Block Positivity and Effective Criteria for Witnesses of Quantum Entanglement

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1. Introduction

Quantum Informantion is a field of study which emearged over the recent decades and at this point needs no introduction for an attentive reader. Its main principles and achievements were described in multiple reviews, for more details see [6] . In simple terms it can be wieved as a language for describing behaviour of quantum systems. A fundamental feature of such systems, governing the language of quantum information is entanglement. This property appears in the form of correlations between different parts of the system that cannot be achieved solely through local and classical commucation. From the perspective of quantum information algorithms, quantum entanglement often appears as a resource necessary in order to perform said algorithm. Most prominent examples include quantum teleportation and quantum dense coding. In the former, the task of teleporting a state between the sender and the receiver requires 'spending' of the entanglement between the two and in the latter one can exchange the entanglement for the improvement in the efficiency of a communication channel. An intresting problem, which arises as an immediate consequence of this point of view, is that of measuring quantum entanglement. The task of measuring, in and of itself, can be understood in two different ways, one of which is quantifying how entangled a given state is, and the other being discerning between entangled and non-entangled systems. The aim of this thesis is to focus on the latter, and in particular on the characterization of the means in which this distinguishment can be achieved. The means in question are operators detecting entangled states known as entanglement witnesses.

Section 2 introduces some preliminary notions. Its aim is to provide a brief characterization of the spaces of quantum states and operators acting on them. From a storytelling perspective one can view this section as setting the scene on which the later sections unfold. Section 3 discusses some of the separability criteria and introduces the definition and main features of entanglement witnesses. By the end of this section, we present conditions for an operator to be an entanglement witness and narrow down the scope to low dimensions. Section 4 presents the main achievement of this thesis, which is an algoritm evaluating whether an operator acting on systems in $\mathcal{C}^2 \otimes \mathcal{C}^2$ is an entanglement witness. The section starts with a short detour on properties of polynomials, employed in the algorithm, and then walks the reader through the algorithm itself. In section 5 we explore application of the algorithm to chosen examples of families of operators.

2. Setting the Scene

2.1 Convexity

Before delving into the world of quantum states and operators, it is instructive to start by introducing some preliminary mathematical concepts. For the purpose of this section, it is assumed that all discussed sets are subsets of some affine space $\mathcal{A}$. The detailed structure of the space is not crucial to the discussion, as the assumption is made mostly to allow for the mixing of one element of the space with another. Let X be one of such sets and let $x_1, x_2 \in X$. A convex combination of x_1 and x_2 is defined as a mixture

$$\theta x_1 + (1-\theta)x_2 \quad \theta \in [0,1]. \tag{2.1}$$

From a geometric perspective this can be interpreted as a line segment between x_1 and x_2. Convex combination can be generalized to more than two points by

$$\theta_1 x_1 + \theta_2 x_2 + ... + \theta_n x_n, \quad \sum_{i=1}^{n} \theta_i = 1 \ \wedge \ \theta_i \geq 0 \ [2]. \tag{2.2}$$

Definition 2.1 (Convex Set)**.** A set X is convex if any convex combination of its points belongs to X.

One way of constructing a convex set is taking a union of all possible convex combinations of points in X. Such set is called a convex hull of X, or more generally a polytope. By definition it is a smallest possible convex set containing X.

Definition 2.2 (Convex Cone)**.** Set K is a convex cone if it is convex and

$$\forall x \in K \wedge \theta \geq 0, \quad \theta x \in K \ [2]. \tag{2.3}$$

Condition (2.3) by itself defines a cone that is not necessarily convex. One can construct a convex cone from any convex set X by choosing a point $y \notin X$ and taking the union of all half lines starting at y and intersecting with X [1]. Another frequently occurring type of sets in convex analysis is the hyperplane, which is defined as

$$X = \{x | y \cdot x = c\} \tag{2.4}$$

where y is a fixed element of the affine space and c is a constant. Replacing the equality condition in (2.4) by either strong or weak inequality divides the space into to halves known as halfspaces. Intersection between multiple halfspaces and hyperplanes forms a convex set known as a polyhedron. Bounded polyhedra are called polytopes and correspond to convex hulls of other sets. A convex body is defined as a bounded convex set with a non empty interior [1]. A general remark providing a prescription for construction of convex sets is that any intersection of convex sets is also a convex set.

Definition 2.3 (Simplex)**.** Let $X = x_0, x_1, ..., x_k$ be a set of $k+1$ geometrically independent points i.e. set of points that are not confined to a $k-1$ dimensional hyperplane. A convex hull

$$\sigma_k = \left\{ \theta_0 x_0 + \theta_1 x_1 + ... + \theta_k x_k \mid \sum_{i=1}^{k} \theta_i = 1 \ \wedge \ \theta_i \geq 0 \right\} \tag{2.5}$$

of X is called a k-simplex [1, 10].

