determining the trajectory of our ideas during this project. Some of the results of these simulations are presented in this report, and the Jupyter notebook containing all the simulations is available in this link.
- To the best of my knowledge, some parts of the present work, mostly the results in Section V and VI.B, are original.

This report is structured in five main sections. We begin with an exploration of entanglement witnesses in Section II, and then, moving into the other criteria, we provide a list of examples of positive but not completely positive maps in Section III. Section IV is dedicated to a short introduction to the notion of duality for linear maps and some of the useful applications of dual maps in our context. In Section V, we establish a method for finding entanglement witnesses using semidefinite programming, and following that, we bring together all the notions introduced in the first five sections to study the properties of entanglement criteria in Section VI.

#### **II. ENTANGLEMENT WITNESSES**

We start this section by a simple geometric argument.

**Proposition 3.** For every entangled state  $\rho_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ , there exists a Hermitian operator  $W \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$  such that  $\operatorname{tr}(W\rho) < 0$  and  $\operatorname{tr}(W\sigma) \geq 0$  for all separable states  $\sigma$ .

*Proof.* The proof is a consequence of the hyperplane separation theorem, which states that if  $C \subset \mathcal{V}$  is a closed



FIG. 1 An entanglement witness defines a separating hyperplane.

convex proper subset of  $\mathcal{V}$  and  $x \in \mathcal{V} \setminus C$ , then x and C can be strictly separated by a hyperplane. (Horodecki *et al.*, 1996).

Let W be a Hermitian operator its existence is proved by Proposition 3. Since  $tr(W\rho) < 0$ , we can conclude that W is not a positive operator. Moreover, since  $\operatorname{tr}(W\sigma) \geq 0$  for all separable states  $\sigma$ , and especially for all product states  $|\psi_A\rangle \langle \psi_A| \otimes |\psi_B\rangle \langle \psi_B|$ , we conclude that W is an entanglement witness. On the other hand, if W is an entanglement witness with an eigenvector  $|v\rangle$  corresponding to a negative eigenvalue, the state  $|v\rangle\langle v|$  is an entangled state for which the inequality  $\operatorname{tr}(W|v\rangle\langle v|) < 0$  holds. Thus, the set of entanglement witnesses is exactly the set of Hermitian operators obtained from Proposition 3. Moreover, note that we can think of an entanglement witness W as a normal vector, defining a hyperplane consisting of all density matrices  $\tau$ that are perpendicular to W, i.e.  $tr(W\tau) = 0$  (See Figure 1.).

**Example** The SWAP operator, which is defined as:

$$\mathrm{SWAP} := \sum_{i,j} \left| i \right\rangle \left\langle j \right| \otimes \left| j \right\rangle \left\langle i \right|,$$

is an entanglement witness.

We can see that there is a correspondence between entanglement witnesses and positive maps. This correspondence can be obtained by using the Choi matrix.

**Proposition 4.** (Choi–Jamiołkowski isomorphism) The map  $\mathcal{J} : \mathcal{L}(\mathcal{L}_A, \mathcal{L}_B) \to \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ , which is defined as

$$\mathcal{J}(\Phi) := C_{\Phi} = \sum_{i,j=1}^{d_A} |i\rangle \langle j| \otimes \Phi(|i\rangle \langle j|)$$
(3)

defines a bijection between the set of all positive but not completely positive maps in  $\mathcal{L}(\mathcal{L}_A, \mathcal{L}_B)$  and the set of all entanglement witnesses in  $\mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ .

*Proof.* The map  $\mathcal{J}$  defines an isomorphism between  $\mathcal{L}(\mathcal{L}_A, \mathcal{L}_B)$  and  $\mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ . Therefore, it suffices to show that  $\mathcal{J}(\Phi)$  is an entanglement witness iff  $\Phi$  is positive but not completely positive.

 $\Phi$  is positive iff for all  $|x\rangle \in \mathcal{H}_A$ ,  $\Phi(|x\rangle \langle x|) \geq 0$ , which means that for all  $|y\rangle \in \mathcal{H}_B$ ,  $\langle y| \Phi(|x\rangle \langle x|) |y\rangle \geq 0$ . Note that

$$\Phi(\ket{x}ra{x}) = \sum_{i,j}ra{i}x
angle \langle x|j
angle \Phi(\ket{i}ra{j}).$$

Using the above equality, we obtain

$$egin{aligned} &\langle y | \, \Phi(|x 
angle \left\langle x | 
ight) | y 
angle &= \sum_{i,j} \left\langle ar{x} | i 
angle \left\langle j | ar{x} 
ight
angle \left\langle y | \, \Phi(|i 
angle \left\langle j |) \left| y 
ight
angle \ &= \sum_{i,j} \left\langle ar{x} y | \left( | i 
angle \left\langle j | \otimes \Phi(|i 
angle \left\langle j |) 
ight) | ar{x} y 
angle \end{aligned}$$

Therefore,  $\Phi$  is positive iff for every  $|x\rangle \in \mathcal{H}_A$  and  $|y\rangle \in \mathcal{H}_B$ ,

$$\operatorname{tr}(\mathcal{J}(\Phi)|\bar{x}\rangle\langle\bar{x}|\otimes|y\rangle\langle y|)\geq 0$$

or equivalently, for all  $\rho_{AB} \in \mathsf{SEP}$ ,  $\operatorname{tr}(\mathcal{J}(\Phi)\rho_{AB}) \geq 0$ . Now, assume that there exists a state  $\rho_{AB}$  such that  $\operatorname{tr}(\mathcal{J}(\Phi)\rho_{AB}) < 0$ . Then there exists a vector  $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$  s.t.  $\langle \psi | \mathcal{J}(\Phi) | \psi \rangle < 0$ , which means that  $\mathcal{J}(\Phi)$  is not PSD. Note that  $\mathcal{J}(\Phi)$  is the Choi matrix of the map  $\Phi$ . Hence  $\Phi$  is not completely positive. Finally, to prove the other direction, one can see that  $\rho_{AB} = |x\rangle \langle x|$ , where  $|x\rangle$  is one of the negative eigenvectors of  $\Phi$ 's Choi matrix, yields  $\operatorname{tr}(\mathcal{J}(\Phi)\rho_{AB}) < 0$ .

As we mentioned earlier, positive but not completely positive maps and entanglement witnesses can be related in different ways. Note that the above proposition provides one of such connections: every entanglement witness specifies a positive map and from any positive but not completely positive map, an entanglement witness can be constructed.

#### **III. POSITIVE MAPS**

In this section we survey a number of well known positive but not completely positive maps. It is important to note that these maps do not necessarily correspond to physically implementable maps, but as we discussed earlier, they provide us useful tools in the study of quantum entanglement. Before delving into the examples, it is useful to mention a result by Yu (Yu, 2000), and discuss a corollary derived from it, as it will be used later.

**Theorem 5.** Every positive map can be written as the difference of two completely positive maps.

**Corollary 6.** Positive maps are Hermitian preserving, in the sense that if  $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$  is a positive map, then for all  $X \in \mathcal{L}(\mathcal{H}_A)$ ,

$$\Phi(X^{\dagger}) = \Phi(X)^{\dagger}$$

*Proof.* By Theorem 5, we have  $\Phi = \Phi_1 - \Phi_2$ , where  $\Phi_1$  and  $\Phi_2$  are completely positive. Suppose that the Kraus decompositions of  $\Phi_1$  and  $\Phi_2$  are  $\sum_i K_i X K_i^{\dagger}$  and  $\sum_i J_j X J_j^{\dagger}$ , respectively. Therefore,

$$\Phi(X^{\dagger}) = \sum_{i} K_{i} X^{\dagger} K_{i}^{\dagger} - \sum_{j} J_{j} X^{\dagger} J_{j}^{\dagger}$$

$$\tag{4}$$

$$=\left[\sum_{i}K_{i}XK_{i}^{\dagger}-\sum_{j}J_{j}XJ_{j}^{\dagger}\right]^{\dagger}=\Phi(X)^{\dagger} \quad (5)$$

In the following, we will list some examples of the positive but not completely positive maps.