Exemplary simplexes being points ($k = 0$), line segments ($k = 1$) and triangles ($k = 2$). For any convex set X it is possible to find a sequence $\mathcal{I} = \{0, ..., i\}$ such that for all $n \in \mathcal{I}$ there exists a n-simplex contained in X. The largest $n \in \mathcal{I}$ corresponds to the dimension of X. Narrowing down the scope of the discussion to convex bodies, one can distinguish between pure and mixed points. The former are defined as ones that cannot be expressed as mixtures of others, while the latter correspond to all non-pure points. One example of pure points are vertices of a k-simplex. In the definition 2.3 these points are labeled as set

X. Another example, more relevant for quantum mechanics, is the outer surface of a 2-ball, which for physicists is known as the Bloch sphere.

Considering a k-simplex σ_k one can construct q-simplexes σ_q of lower dimensions by choosing $q+1 < k+1$ pure points of σ_k and taking their convex hull. All possible σ_q simplexex obtained from σ_k form a set of $\binom{k+1}{q+1}$ q-faces of σ_k [10]. The notion of faces can be generalized to any convex set X so that a q-face F of X is a q-dimensional convex subset of X such that

$$x = \theta x_1 + (q-\theta)x_2 \in F \iff x_1, x_2 \in F \text{ [1]}. \tag{2.6}$$

Notice that the condition (2.6) is more restricting than just the requirement for convexity. A mixture of pure points belongs to a face F of X if and only if the pure points in question also belong to F. This is not necessarily true for any general convex subset of X. In broad terms set of faces of a convex set X forms its boundaries.

Combining the properties of convex sets with the definition of hyperplanes leads to the Hahn Banach theorem, also known as separating hyperplane theorem, which turns out to be extremely valueable when considering sets of quantum states.

Theorem 2.1 (Separarating Hyperplane Theorem)**.** *Let Z and Y be two convex sets in an affine space $\mathcal{A}$, such that $Z \cap Y = \emptyset$. There exists a hyperplane $H = \{x | a \cdot x = c,\ a \in \mathcal{A}\}$, admiting a linear function $f(x) = a \cdot x - c$ on $\mathcal{A}$ such that*

$$\forall x \in Z,\ f(x) \geq 0 \ \wedge\ \forall x \in Y\ f(x) < 0. \tag{2.7}$$

The hyperplane H is called a separating hyperplane of sets Z and Y [1, 2].

By combining theorem 2.1 with the remark that intersection of convex sets is itself convex, one can deine supporting hyperplanes.

Definition 2.4 (Supporting Hyperplane)**.** Let X be a n-dimensional convex set and let x_0 be a point on one of the q-faces of X where $q < n$. Let $H = \{x | y \cdot x = y \cdot x_0\}$ be a hyperplane such that for all $x \in X$, $y \cdot x \leq x_0$. Such hyperplane H is called a supporting hyperplane of X at point x_0 [2].

Definition 2.5 (Dual of a convex set)**.** Let X be a convex set. The dual X^* of X is defined as

$$X^* = \{y | x \cdot y \geq c,\ \forall x \in X\} \text{ [2]}. \tag{2.8}$$

In some cases investigating duals or supporting hyperplanes at specific points, provides valuable information about the convex set itself.

2.2 Space of quantum states

Being equipped with the notions from the previous section, one can now move on to investigating the sets of quantum states. It is important to keep in mind that many of the sets considered throughout all the chapters are in fact convex. This means that all the properties and definitions from before are still applicable, even if opfuscated by a slightly different notation. For the purpose of the discussion, the state is understood as some form of mathematical representation of knowledge about a quantum system.

Let $\mathcal{H}^n$ be a Hilbert space of dimension n. Each pure quantum state corresponds to a class of normalized vectors in $\mathcal{H}^n$, equivalent up to a phase, and is represented using Dirac notation by a ket

$$|\psi\rangle = \sum_{i=1}^{n} c_i |i\rangle. \tag{2.9}$$

Kets $|i\rangle$ are elements of a basis of $\mathcal{H}^n$ with the inner product defined by $\langle i|j\rangle = \delta_{ij}$. The Hilbert space itself can be a multipartite system i.e. a tensor product of multiple subsystems of lower dimension $\mathcal{H}^{\otimes n}$, in which case a pure state

$$|\psi\rangle = \sum_{i_n} c_{i_n} |i_n\rangle, \tag{2.10}$$

is a sum over a multi-index i_n and $|i_n\rangle$ is a tensor product of the basis vectors of individual subsystems [6]. The naming scheme is not coincidental as one can form convex combinations of pure states and thus explore the complete space of quantum states. These combinations are more straight forward in density matrix formalism, where pure states, represented by projectors

$$\rho = |\psi\rangle\langle\psi|, \tag{2.11}$$

combine into mixed states of the form

$$\rho = \sum_{i=1}^{n} p_i |\psi_i\rangle\langle\psi_i|, \quad \sum_i p_i = 1. \tag{2.12}$$

A matrix $\rho \in \mathcal{L}(\mathcal{H}^n)$ is a density matrix if it is hermitian, positive-semidefinite and trace normalised [1]. These condtitions allow for the definition

$$\mathcal{S}^n = \{\rho | \rho \in \mathcal{L}(\mathcal{H}^n) \ \wedge \ \rho^\dagger = \rho \ \wedge \ \rho \geq 0 \ \wedge \ \mathrm{Tr}(\rho) = 1\} \tag{2.13}$$

of the set of density matrixes of dimension n. The space $\mathcal{L}(\mathcal{H}^n)$ can be equipped with the Hilbert-Schmidt inner product

$$(A, B)_{HS} = \mathrm{Tr}\left(A^\dagger B\right), \quad A, B \in \mathcal{L}(\mathcal{H}^n), \tag{2.14}$$

inducing the same inner product on elements of $\mathcal{S}^n$. From now on, unless relevant, the indecees representing hilbert space dimensions will be dropped.