**Transpose Map (Peres, 1996)** The most famous example of a positive map that is not completely positive is the transposition map  $\theta : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$ , which is defined as  $\theta(X) := X^T$  for all  $X \in \mathcal{H}(A)$ . For a PSD matrix  $\rho$ , suppose that the spectral decomposition of  $\rho$  is  $\sum_i \lambda_i |v_i\rangle \langle v_i|$ . Then  $\rho^T = \sum_i \lambda_i \overline{|v_i\rangle} \langle v_i|$  which is PSD, and this implies the positivity of  $\theta$ .

To see that  $\theta$  is not completely positive, we show that the Choi matrix corresponding to  $\theta$  is not PSD. The Choi matrix  $C_{\theta}$  of the transposition map is computed by:

$$egin{aligned} C_{ heta} &= \sum_{i,j} \ket{i} ig\langle j 
vert \otimes heta(\ket{i} ig\langle j ert) \ &= \sum_{i,j} \ket{i} ig\langle j ert \otimes ert j ig
angle \, \ket{j} ig\langle i ert \end{aligned}$$

A vector  $|v\rangle = \sum_{i,j} \lambda_{i,j} |ij\rangle$  is an eigenvector for  $C_{\theta}$  iff  $C_{\theta} |v\rangle = \alpha |v\rangle$  for an  $\alpha \in \mathbb{C}$ . One can see that  $C_{\theta} |v\rangle = \sum_{i,j} \lambda_{j,i} |ij\rangle$ , and for all i < j, the vectors  $|v_{i,j}\rangle := |ij\rangle - |ji\rangle$  are the eigenvectors of  $C_{\theta}$ , corresponding to the eigenvalue  $\alpha = -1$ . Since  $C_{\theta}$  has a negative eigenvalue, it is not PSD, and  $\theta$  is not completely positive.

**Remark** By the definition of (partial) transpose, it is clear that it is not canonical and depends on the choice of basis. However, the eigenvalues of the partial transpose of an operator do not depend on the choice of basis.

**Remark** If we work with a block matrix  $(A_{ij})$ , where  $A_{ij} \in \mathcal{L}(\mathcal{H}_B)$ , the partial transpose of the matrix with respect to the first and second components are  $(A_{ji})$  and  $(A_{ij}^{T})$ , respectively. An example for a two qubit system

is illustrated below.

$$\rho_{AB} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix},$$
$$(\mathcal{I} \otimes \theta) \rho_{AB} = \begin{bmatrix} a_{11} & a_{21} & a_{13} & a_{23} \\ a_{12} & a_{22} & a_{14} & a_{24} \\ a_{31} & a_{41} & a_{33} & a_{43} \\ a_{32} & a_{42} & a_{34} & a_{44} \end{bmatrix},$$
$$(\theta \otimes \mathcal{I}) \rho_{AB} = \begin{bmatrix} a_{11} & a_{21} & a_{31} & a_{32} \\ a_{12} & a_{22} & a_{41} & a_{42} \\ a_{13} & a_{14} & a_{33} & a_{43} \\ a_{23} & a_{24} & a_{34} & a_{44} \end{bmatrix}$$

**Remark** It is worth noting that the transposition has a physical meaning in terms of the notion of *time reversal* (Sanpera *et al.*, 1997).

Reduction Map (Horodecki and Horodecki, 1999) The reduction map  $\Lambda : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$  is defined as:

$$\Lambda(\rho) := \operatorname{tr}(\rho)\mathbb{I}_{\mathcal{H}} - \rho.$$

The positivity of the map follows from the fact that for a positive matrix H,  $\operatorname{tr}(H) \geq \lambda_{max} = \max_{\operatorname{unit vector } |\psi\rangle} \langle \psi | H | \psi \rangle$ . Another way to prove the positivity of  $\Lambda$  is by considering the spectral decomposition of  $\rho$ :

$$\operatorname{tr}(\rho)\mathbb{I} - \rho = (\sum_{i} \lambda_{i})\mathbb{I} - \sum_{i} \lambda_{i} |v_{i}\rangle \langle v_{i}|$$
$$= \sum_{i} (\sum_{j} \lambda_{j} - \lambda_{i}) |v_{i}\rangle \langle v_{i}| \ge 0$$

The reduction map is not completely positive. To prove this, let us consider the Choi matrix  $C_{\Lambda}$  associated to it:

$$C_{\Lambda} = \sum_{i,j} |i\rangle \langle j| \otimes \Lambda(|i\rangle \langle j|)$$
  
=  $\sum_{i,j} |i\rangle \langle j| \otimes (\operatorname{tr}(|i\rangle \langle j|)\mathbb{I} - |i\rangle \langle j|)$   
=  $\sum_{i,j} |i\rangle \langle j| \otimes \operatorname{tr}(|i\rangle \langle j|)\mathbb{I} - \sum_{i,j} |i\rangle \langle j| \otimes |i\rangle \langle j|)$   
=  $\sum_{i} |i\rangle \langle i| \otimes \mathbb{I} - |\Omega\rangle \langle \Omega|$   
=  $\mathbb{I} - |\Omega\rangle \langle \Omega| = \mathbb{I} - d |\Omega'\rangle \langle \Omega'|,$ 

where  $|\Omega'\rangle = \frac{1}{\sqrt{d}} \sum_{i} |ii\rangle$ . Since  $\lambda_{min}(C_{\Lambda}) \leq \langle \Omega' | C_{\Lambda} | \Omega' \rangle < 0$ ,  $\Lambda$  is not completely positive.

The positivity of a state under the partial application of the reduction map can be equivalently formulated, as presented below. **Proposition 7.** (Reduction criterion) Consider a bipartite state  $\rho_{AB}$ . The following conditions are equivalent:

1. 
$$(\mathcal{I} \otimes \Lambda) \rho_{AB} \ge 0.$$

2.  $\rho_A \otimes \mathbb{I} \geq \rho_{AB}$ .

*Proof.* Let  $\sum_{i} |u_i\rangle \langle u_i|$  be the spectral decomposition of  $\rho_{AB}$ , where  $|u_i\rangle$ s are (possibly) unnormalized vectors, and suppose that  $|u_i\rangle = \sum_{a,b} u_i^{a,b} |a\rangle |b\rangle$ , where  $|a\rangle$ s and  $|b\rangle$ s form a basis for  $\mathcal{H}_A$  and  $\mathcal{H}_B$  respectively. Then we have:

$$\begin{aligned} (\mathcal{I} \otimes \Lambda)\rho_{AB} \\ &= (\mathcal{I} \otimes \Lambda) \sum_{i} \sum_{\substack{a,b,c,d \\ i}} u_{i}^{a,b} \overline{u_{i}^{c,d}} (|a\rangle \langle c| \otimes |b\rangle \langle d|) \\ &= \sum_{i} \sum_{\substack{a,b,c,d \\ i}} u_{i}^{a,b} \overline{u_{i}^{c,d}} |a\rangle \langle c| \otimes (\operatorname{tr}(|b\rangle \langle d|) \mathbb{I} - |b\rangle \langle d|) \\ &= \rho_{A} \otimes \mathbb{I} - \rho_{AB}. \end{aligned}$$

The next proposition shows that the set of positive but not completely positive maps is not closed under the composition of maps.

**Proposition 8.** The composition of the transpose and the reduction map is a completely positive map.

*Proof.* First note that  $\theta \Lambda = \Lambda \theta$ . The Choi matrix corresponding to  $\theta \Lambda$  is:

$$\begin{split} C_{\theta\Lambda} &= \sum_{i,j} |i\rangle \langle j| \otimes \theta\Lambda(|i\rangle \langle j|) \\ &= \sum_{i,j} |i\rangle \langle j| \otimes (\operatorname{tr}(|i\rangle \langle j|)\mathbb{I} - |j\rangle \langle i|) \\ &= \mathbb{I} - \sum_{i,j} |ij\rangle \langle ji| \end{split}$$

We saw earlier that the eigenvalues of the operator  $\sum_{i,j} |ij\rangle \langle ji|$  are  $\pm 1$ , and we know that for a Hermitian matrix  $H, H \leq \lambda_{max}(H)\mathbb{I}$ . Putting these together, it can be implied that  $C_{\theta\Lambda}$  is PSD.

#### Breuer-Hall maps (Breuer, 2006; Hall, 2006)

Consider the family of maps defined on  $\mathcal{L}(\mathcal{H})$  as

$$T_{BH}(\rho) = \operatorname{tr}(\rho)\mathbb{I}_{\mathcal{H}} - \rho - U\rho^T U^{\dagger},$$

for any  $U : \mathcal{H} \to \mathcal{H}$  with  $U^T = -U$  and  $U^{\dagger}U \leq \mathbb{I}$ , which are known as Breuer-Hall maps.

To prove the positivity of  $T_{BH}$ , it is enough to prove that for any unit vector  $|\psi\rangle$ ,  $T_{BH}(|\psi\rangle\langle\psi|)$  is PSD. We have:

$$T_{BH}(|\psi\rangle\langle\psi|) = \mathbb{I} - |\psi\rangle\langle\psi| - U\overline{|\psi\rangle\langle\psi|}U^{\dagger}$$
(6)

$$= \mathbb{I} - |\psi\rangle \langle \psi| - |\tilde{\psi}\rangle \langle \tilde{\psi}|, \qquad (7)$$

where  $|\tilde{\psi}\rangle := U |\overline{\psi}\rangle$ . On the other hand, since  $U^T = -U$ , we conclude that:

$$\langle \psi | \tilde{\psi} \rangle = \langle \psi | U | \overline{\psi} \rangle = - [\langle \psi | U | \overline{\psi} \rangle]^T = 0,$$

which implies the orthogonality of  $|\psi\rangle$  and  $|\tilde{\psi}\rangle$ . We know that the set  $\{|\psi\rangle, \frac{|\tilde{\psi}\rangle}{||\tilde{\psi}\rangle|}\}$  can be extended to an orthonormal basis  $\{|\psi\rangle, \frac{|\tilde{\psi}\rangle}{||\tilde{\psi}\rangle|}, |\phi_1\rangle, \dots, |\phi_{d-2}\rangle\}$ , and  $\mathbb{I}$  can be written as  $\mathbb{I} = |\psi\rangle \langle \psi| + \frac{|\tilde{\psi}\rangle \langle \tilde{\psi}|}{||\tilde{\psi}\rangle|^2} + \sum_i |\phi_i\rangle \langle \phi_i|$ . Hence (7) can be rewritten as:

$$T_{BH}(|\psi\rangle\langle\psi|) = |\tilde{\psi}\rangle\langle\tilde{\psi}|\frac{1-||\tilde{\psi}\rangle|^2}{||\tilde{\psi}\rangle|^2} + \sum_i |\phi_i\rangle\langle\phi_i|.$$
 (8)

Since  $U^{\dagger}U \leq \mathbb{I}$ ,

$$\left|\left|\tilde{\psi}\right\rangle\right|^{2} = \left<\tilde{\psi}\right|\tilde{\psi}\right> = \left<\overline{\psi}\right|U^{\dagger}U\left|\overline{\psi}\right> \le \left<\overline{\psi}\right|\overline{\psi}\right> = 1,$$

and the right hand side of (8) will be positive.

Now we prove that  $T_{BH}$  is not completely positive in a similar way to what we did for the reduction map.

$$C_{T_{BH}} = \sum_{i,j} |i\rangle \langle j| \otimes T_{BH}(|i\rangle \langle j|)$$
  
=  $\sum_{i,j} |i\rangle \langle j| \otimes (\operatorname{tr}(|i\rangle \langle j|)\mathbb{I} - |i\rangle \langle j| - U |j\rangle \langle i| U^{\dagger})$   
=  $\mathbb{I} - d |\Omega'\rangle \langle \Omega'| - \sum_{i,j} |i\rangle \langle j| \otimes U |j\rangle \langle i| U^{\dagger}$ 

Moreover,

$$\begin{split} &\langle \Omega | \left( \sum_{i,j} |i\rangle \langle j| \otimes U |j\rangle \langle i| U^{\dagger} \right) |\Omega \rangle \\ &= \sum_{\ell} \langle \ell \ell | \left( \sum_{i,j} |i\rangle \langle j| \otimes U |j\rangle \langle i| U^{\dagger} \right) \sum_{k} |kk\rangle \\ &= \sum_{i,j,\ell,k} \langle \ell |i\rangle \langle j|k\rangle \otimes \langle \ell |U|j\rangle \langle i|U^{\dagger}|k\rangle \\ &= \sum_{i,j} \langle i|U|j\rangle \langle i|U^{\dagger}|j\rangle \\ &= \sum_{i,j} U_{ij} U_{ij}^{\dagger} = \sum_{i,j} -U_{ij} \overline{U_{ij}}, \end{split}$$

where the last equality is derived by the fact that U is antisymmetric. Therefore,

$$\left\langle \Omega' \right| C_{T_{BH}} \left| \Omega' \right\rangle = 1 - d + \frac{\sum_{i,j} \left| U_{ij} \right|^2}{d}.$$

Note that  $U^{\dagger}U \leq \mathbb{I}$  implies that  $(U^{\dagger}U)_{jj} \leq 1$  for all j's. Hence,

$$d \ge \sum_{j} (U^{\dagger}U)_{jj} = \sum_{i,j} U_{ji}^{\dagger}U_{ij} = \sum_{i,j} \overline{U_{ij}}U_{ij} = \sum_{i,j} |U_{ij}|^2.$$

For d > 2,  $\langle \Omega' | C_{T_{BH}} | \Omega' \rangle < 0$  and consequently  $\lambda_{min} < 0$ , which implies that  $C_{T_{BH}}$  is not PSD.

When d is even, we know that there are anti-symmetric unitaries  $U_{d\times d}$ , that could be constructed using the anti-symmetric unitary  $D = \sum_{k=0}^{\frac{d}{2}} |2k\rangle \langle 2k+1| - |2k+1\rangle \langle 2k|$ . In fact, for an arbitrary real unitary  $V_{d\times d}$ ,  $VDV^{\dagger}$  is an anti-symmetric unitary.

Before proceeding to the next example, it is worth mentioning that there is a well established correspondence between linear superoperators and biforms. Let  $\mathbb{R}[x, y]$  be the vector space of polynomials in the variables  $\mathbf{x} := (x_1, \ldots, x_n)$  and  $y := (y_1, \ldots, y_m)$ , and  $\mathbb{R}[x, y]_{k_1, k_2}$ be the subspace of biforms of bidegree  $(k_1, k_2)$ , that is polynomials in  $\mathbb{R}[x, y]$  that are homogeneous of degree  $k_1$  and  $k_2$  in x and y, respectively.

In the case of real vector spaces, we can define this bijection  $\mu : \mathcal{L}(\mathbb{S}^n, \mathbb{S}^m) \to \mathbb{R}[x, y]_{2,2}$ , where  $\mathbb{S}^n$  denotes the set of all symmetric  $n \times n$  real matrices, as:

$$\mu(\Phi) = p_{\Phi}(x, y) = \langle y | \Phi(|x\rangle \langle x|) | y \rangle.$$

The following theorem shows that through this correspondence, (complete) positivity has a nice translation within the realm of biforms.

**Theorem 9.** Let  $\Phi : \mathbb{S}_n \to \mathbb{S}_m$  be a linear map. Then *(Klep* et al., 2019):

#### 1. $\Phi$ is positive iff $p_{\Phi}$ is nonnegative.

2.  $\Phi$  is completely positive iff  $p_{\Phi}$  is a sum of squares.