Definition 2.6. (Positive-semidefinite operator) Let A be an operator acting on hilbert space $\mathcal{H}$. Operator A is positive-semidefinite iff

$$\forall |\psi\rangle \in \mathcal{H}, \quad \langle A \rangle = \langle \psi | A | \psi \rangle \geq 0. \tag{2.15}$$

The set of all positive-semidefinite operators in $\mathcal{L}(\mathcal{H})$ is denoted as $\mathcal{L}^+(\mathcal{H})$. In the language of density matrices one can rephrase the condition for positivity as

$$\langle A \rangle = \mathrm{Tr}\left(A\rho\right) \geq 0, \tag{2.16}$$

for all projectors ρ of the form (2.11).

Remark 1. *Set of positive-semidefinite operators $\mathcal{L}^+(\mathcal{H})$ is a convex cone.*

Proof. Let $A_1, A_2 \in \mathcal{L}^+(\mathcal{H})$ it is clear that:

i) $\forall|\psi\rangle \in \mathcal{H} \wedge \forall\theta \geq 0,\ \langle\psi|\theta A_1|\psi\rangle = \theta\langle\psi|A_1|\psi\rangle \geq 0$; and

ii) $\forall|\psi\rangle \in \mathcal{H} \wedge \theta \in [0,1],\ \langle\psi|(\theta A_1 + (1-\theta)A_2)|\psi\rangle = \theta\langle\psi|A_1|\psi\rangle + (1-\theta)\langle\psi|A_2|\psi\rangle \geq 0.$

□

One can easily see that $\mathcal{S}$ is a convex set by simply considering the convex combination

$$\theta\rho_1 + (1-\theta)\rho_2, \quad \theta \in [0,1] \tag{2.17}$$

of two density matrices, which clearly preserves hermicity, positivity and unit trace. This is equivalent to viewing the set $\mathcal{S}$ as an intersection of the set of positive hermitian matrices and the hyperplane $\{\rho|\operatorname{Tr}(\mathbb{1}\rho) = 1\}$, both individually convex sets yielding a convex intersection. The dimension of $\mathcal{S}^n$ is $n^2 - 1$ with pure states forming a $2n-2$ dimensional subset.

Working in a specific basis one can define an eigenvalue $n-1$-simplex such that

$$\rho = \sum_{i=1}^{n} \lambda_i |i\rangle\langle i|, \tag{2.18}$$

is an element of that simplex, where $|i\rangle$ are basis vectors corresponding to λ_i which add up to one. This eigenvalue simplex forms a $n-1$ dimensional subset of $\mathcal{S}^n$ in which each state is expressed as a diagonal matrix. Each density matrix ρ is an element of some eigenvalue simplex [1]. This is equivalent to saying that a maximal number of pure states required to express any state $\rho \in \mathcal{S}^n$ is equal to n.

Pure states in bipartite systems of the form $\mathcal{H}_A \otimes \mathcal{H}_B$, which will be subjects of later disscussion, admit a Schmidt decomposition

$$|\psi\rangle = \sum_{i=1}^{r} c_i |e_i\rangle \otimes |f_i\rangle \tag{2.19}$$

where $|e_i\rangle$ and $|f_i\rangle$ are the basis vectors of $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively. Coeficients c_i are known as Schmidt coefficients and satisfy $\sum_i^r |c_i|^2 = 1$. The number r is known as the Schmidt rank of the state $|\psi\rangle$ and satisfies $1 \leq r \leq \min(\dim(\mathcal{H}_A), \dim(\mathcal{H}_B))$ [4].

Definition 2.7 (Schmidt Number [15])**.** A density matrix ρ has a schmidt number r if for any decomposition

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \tag{2.20}$$

the rank of at least one of the vectors $|\psi\rangle$ is at least r, and there exists a decomposition where there rank of all vectorst $|\psi_i\rangle$ is at most r.

Examining multipartite pure states of the form (2.10), it is easy to see that not all of them can be expressed as tensor products of individual subsystems. Such states are called entangled states. A good example of that, is a maximally entangled state

$$|\phi^+\rangle = \frac{1}{\sqrt{n}} \sum_i^n |i\rangle|i\rangle. \tag{2.21}$$

in a bipartite system. The name of $|\phi^+\rangle$ suggests that some states can be more entangled than others, however, the strength of the entanglement will not be the subject of this discussion. Entanglement of pure states can be swiftly defined in terms of the Schmidt rank.

Definition 2.8 (Entanglement of pure states [4])**.** A pure state $|\psi\rangle \in \mathcal{H}$ is separable iff its Schmidt rank is equal to 1. Otherwise, the state $|\psi\rangle$ is entangled.