**Choi map (Choi, 1975b)** Choi proved that there is a non-negative biquadratic form that can not be expressed as sum of squares. The corresponding superoperator  $\Phi$ :  $M_3(\mathbb{R}) \to M_3(\mathbb{R})$  can be written as:

$$X = \begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix}$$
  
$$\mapsto \Phi(X) = \begin{pmatrix} x_{11} + x_{33} & -x_{12} & -x_{13} \\ -x_{21} & x_{22} + x_{11} & -x_{23} \\ -x_{31} & -x_{32} & x_{33} + x_{22} \end{pmatrix}.$$

There are generalizations of the original Choi map that are known as Choi-type maps. The reader can find a list of different variations of Choi-type maps in (Ha and Kye, 2012).

**Positive maps based on UPBs** To introduce this family of maps, we need to first, introduce the notion of an unextendible product basis.

**Definition** Let  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$  be a bipartite system. An unextendible product basis (UPB) S is a set of orthogonal product vectors such that Span(S) is a proper subset of  $\mathcal{H}$ , and  $(\text{Span}(S))^{\perp}$  contains no product vector (Bennett et al., 1999). The reader can find some examples of UPBs in (Bennett *et al.*, 1999; Terhal, 2001). Suppose that  $S = \{|\psi_i\rangle = |\alpha_i\rangle |\beta_i\rangle\}_{i=1}^n$  is a UPB. We define a bipartite state  $\rho_{AB}$  as follows:

$$\rho = \frac{1}{\dim \mathcal{H} - |\mathbf{S}|} \left( \mathbb{I}_{AB} - \sum_{i} |\alpha_{i}\rangle \langle \alpha_{i}| \otimes |\beta_{i}\rangle \langle \beta_{i}| \right).$$
(9)

 $\rho$  is a projection on  $\text{Span}(\mathcal{S})^{\perp}$ , hence its range contains no products, and this implies that  $\rho$  is entangled. For this entangled state, we know that an entanglement witness exists. One can prove that the following Hermitian operator is an entanglement witness for  $\rho$ .

$$\mathbf{H} = \sum_{i=1}^{|\mathbf{S}|} |\psi_i\rangle \langle\psi_i| - d\epsilon |\Psi\rangle \langle\Psi|,$$

where  $|\Psi\rangle$  is a maximally entangled state s.t.

$$\langle \Psi | \rho | \Psi \rangle > 0, \tag{10}$$

and

$$\epsilon = \min_{|\phi_A\rangle\otimes|\phi_B\rangle} \sum_{i=1}^{|\mathcal{S}|} \left|\langle\phi_A \mid \alpha_i\rangle\right|^2 \left|\langle\phi_B \mid \beta_i\rangle\right|^2, \qquad (11)$$

where the minimum is taken over all pure states  $|\phi_A\rangle \in \mathcal{H}_A$  and  $|\phi_B\rangle \in \mathcal{H}_B$ . For any unextendible product basis S it is possible to find a maximally entangled state  $|\Psi\rangle$  such that (10) holds.

To prove that H is an entanglement witness we need to show that  $\operatorname{tr}(\operatorname{H}\rho) < 0$  and for any separable state  $\sigma$ ,  $\operatorname{tr}(\operatorname{H}\sigma) \geq 0$ . Since  $\rho$  is a projector on  $\operatorname{Span}(\mathcal{S})^{\perp}$ ,  $\operatorname{tr}(\sum_{i} |\psi_{i}\rangle \langle \psi_{i}| \rho) = 0$ , and since (10) holds, we conclude that  $\operatorname{tr}(-d\epsilon |\Psi\rangle \langle \Psi| \rho) < 0$ , which implies that  $\operatorname{tr}(\operatorname{H}\rho) < 0$ . Note that  $\epsilon > 0$ . It is because of the fact that the function  $|\phi_{A}\rangle |\phi_{B}\rangle \mapsto \sum_{i=1}^{|\mathcal{S}|} |\langle \phi_{A} | \alpha_{i}\rangle|^{2} |\langle \phi_{B} | \beta_{i}\rangle|^{2}$ is continuous and the set of all product vectors is compact, hence the minimum is taken by a product vector  $|\phi_{A}\rangle |\phi_{B}\rangle$ , and if the value of function for this product vector is zero, it contradicts the fact that S is a UPB.

To prove that for all separable states  $\sigma$ , tr(H $\sigma$ )  $\geq 0$ , it is enough to show that for all vectors  $|\phi_A\rangle$  and  $|\phi_B\rangle$ ,

$$\operatorname{tr}(\mathrm{H} |\phi_A\rangle \langle \phi_A | \otimes |\phi_B\rangle \langle \phi_B |) \ge 0.$$

For a maximally entangled state  $|\Psi\rangle$ , we have  $|\langle \Psi | \phi_A \rangle \otimes | \phi_B \rangle|^2 \leq \frac{1}{d}$ . Therefore:

$$\begin{aligned} \operatorname{tr}(\mathbf{H} |\phi_A\rangle \langle \phi_A | \otimes |\phi_B\rangle \langle \phi_B |) \\ &= \operatorname{tr}((\sum_{i=1}^{|\mathbf{S}|} |\psi_i\rangle \langle \psi_i | - d\epsilon |\Psi\rangle \langle \Psi |) |\phi_A\rangle \langle \phi_A | \otimes |\phi_B\rangle \langle \phi_B |) \\ &= \sum_{i=1}^{|\mathbf{S}|} |\langle \phi_A | \alpha_i\rangle|^2 |\langle \phi_B | \beta_i\rangle|^2 - d\epsilon |\langle \Psi | \phi_A\rangle \otimes |\phi_B\rangle |^2 \\ &\geq \epsilon - d\epsilon \frac{1}{d} = 0. \end{aligned}$$

#### IV. DUAL OF A MAP

In this section, we introduce the notion of the dual of a linear map, which will be important for the rest of our discussion.

**Proposition 10.** Let  $\mathcal{H}_1$  and  $\mathcal{H}_2$  be two (finite dimensional) Hilbert spaces. For any linear map T:  $\mathcal{H}_1 \to \mathcal{H}_2$ , there exist a unique linear map  $T^*: \mathcal{H}_2 \to \mathcal{H}_1$  such that for all  $x \in \mathcal{H}_1$  and  $y \in \mathcal{H}_2$ ,

$$\langle Tx, y \rangle_{\mathcal{H}_2} = \langle x, T^*y \rangle_{\mathcal{H}_1}, \tag{12}$$

where  $\langle ., . \rangle_{\mathcal{H}_i}$  denotes the inner product over the space  $\mathcal{H}_i$ . The map  $T^*$  is called the dual of T.

One can see that for a Hilbert space  $\mathcal{H}$ , the map  $\langle ., . \rangle$ :  $\mathcal{L}(\mathcal{H}) \times \mathcal{L}(\mathcal{H}) \to \mathbb{C}$  which is defined as

$$\langle A, B \rangle := \operatorname{tr}(AB^{\dagger}),$$

is an inner product on  $\mathcal{L}(\mathcal{H})$ . Thus, for a map  $\Phi$ :  $\mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H}')$  we can rewrite Equation (12) as

$$\operatorname{tr}(\Phi(X)Y^{\dagger}) = \operatorname{tr}(X(\Phi^*(Y))^{\dagger}).$$

Furthermore, note that

$$\begin{split} \Phi(|i\rangle\langle j|)_{k,l} &= \langle k|\Phi(|i\rangle\langle j|)|l\rangle \\ &= \operatorname{tr}(\Phi(|i\rangle\langle j|)|l\rangle\langle k|) \\ &= \operatorname{tr}(|i\rangle\langle j|(\Phi^*(|k\rangle\langle l|))^{\dagger}) \\ &= \langle i|\Phi^*(|k\rangle\langle l|)|j\rangle \\ &= \Phi^*(|k\rangle\langle l|)_{i,j}, \end{split}$$

which can be used to find the dual of a given map  $\Phi$ .

**Example** We can see that the transposition, reduction and Breuer-Hall maps are *self-dual*, meaning that they are equal to their duals. However, the Choi map is not self-dual, since it maps  $|0\rangle \langle 0|$  to  $\frac{1}{2}(|0\rangle \langle 0| + |2\rangle \langle 2|)$ , while its dual maps  $|0\rangle \langle 0|$  to  $\frac{1}{2}(|0\rangle \langle 0| + |1\rangle \langle 1|)$ .

**Proposition 11.** 1.  $\Phi$  is positive iff  $\Phi^*$  is positive.

2.  $\Phi$  is completely positive iff  $\Phi^*$  is completely positive.

Proof. 1.  $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$  is positive iff for all  $|x\rangle \in \mathcal{H}_A, \ \Phi(|x\rangle \langle x|) \ge 0$  iff for all  $|x\rangle \in \mathcal{H}_A$  and  $|y\rangle \in \mathcal{H}_B,$ 

$$\operatorname{tr}(\Phi(|x\rangle \langle x|) |y\rangle \langle y|) = \operatorname{tr}(|x\rangle \langle x| \Phi^*(|y\rangle \langle y|)) \ge 0,$$

iff  $\Phi^*$  is positive.

2.  $\Phi$  is completely positive iff for any Hilbert space  $\mathcal{H}_C$ , the map  $(\mathcal{I}_C \otimes \Phi)$  is positive. From the previous part we know that  $(\mathcal{I}_C \otimes \Phi)$  is positive iff  $(\mathcal{I}_C \otimes \Phi)^* = (\mathcal{I}_C \otimes \Phi^*)$  is positive.

Henceforth, we use an alternative construction for establishing an entanglement witness from a positive but not completely positive maps, using the concept of the dual of a map.  $\Box$ 

**Proposition 12.** The map  $C : \mathcal{L}(\mathcal{L}_B, \mathcal{L}_A) \to \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ , which is defined as

$$\mathcal{C}(\Phi) = \sum_{i,j=1}^{d_A} |i\rangle \langle j| \otimes \Phi^*(|i\rangle \langle j|), \qquad (13)$$

defines a bijection between the set of all positive but not completely positive maps in  $\mathcal{L}(\mathcal{L}_B, \mathcal{L}_A)$  and the set of all entanglement witnesses in  $\mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ .

*Proof.* The statement is a direct implication of Propositions 11 and 4.  $\Box$ 

**Proposition 13.** Let  $\Phi : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$  be a positive but not completely positive map, and  $\rho \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$  be a state such that  $\operatorname{tr}(\mathcal{C}(\Phi)\rho) < 0$ . Then,  $\rho \notin \mathsf{PP}\Phi$ .

*Proof.* Note that

$$\operatorname{tr}(\mathcal{C}(\Phi)\rho) = \operatorname{tr}((\mathcal{I}\otimes\Phi^*)|\Omega\rangle \langle \Omega|\rho) = \operatorname{tr}(|\Omega\rangle \langle \Omega| (\mathcal{I}\otimes\Phi)\rho).$$

Thus, if  $\operatorname{tr}(\mathcal{C}(\Phi)\rho) < 0$ ,  $(\mathcal{I} \otimes \Phi)\rho$  is not positive, i.e.  $\rho \notin \mathsf{PP}\Phi$ .

The above proposition justifies our preference for using the latter version of the Choi-Jamiołkowski isomorphism, as the witness criterion obtained from a positive map using the latter version would have a canonical relation with the  $\mathsf{PP}\Phi$  criterion associated to the map.

**Proposition 14.** Let  $\Phi : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$  be a positive but not completely positive map. Then  $\mathsf{PP}\Phi$  is a proper subset of  $\mathsf{D}$ .

*Proof.* Since  $\Phi$  is not completely positive, by Proposition 11, we conclude that  $\Phi^*$  is not completely positive either. Thus, the Choi matrix of  $\Phi^*$ , which is  $C_{\Phi^*} = (\mathcal{I} \otimes \Phi^*) |\Omega\rangle \langle \Omega|$  is not PSD, and has a negative eigenvalue corresponding to an eigenvector  $|v\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ . Note that

$$\operatorname{tr}(C_{\Phi^*} |v\rangle \langle v|) = \operatorname{tr}(|\Omega\rangle \langle \Omega| (\mathcal{I} \otimes \Phi) |v\rangle \langle v|) < 0.$$

Since  $|\Omega\rangle \langle \Omega|$  is PSD, then  $(\mathcal{I} \otimes \Phi) |v\rangle \langle v|$  is not PSD, which implies that  $\frac{|v\rangle \langle v|}{||v\rangle|^2} \notin \mathsf{PP}\Phi$ .

### V. ENTANGLEMENT WITNESSES AND SDP'S

In this section, we discuss another method for obtaining an entanglement witness which detects a state  $\rho_{AB}$  when  $\rho_{AB} \notin \mathsf{PP}\Phi$  for a positive but not completely positive map  $\Phi$ . In this method, we use semidefinite programming, that is an optimisation paradigm in which linear functions are optimized over spectrahedra. We assume that the reader is familiar with the basic concepts of semidefinite programming, and if it is not the case, we refer her to relevant references such as (Boyd and Vandenberghe, 2004).

Let  $\Phi : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$  be a positive but not completely positive map. Consider the following optimization problem:

$$\max_{t} \quad t \quad (14)$$
  
s.t.  $(\mathcal{I}_A \otimes \Phi) \rho_{AB} \ge t \mathbb{I}_{AB}.$ 

We can see that the above optimization problem is a SDP, and there exist methods (e.g. interior point methods) that can be used to efficiently solve the problem.

The above SDP computes the minimum eigenvalue of  $(\mathcal{I}_A \otimes \Phi)\rho_{AB}$ . Therefore, the optimal value of the above SDP, which is denoted by  $t^*$ , is negative iff  $(\mathcal{I}_A \otimes \Phi)\rho_{AB}$  has a negative eigenvalue, iff  $\rho_{AB} \notin \mathsf{PP}\Phi$ .

Now, we write the dual of the above SDP:

$$\min_{W} \operatorname{tr} \left( W(\mathcal{I}_{A} \otimes \Phi) \rho_{AB} \right) \\
\text{s.t.} \quad \operatorname{tr}(W) = 1, \qquad (15) \\
W \ge 0.$$

Since both primal and dual are strictly feasible, by the Slater's theorem the strong duality holds, and we conclude that  $\rho \notin \mathsf{PP}\Phi$  if and only if  $\operatorname{tr}(W^*(\mathcal{I}_A \otimes \Phi)\rho_{AB}) = \operatorname{tr}((\mathcal{I}_A \otimes \Phi^*)W^*\rho_{AB}) < 0$ , where  $W^*$  is the optimal solution of the dual problem.

Moreover, for any pure product state  $|x\rangle \langle x| \otimes |y\rangle \langle y|$ ,

$$\operatorname{tr} \left( \left( \mathcal{I}_A \otimes \Phi^* \right) W^* \left| x \right\rangle \left\langle x \right| \otimes \left| y \right\rangle \left\langle y \right| \right) \\ = \operatorname{tr} \left( W^* \left( \mathcal{I}_A \otimes \Phi \right) \left| x \right\rangle \left\langle x \right| \otimes \left| y \right\rangle \left\langle y \right| \right) \\ = \operatorname{tr} \left( W^* \left| x \right\rangle \left\langle x \right| \otimes \Phi \left( \left| y \right\rangle \left\langle y \right| \right) \right) \ge 0.$$

In fact, we can similarly show that for any state  $\rho \in \mathsf{PP}\Phi$ , tr $((\mathcal{I}_A \otimes \Phi^*)W^*\rho) \geq 0$ . Therefore, if  $\rho_{AB}$  is an entangled state that is not in  $\mathsf{PP}\Phi$ ,  $(\mathcal{I}_A \otimes \Phi^*)W^*$  is an entanglement witness, witnessing  $\rho_{AB}$ .