The Schmidt rank of the state (2.21) is equal to the dimension of the hilbert space n, which is always the case for maximally entangled states. In the case of mixed states, the easiest way to define entanglement is to say that all density matrices in n-partite systems that can be expressed in the form

$$\rho = \sum_i p_i \rho_1^i \otimes \rho_2^i \otimes ... \otimes \rho_n^i \tag{2.22}$$

are seperable, and all non separable states are entangled [6]. Following (2.22) it can be seen that the set $\mathcal{S}_{SEP}$ of separable density matrices is convex whereas the set $\mathcal{S}_{ENT}$ of entangled states is not. As an example showing that $\mathcal{S}_{ENT}$ is not convex, one can take a convex combination of two bell states

$$|\phi^\pm\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle \pm |11\rangle\right), \tag{2.23}$$

such that

$$\rho = \frac{1}{2}\left(|\phi^+\rangle\langle\phi^+| + |\phi^-\rangle\langle\phi^-|\right) = \frac{1}{2}\left(|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|\right). \tag{2.24}$$

According to (2.22) such state ρ is separable.

2.3 Space of Maps

The discussion on quantum states would not be complete without mentioning the maps that connect different spaces of density matrices. Let $\mathcal{L}\left(\mathcal{L}(\mathcal{H}_A), \mathcal{L}(\mathcal{H}_B)\right)$ denote the space of maps $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ that take an operator on the hilbert space $\mathcal{H}_A$ and map it onto an operator on $\mathcal{H}_B$. A subset of this space corresponds to a set of physical operations that can be performed on density matrices $\mathcal{S}_A$. Such a physical operation takes a state from $\mathcal{S}_A$ as an input and gives an output in the form of a state from $\mathcal{S}_B$. The space $\mathcal{L}(\mathcal{H}_B)$ can, but does not have to, be of different dimension than $\mathcal{L}(\mathcal{H}_A)$. As one can imagine, these requirements provide some restrictions on the subset of maps that represent physical operations. Let A be an operator acting on $\mathcal{H}_A$. A map $\Phi \in \mathcal{L}\left(\mathcal{L}(\mathcal{H}_A), \mathcal{L}(\mathcal{H}_B)\right)$ connects spaces of density matrices $\mathcal{S}_A$ and $\mathcal{S}_B$, if it satisfies

1) $(\Phi(A))^\dagger = \Phi(A^\dagger)$,

2) $\mathrm{Tr}(\Phi(A)) = \mathrm{Tr}(A)$

3) and $\Phi(A) \geq 0,\ \forall A \geq 0$ [1, 4].

Maps satisfying condition 1) are known as hermicity preserving. Condition 2) defines trace-preserving maps and condition 3) is called positivity. The set of of positive maps Φ is denoted as $\mathcal{P}$.

Remark 2. *All maps $\Phi \in \mathcal{P}$ are hermicity-preserving.*

When performing physical operations on quantum states, it should generally be possible to arbitrarily extend the dimension of the system. After such an extension, a physical operation on an input quantum state should still yield a physical state. Hence, a map representing such operations has to possess a similiar property, leading to the requirement of complete positivity.

Definition 2.9 (Complete positivity [4])**.** Let $\Phi \in \mathcal{L}\left(\mathcal{L}(\mathcal{H}_A), \mathcal{L}(\mathcal{H}_B)\right)$ be a positive, trace-preserving map. If an extension

$$\Phi \otimes \mathbb{1}_k : \mathcal{L}(\mathcal{H}_A^n) \otimes \mathbb{C}^{k\times k} \to \mathcal{L}(\mathcal{H}_B^n) \otimes \mathbb{C}^{k\times k} \tag{2.25}$$

is a positive map for any dimension n, then Φ is completely positive. A map ϕ with a positive extension (2.25) for dimension k is k-positive. The set of completely positive maps and k-positive maps is denoted as $\mathcal{CP}$ and $\mathcal{P}^k$ respectively. The definition is a restriction on the set of positive maps, so it follows that $\mathcal{CP} \subset \mathcal{P}$.

An importat observation, which allows for additional criteria for positivity and complete positivity of maps, is that the space $\mathcal{L}\left(\mathcal{L}(\mathcal{H}_A), \mathcal{L}(\mathcal{H}_B)\right)$ is isomorphic to $\mathcal{L}\left(\mathcal{H}_{AB}\right)$ i.e. the space of operators acting on the bipartite system $\mathcal{H}_A \otimes \mathcal{H}_B$ of dimension $n = \dim(\mathcal{H}_A) \cdot \dim(\mathcal{H}_B)$.

Definition 2.10 (Choi-Jamiołkowski isomorphism [4, 13])**.** Let $\Phi \in \mathcal{L}\left(\mathcal{L}(\mathcal{H}_\mathcal{A}), \mathcal{L}(\mathcal{H}_\mathcal{B})\right)$ and let $|\phi^+\rangle$ be a maximally entangled state (2.21) in $\mathcal{H}_A^{\otimes 2}$. Choi-Jamiołkowski isomorphism is a map

$$\mathcal{J} : \mathcal{L}\left(\mathcal{L}(\mathcal{H}_\mathcal{A}), \mathcal{L}(\mathcal{H}_\mathcal{B})\right) \ni \Phi \mapsto \left(\mathbb{1}_A \otimes \Phi\right) |\phi^+\rangle\langle\phi^+| \in \mathcal{L}(\mathcal{H}_{AB}), \tag{2.26}$$

where $\mathcal{J}(\Phi)$ is often expressed as a matrix C_Φ and called the Choi matrix.