**Proposition 15.** Let  $W^*$  be the optimal solution of the dual problem, and define  $\Pi_{\lambda_{\min}}$  to be the projector on the eigenspace of the minimum eigenvalue of the operator  $(\mathcal{I}_A \otimes \Phi)\rho_{AB}$ . Then,  $\operatorname{Im}(W^*) \subseteq \operatorname{Supp}(\Pi_{\lambda_{\min}})$ .

*Proof.* Define  $M := (\mathcal{I}_A \otimes \Phi)\rho_{AB}$ , and let  $\lambda_{\min}$  be the minimum eigenvalue of M, which is equal to the optimal value of the primal. Since the strong duality holds, we have  $\lambda_{\min} = \operatorname{tr}(W^*M)$ , which can be rewritten as

$$\operatorname{tr}(W^*(M - \lambda_{\min} \mathbb{I}_{AB})) = 0.$$

Since  $W^*$  and  $M - \lambda_{\min} \mathbb{I}_{AB}$  are both PSD, we conclude that  $W^*(M - \lambda_{\min} \mathbb{I}_{AB}) = (M - \lambda_{\min} \mathbb{I}_{AB})W^* = 0$ , and using the fact that all the non-zero eigenvalues of  $M - \lambda_{\min} \mathbb{I}_{AB}$  are strictly positive, and  $\ker(M - \lambda_{\min} \mathbb{I}_{AB}) = \operatorname{Supp}(\Pi_{\lambda_{\min}})$ , it is implied that  $\operatorname{Im}(W^*) \subseteq \operatorname{Supp}(\Pi_{\lambda_{\min}})$ .  $\Box$ 

# VI. PROPERTIES OF ENTANGLEMENT CRITERIA AND THEIR CONNECTIONS

# A. Properties of $PP\Phi$ 's

We defined the PP $\Phi$  set in Section I.B for any positive but not completely positive map  $\Phi$ , and showed that SEP  $\subseteq$  PP $\Phi$ . We know, in particular, that SEP  $\subseteq$  PPT. It is an interesting question to investigate whether or not this inclusion is strict. As we will see in the following, the inclusion is strict unless the local dimensions are (2, 2), (2, 3) and (3, 2).

The next proposition shows that the set of all  $\mathsf{PP}\Phi$  criteria is in some sense *complete*, meaning that if a state  $\rho_{AB}$  is entangled, there exists a positive but not completely positive map  $\Phi : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$  such that  $(\mathcal{I}_A \otimes \Phi)\rho_{AB}$  is not PSD.

**Theorem 16.** A state  $\rho_{AB}$  is separable iff for all positive maps  $\Phi : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A), \ \rho_{AB} \in \mathsf{PP}\Phi$  (Horodecki et al., 1996).

*Proof.* The proof of the "only if" direction is obvious. For the other direction, suppose that the state  $\rho_{AB} \notin \mathsf{SEP}$ . Then, by Proposition 3, there exists an entanglement witness W detecting  $\rho_{AB}$ . Using the Choi–Jamiolkowski isomorphism, we know that there exists a positive map  $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$  such that:

$$W = (\mathcal{I}_A \otimes \Phi) |\Omega\rangle \langle \Omega|.$$

Then we have:

$$0 > \operatorname{tr}(W\rho_{AB}) = \operatorname{tr}((\mathcal{I} \otimes \Phi) |\Omega\rangle \langle \Omega| \rho_{AB})$$
$$= \operatorname{tr}(|\Omega\rangle \langle \Omega| (\mathcal{I} \otimes \Phi^*)\rho_{AB}),$$

which yields  $(\mathcal{I} \otimes \Phi^*)\rho_{AB} \not\geq 0$ , where  $\Phi^* : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$  is a positive map.

**Definition** A linear map  $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$  is called decomposable if it can be written as:

$$\Phi = T_1 + T_2\theta,$$

where  $T_1$  and  $T_2$  are completely positive maps, and  $\theta$  is the transposition map.

**Theorem 17.** All positive maps are decomposable when  $(dim(\mathcal{H}_A), dim(\mathcal{H}_B)) \in \{(2, 2), (2, 3), (3, 2)\}$  (Woronow-icz, 1976).

**Proposition 18.** If  $\rho_{AB} \in \mathsf{PPT}$ , then for any decomposable map  $\Phi : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$ ,  $\rho_{AB} \in \mathsf{PP\Phi}$ .

*Proof.* We have

$$\begin{aligned} (\mathcal{I} \otimes \Phi)\rho_{AB} &= (\mathcal{I} \otimes (T_1 + T_2\theta))\rho_{AB} \\ &= (\mathcal{I} \otimes T_1)\rho_{AB} + (\mathcal{I} \otimes T_2)(\mathcal{I} \otimes \theta)\rho_{AB}. \end{aligned}$$

Since  $\rho_{AB} \in \mathsf{PPT}$ ,  $(\mathcal{I} \otimes \theta)\rho_{AB} \geq 0$ , and we know that the positivity of matrices is preserved under the partial application of completely positive maps. Hence  $(\mathcal{I} \otimes \Phi)\rho_{AB} \geq 0$ , and  $\rho_{AB} \in \mathsf{PP\Phi}$ .

**Proposition 19.** The reduction criterion is weaker than the PPT criterion, meaning that  $PPT \subseteq PP\Lambda$ .

*Proof.* Once we can prove that the reduction map is decomposable, the above proposition becomes an immediate implication of Proposition 18. To show that  $\Lambda$  is decomposable, note that:

$$\begin{aligned} \theta \circ \Lambda \circ \theta(\rho) &= \theta \circ \Lambda(\rho^T) \\ &= \theta(\operatorname{tr}(\rho^T)\mathbb{I} - \rho^T) \\ &= \operatorname{tr}(\rho)\mathbb{I} - \rho \\ &= \Lambda(\rho) \end{aligned}$$

We saw in Proposition 8 that  $\theta \Lambda$  is completely positive, which implies  $\Lambda$  is decomposable.

**Remark** Although the reduction map is decomposable, and the reduction criterion is weaker than the PPT criterion, it plays an important role in entanglement distillation. In fact, it was proved in (Horodecki and Horodecki, 1999) that any state violating the reduction criterion can be distilled.

Putting together Theorems 16, 17 and Proposition 18, the following theorem is obtained.

**Theorem 20.** A state  $\rho_{AB}$  acting on  $\mathbb{C}^2 \otimes \mathbb{C}^2$  or  $\mathbb{C}^2 \otimes \mathbb{C}^3$ is separable iff its partial transposition is PSD, but in higher dimensions,  $(\mathcal{I} \otimes \theta)\rho_{AB} \geq 0$  is not a sufficient condition for separability (Horodecki et al., 2001).

Knowing that PPT is strictly greater than SEP in higher dimensions, we came up with the idea of intersecting PPT with other  $PP\Phi$ 's in order to find better approximations of SEP. To that purpose, I undertook a numerical simulation to estimate the volume of  $\mathsf{PP}\Phi\mathsf{s}$  for the above-mentioned positive maps. Volumes are calculated as the fraction of the number of states that satisfy the  $\mathsf{PP}\Phi$  criteria in a random sample of quantum states. I used the transpose map, reduction map, a Choi-type map (the original map introduced by Choi), a Breuer-Hall map (only for cases where the local dimension is even  $\geq 4$ , using the anti-symmetric unitary  $D = \sum_{k=0}^{\frac{\pi}{2}} |2k\rangle \langle 2k+1| - |2k+1\rangle \langle 2k| \rangle$ , and a special map based on UPBs (using the first example of such maps discussed in (Terhal, 2001)), which we call it the Terhal map henceforth.

The results are obtained in each dimension with a sample size of 100000 density matrices generated at random according to the Haar measure, using the random density matrix generator provided in 'toqito' (Russo, 2021); a software tool for studying quantum information theory.

Figure 2 depicts the results. I also tried to find states that are in PPT, but they are not in other PP $\Phi$ s, which was not successful as the number of PPT samples is too small.

As we proved earlier, the PP $\Phi$  corresponding to the reduction map contains PPT, which agrees with our results. We also expect that the volume of the PP $\Phi$  associated to the Breuer-Hall map be less than the volume of the PP $\Phi$  associated to the reduction map, which is consistent with the results.

Let us denote the Terhal map by  $\Phi$ . As can be seen, all of our samples satisfy the PP $\Phi$  criteria. We do know, however, that there exist PPT entangled states that are not in PP $\Phi$ . As a result, PP $\Phi$  cuts PPT, and their intersection is strictly smaller than PPT.

I also tried to illustrate this cut by demonstrating  $PP\Phi$  and PPT in the convex hull of three well-chosen states. Our three states are an adequate convex combination of a state in SEP, a state in PPT but not in PP $\Phi$ , and a state in PP $\Phi$  but not in PPT. The maximally mixed state  $\frac{\mathbb{I}}{9}$  is utilised for the first state, and the state used to define the Terhal map for the second one. The third state belongs to the Werner state family, which are defined as

$$\rho_{AB} = \frac{1}{d^2 - d\alpha} \left( \mathbb{I}_{d^2 \times d^2} - \alpha \mathbb{F}_{AB} \right),$$

where  $\mathbb{F}_{AB} = \sum_{ij} |i\rangle \langle j|_A \otimes |j\rangle \langle i|_B$ , dim $(\mathcal{H}_A) =$ dim $(\mathcal{H}_B) = d$ , and  $\alpha \in [-1, 1]$ . It is known that all Werner states with  $p < \frac{1}{2}$  are entangled if we write  $\alpha$  as

$$\alpha = \frac{((1-2p)d+1)}{(1-2p+d)}.$$

These entangled Werner states violate the PPT condition.

Let  $\rho'$  be the 9 × 9 Werner state with  $\alpha = 0.6$ . Then we define our states  $\sigma_i$  for i = 1, 2, 3 as:

$$\sigma_1 = 0.07(0.01 \frac{\mathbb{I}}{9} + 0.99\rho) + 0.93(0.003\rho' + 0.997\rho),$$
  
$$\sigma_2 = \rho, \quad \sigma_3 = 0.004\rho' + 0.996\rho.$$

In Figure 3, we represented the intersection of PPT and PP $\Phi$  with the convex hull of the states  $\{\sigma_i\}_i$ . It is obvious that PPT  $\cap$  PP $\Phi$  is strictly smaller than PPT, and using this set as an approximation of SEP leads to a better relaxation. It is also noteworthy that the membership of this set can be determined efficiently.

We end this part with a characterization of  $\mathsf{PP}\Phi$  in terms of entanglement witnesses. The following proposition is the generalization of a result stated in (Horodecki *et al.*, 2009).

	fraction										
Map	(2,2)	(3,2)	(2,3)	(3,3)	(2,4)	(4, 2)	(3,4)	(4, 3)	(2, 5)	(5,2)	(4, 4)
transpose	0.24156	0.02112	0.0217	0.0002	0.00074	0.00079	0.0	0.0	0.00001	0.00002	0.0
reduction	0.24156	0.02112	0.79969	0.5103	0.99025	0.00079	0.96034	0.27982	0.99993	0.00002	0.90626
Choi-type				0.9669				0.94195			
Terhal				1.0				1.0			
Breuer-Hall					0.817		0.56515				0.32796

FIG. 2 Computing the volume of  $\mathsf{PP}\Phi$ 's



FIG. 3 The set of states  $\rho = (1 - p - q)\sigma_1 + p\sigma_2 + q\sigma_3$  and its intersection with PP $\Phi$  and PPT.

**Proposition 21.** For any positive but not completely positive map  $\Phi : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$ , the family of witnesses of the form

$$W_{|\psi\rangle} = (\mathcal{I} \otimes \Phi^*) \ket{\psi} \langle \psi |_{\mathcal{I}}$$

where  $|\psi\rangle$  is an entangled vector in  $\mathcal{H}_A \otimes \mathcal{H}_A$ , are enough to describe PP $\Phi$ , meaning that for  $\rho_{AB} \notin PP\Phi$ , if and only if there exists a member of this family witnessing  $\rho_{AB}$ .

*Proof.* Suppose that  $\rho \notin \mathsf{PP}\Phi$ . Then  $(\mathcal{I} \otimes \Phi)\rho \ngeq 0$ , and  $(\mathcal{I} \otimes \Phi)\rho$  has an eigenvector  $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_A$  corresponding to a negative eigenvalue, which is necessarily entangled. Thus, we have

$$0 > \operatorname{tr}((\mathcal{I} \otimes \Phi)\rho |\psi\rangle \langle \psi|) = \operatorname{tr}((\mathcal{I} \otimes \Phi^*) |\psi\rangle \langle \psi| \rho)$$

On the other hand, if  $W_{|\psi\rangle} = (\mathcal{I} \otimes \Phi^*) |\psi\rangle \langle \psi|$  is a witness for a state  $\rho$ , then tr $((\mathcal{I} \otimes \Phi^*) |\psi\rangle \langle \psi| \rho) < 0$ , implying that  $(\mathcal{I} \otimes \Phi)\rho \geq 0$ .

#### **B.** Properties of SDP Witnesses

In Section V, We discussed a method to find an entanglement witness W for a positive but not completely

positive map  $\Phi$ , witnessing a given state  $\rho \notin \mathsf{PP}\Phi$ . When we obtain such a witness, it is possible to find a positive but not completely positive map  $\Phi'$  using the Choi–Jamiolkowski isomorphism, such that  $\mathcal{J}(\Phi') = W$ . We might ask what is the relationship between the volume of  $\mathsf{PP}\Phi$  and  $\mathsf{PP}\Phi'$ .

In order to answer this question, I used some numerical simulations. First, I chose the initial entangled state  $\rho$  to be the maximally entangled state  $\frac{1}{d} |\Omega\rangle \langle \Omega|$ . For each map  $\Phi$ , I estimated the volume of PP $\Phi$  and PP $\Phi'$  in dimensions (2, 2) and (3, 3), where  $\Phi'$  is the map obtained from the above procedure. The sample size of 10000 density matrices has been chosen, and for each map, the matrices has been sampled separately. Results are shown in Figure 4.

Then, I repeated the procedure by changing the initial state to be a random entangled state that is not in  $\mathsf{PP}\Phi$ . For all the considered maps, except the transposition, remained equal. However, I observed that the volume of PPT varies when I change the initial state, and there exist initial states such that starting from them, the volume of  $\mathsf{PPT}'$  is equal to the volume of  $\mathsf{PPT}$ . For the other cases, I wondered it might be the case that  $\Phi = \Phi'$ , and the equality of the volumes comes from this equality. To answer this question, I computed  $\mathcal{J}(\Phi)$  and checked whether it is an optimal solution of the dual SDP. The answer was positive for the reduction, Breuer-Hall and Choi map, but it was negative for the transposition and Terhal map. Therefore, the entanglement witnesses obtained from the first three maps by Choi–Jamiołkowski isomorphism are SDP witnesses.

We also conjectured that the SDP witnesses are optimal, in the sense that for any SDP witness W, there are no other witness W' such that W' witnesses all the entangled states that are witnessed by W. To verify this hypothesis, I plotted cross-sections of the set of states and examine whether this optimality holds.