Remark 3. *The Choi-Jamiołkowski isomorphism $\mathcal{J} : \mathcal{L}\left(\mathcal{L}(\mathcal{H}_\mathcal{A}), \mathcal{L}(\mathcal{H}_\mathcal{B})\right) \to \mathcal{L}(\mathcal{H}_{AB})$ is an isometry, that is*

$$(\Phi, \Psi) = (\mathcal{J}(\Phi), \mathcal{J}(\Psi)) \tag{2.27}$$

for any Φ and Ψ in $\mathcal{L}\left(\mathcal{L}(\mathcal{H}_\mathcal{A}), \mathcal{L}(\mathcal{H}_\mathcal{B})\right)$ [13].

It is easy to see that if Φ is a physical operation on states in $\mathcal{S}_A$ then its image under $\mathcal{J}$ is a state in bipartite system $\mathcal{S}_{AB}$. This is equivalent to saying that the space of physical operations, acting on an input system and resulting in some output, is isomorphic to a tensor product of the input and the output systems [8]. Another characteristic akin to positivity of operators, which is relevant when considering bipartite systems, is block positivity.

Definition 2.11 (Block-positivity)**.** Let A be an operator acting on bipartite system $\mathcal{H}_{AB}$, of the form $\mathcal{H}_A \otimes \mathcal{H}_B$. Operator A, such that

$$\forall v \in \mathcal{H}_A \wedge \forall w \in \mathcal{H}_B, \quad \langle v \otimes w | A | v \otimes w \rangle \geq 0, \tag{2.28}$$

is called block-positive. Let $\mathcal{L}^{B+}(\mathcal{H})$ denote the set of block-positive operators acting on $\mathcal{H}$.

From definitions 2.6 and 2.11 it should be clear that $\mathcal{L}^{B+}(\mathcal{H}) \subset \mathcal{L}^{+}(\mathcal{H})$. The property of block-positivity will be crucial when defining entanglement witnesses. The notion can be easily generalized, if needed, for other multipartite systems comprising more that two subsystems. Analysis of Choi matrices C_Φ from definition 2.10 allows for the following theorems on maps Φ.

Theorem 2.2 (Jamiołkowski's theorem [7])**.** *A map $\Phi \in \mathcal{L}\left(\mathcal{L}(\mathcal{H}_\mathcal{A}), \mathcal{L}(\mathcal{H}_\mathcal{B})\right)$ is positive if and only if the coresponding $C_\Phi \in \mathcal{L}^{B+}(\mathcal{H}_{AB})$.*

Theorem 2.3 (Choi's theorem [3])**.** *A map $\Phi \in \mathcal{L}\left(\mathcal{L}(\mathcal{H}_\mathcal{A}), \mathcal{L}(\mathcal{H}_\mathcal{B})\right)$ is completely positive if and only if the coresponding $C_\Phi \in \mathcal{L}^{+}(\mathcal{H}_{AB})$.*

Following the definition 2.5 and remark 3 it is now possible to find the duals of sets $\mathcal{P}$ and $\mathcal{CP}$. The dual set of completely positive maps is defined as

$$\mathcal{CP}^* = \{\Phi | (\Psi, \Phi) \geq 0, \forall \Psi \in \mathcal{CP}\}, \tag{2.29}$$

where $(\Psi, \Phi) = \mathrm{Tr}\left\{C_\Psi^\dagger C_\Phi\right\} = \mathrm{Tr}\{C_\Psi C_\Phi\}$ is greater than zero if both Choi matrices are positive. Hence, Φ is also completely positive and the set $\mathcal{CP}$ is self dual meaning $\mathcal{CP} = \mathcal{CP}^*$. In the case of positive maps one defines the set

$$\mathcal{SP} = \mathcal{P}^* = \{\Phi | (\Psi, \Phi) \geq 0, \forall \Psi \in \mathcal{P}\} \tag{2.30}$$

of super positive maps [1]. The condition (2.30) implies that the set of super positive maps is isomorphic to the set of Choi matrices whose inner product with block positive matrices is nonnegative.

3. Section 3

3.1 First Look at Entanglement Witnesses

Following the discussion on quantum states one can now dive into the problem directly related to entanglement witnesses, that is, distinguishing between the separable and entangled states. In the following sections, the focus will be on bipartite systems, and only some of the notions can be generalized for other multipartite states. In section 2.2 it was discussed how the set of density matrices $\mathcal{S}_{\mathcal{AB}}$ is a convex subset of $\mathcal{L}(\mathcal{H}_{AB})$, with the subset of separable states being convex itself. The main idea behind separability criteria discussed here, will be examining how a particular state behaves under the action of specific operators.

The first separability criteria comes via entanglement witnesses. One can easily get the intuition behind them, by considering the theorem 2.1 which implies that it should be possible to find an operator in $\mathcal{L}(\mathcal{H}_{AB})$ and construct a hyperplane, separating the set of density matrices containing separable states, from the rest. This notion was consisely expressed in [5] by the following witness lemma.