Figure 5 depicts the set of states  $\rho = (1 - p - q)\sigma_1 + p\sigma_2 + q\sigma_3$ , where  $\sigma_1$  is a random state that is not in PP $\Phi$ ,  $\sigma_2$  is the state used to define the Terhal map, and  $\sigma_3 = \frac{1}{1-0.4} (\frac{\mathbb{I}}{9} - 0.4\sigma_2)$ , and its intersection with PP $\Phi$  and the half-space tr( $W\rho$ ) < 0, where W is the witness obtained from  $\Phi$  using the initial state  $\sigma_1$ . The results for all the considered map were similar, so we only depict three examples of the plots when  $\Phi$  is the transpose map.

	fraction									
			(2,2)		(3,3)					
Φ	$PP\Phi$	$PP\Phi'$	$PP\Phi \setminus PP\Phi'$	$PP\Phi' \setminus PP\Phi$	$PP\Phi$	$PP\Phi'$	$PP\Phi \setminus PP\Phi'$	$PP\Phi' \setminus PP\Phi$		
Transpose	0.2428	0.2428	0.0000	0.0000	0.0001	0.5179	0.0000	0.5178		
Reduction	0.2394	0.2394	0.0000	0.0000	0.5208	0.5208	0.0000	0.0000		
Choi-type					0.9689	0.9689	0.0000	0.0000		
Terhal					1.0000	1.0000	0.0000	0.0000		

FIG. 4 Comparing the volume of  $PP\Phi$  and  $PP\Phi'$ , starting from the maximally entangled state. Note that different samples have been used for different maps.

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As we can see, the SDP witnesses seem to be optimal.

We finish this section by characterizing the SDP witnesses obtained from the transpose map when the local dimensions are (2, 2). We need the following result to prove our statements.

**Theorem 22.** The partial transpose of any entangled two-qubit state is of full rank and has only one negative eigenvalue (Sanpera et al., 1998; Verstraete et al., 2001).

**Proposition 23.** Let  $W \in \mathcal{L}(\mathbb{C}^2 \to \mathbb{C}^2)$  be a SDP witness obtained from the transpose map with the initial state  $\rho \in \mathcal{L}(\mathbb{C}^2 \otimes \mathbb{C}^2)$ . Then W is of the form

$$W = (\mathcal{I} \otimes \theta) \ket{\psi} \bra{\psi},$$

where  $\theta$  is the transpose map and  $|\psi\rangle$  is an entangled vector in  $\mathbb{C}^2 \otimes \mathbb{C}^2$ .

Proof. Let  $W^*$  be the optimal solution of the dual SDP problem. From Proposition 15, we know that  $\operatorname{Im}(W^*) \subseteq$  $\operatorname{Supp}(\Pi_{\lambda_{\min}})$ . Since by Theorem 22,  $\operatorname{Supp}(\Pi_{\lambda_{\min}})$  is one dimensional and  $W^*$  is a PSD operator whose trace is equal to one, we conclude that  $W^* = \Pi_{\lambda_{\min}}$ . Note that the eigenvector of  $(\mathcal{I} \otimes T)\rho$  corresponding to its negative eigenvalue is an entangled vector. The proof is complete by noting that the SDP witness is derived by  $(\mathcal{I} \otimes T)W^*$ .  $\Box$ 

**Proposition 24.** Let W be the SDP witness obtained from the transpose map  $\theta : \mathcal{L}(\mathbb{C}^2) \to \mathcal{L}(\mathbb{C}^2)$  with the initial state  $\frac{1}{2} |\Omega\rangle \langle \Omega|$ , where  $|\Omega\rangle = |00\rangle + |11\rangle$ . Consider the action of the group of the local unitaries  $\{U_1 \otimes U_2 \mid U_1, U_2 : \mathbb{C}^2 \to \mathbb{C}^2 \text{ are unitaries}\}$  on the set of the Hermitian operators over  $\mathbb{C}^4$ , which is defined as  $X \mapsto (U_1 \otimes U_2) X (U_1 \otimes U_2)^{\dagger}$ . The set of the SDP witnesses obtained from the transpose map with pure states as their initial states is equal to the orbit of W under this group action.

*Proof.* One can see that for all entangled vectors  $|\psi\rangle = c_0 |00\rangle + c_1 |11\rangle$ , where  $c_0, c_1 \ge 0$  such that  $c_0^2 + c_1^2 = 1$ , the eigenvectors corresponding to the negative eigenvalue of  $(\mathcal{I} \otimes \theta) |\psi\rangle \langle \psi|$  are the same. Proof of the Proposition 23 shows that we can conclude that the SDP witnesses obtained from the transpose map with the initial state

 $|\psi\rangle \langle \psi|$  are the same, and equal to W. Using the Schmidt decomposition, we know that we can write any two qubit entangled vector  $|\phi\rangle$  as

$$|\phi\rangle = (U_1 \otimes U_2)(c_0 |00\rangle + c_1 |11\rangle),$$

where  $U_1$  and  $U_2$  are unitaries and  $|\psi\rangle = (c_0 |00\rangle + c_1 |11\rangle)$ is entangled. Note that:

$$\lambda_{\min}((\mathcal{I}\otimes\theta)\ket{\phi}ra{\phi}) = \lambda_{\min}((\mathcal{I}\otimes\theta)\ket{\psi}ra{\psi})$$

as one can see that they are equal up to local unitaries, and in particular, have the same spectrum. Thus, we have

$$\begin{split} \lambda_{\min}((\mathcal{I} \otimes \theta) |\phi\rangle \langle \phi|) \\ &= \lambda_{\min}((\mathcal{I} \otimes \theta) |\psi\rangle \langle \psi|) \\ &= \operatorname{tr}(W |\psi\rangle \langle \psi|) \\ &= \operatorname{tr}((U_1 \otimes U_2)W(U_1 \otimes U_2)^{\dagger}(U_1 \otimes U_2) |\psi\rangle \langle \psi| (U_1 \otimes U_2)^{\dagger}) \\ &= \operatorname{tr}((U_1 \otimes U_2)W(U_1 \otimes U_2)^{\dagger} |\phi\rangle \langle \phi|), \end{split}$$

which implies that  $(U_1 \otimes U_2)W(U_1 \otimes U_2)^{\dagger}$  is an optimal solution for the dual SDP.  $\Box$ 

## VII. CONCLUSION AND FUTURE WORK

The problem of detection of the entanglement is a core problem in quantum information theory. Although solving this problem for mixed quantum states is proven to be NP-hard, several entanglement criteria have been developed during the past 30 years, and the study is still ongoing.

In this project we studied two types of entanglement criteria, namely criteria based on positive but not completely positive maps and entanglement witnesses. The study of these criteria have potential connections to various topics in quantum theory, ranging from the physical concept of time reversal to the task of entanglement distillation, as well as connections to other fields of mathematics and computer science, such as algebraic geometry and semidefinite programming.

The two types of criteria that were studied are related to each other and this relationship can be used to find



FIG. 5 The set of states  $\rho = (1 - p - q)\sigma_1 + p\sigma_2 + q\sigma_3$  and its intersection with PPT (red area) and the half-space tr( $W\rho$ ) < 0 (yellow area). The x and y-axis correspond to p and q, respectively. In each plot, the state  $\sigma_1$  has been chosen randomly.

better entanglement criteria. In particular, we discussed a new method for finding entanglement witnesses using semidefinite programming, that might help us to find improved families of both criteria for detection of the entanglement.

Some of the possible directions for the continuing the present work are as follows:

- 1. extending the Proposition 24 to the set of mixed states when the local dimensions are (2,2) and generalising it to higher dimensions.
- 2. proving or disproving the hypothesis that the SDP witnesses are optimal.
- 3. studying the relationship between  $\mathsf{PP}\Phi$  and  $\mathsf{PP}\Phi'$  which was discussed in Section VI.B.
- 4. finding new families of entanglement criteria based on positive but not completely positive maps or entanglement witnesses: Only a few number of positive but not completely positive maps or families of entanglement witnesses are currently known, and some of the recent works in the literature such as (Klep *et al.*, 2019; Siudzińska, 2022) are concerned about introducing new examples.
- 5. understanding the geometry of  $\mathsf{PP}\Phi$ 's: As our numerical simulations show, it seems that the geometric properties of the known positive maps are different, and explaining some of these geometric attributes can help us in obtaining a better understanding of SEP.

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