Lemma 1. *For any entangled state $\rho \in \mathcal{S}_{AB}$ there exists an operator X such that*

$$\mathrm{Tr}(X\rho) < 0 \quad \wedge \quad \mathrm{Tr}(X\sigma) \geq 0 \tag{3.1}$$

for any separable $\sigma \in \mathcal{S}_{AB}$.

The lemma folows directly from the separating hyperplane theorem with space $\mathcal{L}(\mathcal{H}_{AB})$ being equipped with the Hilbert-Schmidt inner product (2.14). The basic idea is illustraded on figure 1, where the line representing the hyperplane separates the convex set S_{SEP} from a clearly convex set of single entangled state ρ_{ENT}. Opperators satisfying (3.1) for at least one entangled state ρ are called entanglement witnesses.

Definition 3.1 (Entanglement Witness [14, 4])**.** An operator $X \in \mathcal{L}(\mathcal{H}_{AB})$ is an entanglement witness iff $X \in \mathcal{L}^{B+}(\mathcal{H}_{AB})$ and $X \notin \mathcal{L}^{+}(\mathcal{H}_{AB})$. Let $\mathcal{W}$ denote the set of entanglement witnesses i.e. the set of block-positive but not positive semidefinite operators in $\mathcal{L}(\mathcal{H}_{AB})$.

One can also require entanglement witnesses to be trace normalized. Such a restriction allows for a convinient justification of the definition 3.1. The condition of block positivity ensures that entanglement witnesses transform all seperable density matrices into density matrices. Not being positive semidefinite ensures that not all entangled states are transformed into states. Hence, it follows that matrices in $\mathcal{W}$ are the ones satisfying the witness lemma.

Considering theorems 2.2 and 2.3 one can see that the set $\mathcal{W}$ is isomorphic to the set of positive but not completely positive maps $\Phi \in \mathcal{L}\left(\mathcal{L}(\mathcal{H}_{\mathcal{A}}), \mathcal{L}(\mathcal{H}_{\mathcal{B}})\right)$. Moreover, the set of separable states represented by σ in lemma 1 satisfies the same condition as the set of states, isomorphic to super positive maps defined in (2.30). Hence, one can conclude that the set $\mathcal{S}_{SEP}^{AB} \subset \mathcal{L}(\mathcal{H}_{AB})$ is isomorphic to the set of maps $\mathcal{SP} \subset \mathcal{L}(\mathcal{L}(\mathcal{H}_{A}), \mathcal{L}(\mathcal{H}_{B}))$. Connection between entanglement witnesses and positive maps ties in to the second separability criterion.

Theorem 3.1 (Positive but not completetly positive maps [5])**.** *Let ρ be a density matrix representing a sate in a bipartite system $\mathcal{H}$. The state ρ is separable iff*

$$(\mathbb{1} \otimes \Phi)\rho \in \mathcal{L}^{+}(\mathcal{H}) \tag{3.2}$$

for all $\Phi \in \mathcal{P} \setminus \mathcal{CP}$.

Proof. Let $\Phi \in \mathcal{L}\left(\mathcal{L}(\mathcal{H}_{B}), \mathcal{L}(\mathcal{H}_{B'})\right)$ be positive but not completely positive. If $\rho_{AB} \in \mathcal{S}_{SEP}$ then from (2.22)

$$(\mathbb{1} \otimes \Phi)\rho_{AB} = \sum_i p_i \rho_A^i \otimes \Phi(\rho_B^i) \overset{(i)}{=} \sum_i p_i \rho_A^i \otimes \tilde{\rho}_{B'}^i = \tilde{\rho}_{AB'} \in \mathcal{L}^{+}(\mathcal{H}), \tag{3.3}$$

where $\tilde{\rho}$ represents a possibly unnormalized density matrix. The equality (i) follows straight from the positivity of the map Φ. Let σ be a density matrix such that $(\mathbb{1}\otimes\Phi)\sigma \in \mathcal{L}^{+}(\mathcal{H}_{AB'})$ for all $\mathcal{P}$ but not $\mathcal{CP}$ maps Φ. From (2.16) it follows that $((\mathbb{1}\otimes\Phi)\sigma, |\psi\rangle\langle\psi|) = (\sigma, (\mathbb{1}\otimes\Phi)^{\dagger}|\psi\rangle\langle\psi|) \geq 0$. Choosing $|\psi\rangle = |\phi^{+}\rangle$ from (2.21) results in a Choi matrix $C_{\Phi^{\dagger}}$ satisfying the definition 3.1 of an entanglement witness. Now, according to lemma 1 if $(\sigma, C_{\Phi^{\dagger}}) = \mathrm{Tr}\{\sigma C_{\Phi^{\dagger}}\} \geq 0$ for any entanglement witness $C_{\Phi^{\dagger}}$, then σ is not an entangled state. □

Criterion via positive but not completely positive maps is both necessary and sufficient for all bipartite systems, however, it is not operational as the characterization of such maps still constitutes an open problem.

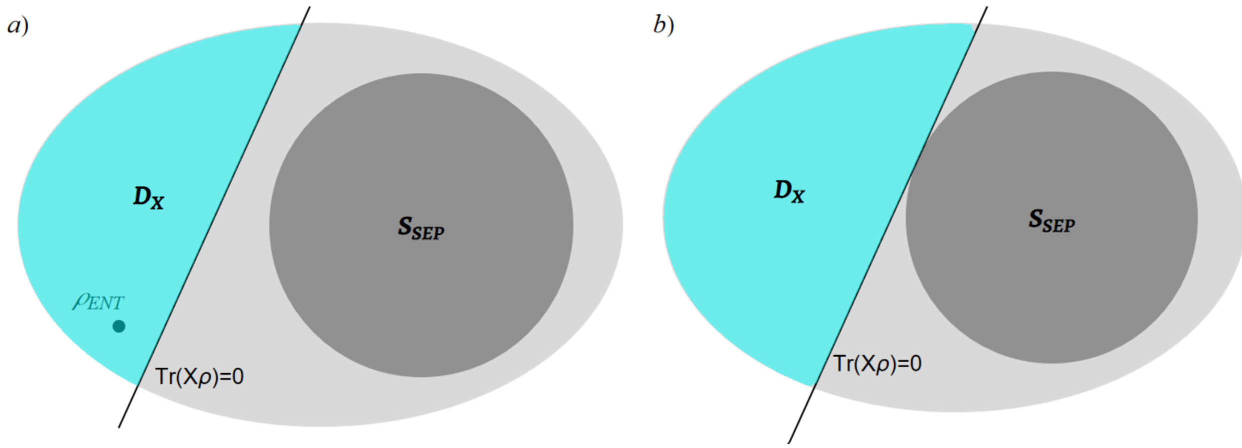

Figure 1: Diagram a) represents the set of quantum states. Subset $\mathcal{S}_{SEP}$ of separable states is separatated from state ρ_{ENT} by a hyperplane constructed by entanglement wtness X. Subset D_X represents all entangled states detected by X. Diagram b) analogous situation, except X is now an optimal entanglement witness. There exists no witness Y such that $D_X \subset D_Y$.

3.2 Positive partial transpose

An interesting conclusion from the discussion on positive but not completely positive maps is that each single map of this type admits a necessary criterion (3.2) for separability. As one can imagine some maps admit a stronger criterion than others. In this context being strongest can be intuitively understood as preserving positivity for the smallest subset of $\mathcal{S}$ containing the set of separable states. A prominent example of such a map is a transposition $T : \mathcal{L}(\mathcal{H})) \to \mathcal{L}(\mathcal{H})$ which is both positive and trace preserving. By applying it to only one of the subsystems one can define the partial transpose

$$\mathbb{1}_A \otimes T_B : \mathcal{L}(\mathcal{H}_{AB}) \to \mathcal{L}(\mathcal{H}_{AB}), \quad (\mathbb{1}_A \otimes T_B)(A \otimes B) = A \otimes B^T. \tag{3.4}$$

By applying partial transposition to the elements of $\mathcal{S}^{AB}$, one can divide the states into two subsets. The first one, denoted as $\mathcal{S}_{PPT}$ contains states which transform into states under partial transposition. Similarly one can define the set $\mathcal{S}_{NPT}$, containing all the density matrices that do not remain positive under partial transpose. PPT in this context stands for positive partial transpose. This of course defines a criterion for separability.

Theorem 3.2 (PPT criterion [11])**.** *If a density matrix $\rho \in \mathcal{S}$ is separable, then $\rho \in \mathcal{S}_{PPT}$, or equivalently $\rho^{T_A} \geq 0$, where T_A represents the partial transpose with respect to one of the subsystems. Conversely, if a density matrix $\sigma \in \mathcal{S}_{NPT}$, implying that σ^{T_A} is not positive semidefinite, then σ reprents an entangled state.*

Mixing two PPT states in itself results in a PPT state and hence the set $\mathcal{S}_{PPT}$ is convex. Remarkably, for low dimensional bipartite systems i.e. $\mathcal{H}^2 \otimes \mathcal{H}^2$ and $\mathcal{H}^2 \otimes \mathcal{H}^3$ PPT provides a both necessary and sufficient condition.

Theorem 3.3 (Peres-Horodeccy criterion [5])**.** *A density matrix ρ acting on $\mathcal{H}^2 \otimes \mathcal{H}^2$ or $\mathcal{H}^2 \otimes \mathcal{H}^3$ is separable if and only if $\rho^{T_A} \geq 0$.*

3.3 Coming Back to Entanglement Witnesses

As celebrated PPT criterion is, it does not necessarily do the trick for bipartite systems of higher dimensions. It is still, however, a very strong starting point, with the remaining problem being determining which of the states in $\mathcal{S}_{PPT}$ are entangled. The problem itself is unfortunately not easy to solve. However, one of the tools aiding the progress are entanglement witnesses. A valuable distinction, when examining PPT states, is between decomposable and nondecomposable witnesses.

Definition 3.2 (Decomposable Entanglement Witnesses [9])**.** An entanglement witness $X \in \mathcal{W} \subset \mathcal{L}(\mathcal{H})$ is decomposable if it can be expressed as

$$X = aA + (1-a)B^T, \tag{3.5}$$

where $a \in [0,1]$ and A, B are positive operators in $\mathcal{L}(\mathcal{H})$.

As it turns out decomposable entanglement witnesses cannot detect entangled PPT states [9]. Hence, entanglement witnesses of the most interest are nondecomposable ones, i.e. those that cannot be expressed as (3.5). As proven in [17], all operators acting on $\mathcal{H}^2 \otimes \mathcal{H}^2$ or $\mathcal{H}^2 \otimes \mathcal{H}^3$ are decomposable, meaning one can only construct decomposable entanglement witnesses acting on these spaces. Such an observation is not surprising, as for the same reason all PPT states in 2×2 and 2×3 systems are separable. Another phrasing of the same statement is that there are no nondecomposable witnesses in 2×2 or 2×3 systems as there are no entangled PPT states to detect. Another handy definition when characterizing entanglement witnesses is a set

$$D_X = \{\rho | \operatorname{Tr}(X\rho) < 0,\ \rho \in \mathcal{S}\} \tag{3.6}$$

containing all entangled states detected by a witness X. This allows for introduction of a relation between two witnesses.

Definition 3.3 (Optimal Entanglement Witness [9])**.** Let X_1 and X_2 be two entanglement witnesses in $\mathcal{W}$. One says that X_1 is finer than X_2 if $D_{X_2} \subset D_{X_1}$. An operator X is an optimal entanglement witness if there is no entaglement witness finer than X.

The idea behind an optimal entanglement witness is illustrated on figure **??**. Let X_1 be a non optimal entanglement witness. In theory, it is always possible to construct an entanglement witness finer than X_1, by subtracting from it some positive-semidefinite operator multiplied by a factor $\epsilon > 0$ [9]. However, even assuming that one has found a suitable operator to subtract, determining whether the result is still an entanglement witness is not a trivial task. This leads to the main problem addressed in this thesis: how to check if an operator is an entanglement witness?

Restating the definition 3.1, an operator X is an entanglement witness if it is block-positive but not positive-semidefinite. Positivity of an operator is equivalent to the positivity of its spectrum, hence, any witness has at least one negative eigenvalue. Applying this logic, one can examine the characteristic equation of an operator

$$\det(\lambda \mathbb{1} - X) = \lambda^N - s_1\lambda^{N-1} + s_2\lambda^{N-2} - ... + (-1)^N s_N = 0. \tag{3.7}$$

In order for X to be an entanglement witess, it has to be hermitian and hence, diagonalizable. In the diagonal form all coefficients s_i in the characteristic equation are just products of eigenvalues of X. This leads to a condition for positive semidefinite matrices.

Proposition 3.1. A hermitian matrix X is positive semidefinite if all coefficients s_i in its characteristic equation (3.7) are nonnegative. The proposition still holds if X is not in a diagonal basis. In such a case the coefficients take form of

$$\begin{gathered} s_1 = \operatorname{Tr} X,\ s_2 = \tfrac{1}{2}(s_1 \operatorname{Tr} X - \operatorname{Tr} X^2), \\ s_k = \tfrac{1}{k}(s_{k-1} \operatorname{Tr} X - s_{k-2} \operatorname{Tr} X^2 + ... + (-1)^{k-1} \operatorname{Tr} X^k).\ [1] \end{gathered} \tag{3.8}$$

Another way of obtaning similar positivity conditions for hermitian matrices is by finding their principal minors, which are positive if hermitian X is positive-semidefinite.

Proposition 3.2. A 2×2 hermitian matrix A is positive semidefinite iff

$$\operatorname{Tr}(A) \geq 0\ \wedge \det(A) \geq 0. \tag{3.9}$$

Proof. Substituting elements of a 2×2 matrix A into the coefficient s_2 in (3.8) results in the determinant of A. □

Conditions for block-positivity of an operator turn out to be more complicated. One can however, slightly rephrase definition 2.11 of block-positivity.

Proposition 3.3. Let X be an operator in $\mathcal{L}(\mathcal{H}^k \otimes \mathcal{H}^l)$ and w be an element of $\mathcal{H}^k$. One can define an operator $X_w \in \mathcal{L}(\mathcal{H}^l)$, such that

$$(X_w)_{ii'} = X_{ij,i'j'} \overline{w}_j w_{j'}, \tag{3.10}$$

where w_i represent components of w. The operator X is block-positive if for all $w \in \mathcal{H}^k$, thus defined matrix X_w is positive-semidefinite.

One can instead define a matrix X_v with v being an element of $\mathcal{H}^l$, yielding analogous requirements for block-positivity. The proposition 3.3 can be understood as changing the problem from checking if an operator X has a positive expectation value for all product states, into checking if all possible possible operators X_w are positive-semidefinite. This approach does not immediately solve the problem. However, it allows for application of already known criteria for positivity, e.g. the ones from proposition 3.1. One can now define entanglement witnesses as follows.

Proposition 3.4. An operator $X \in \mathcal{L}(\mathcal{H}_{AB})$ is an entanglement witness if and only if

$$X \notin \mathcal{L}^+(\mathcal{H}_{AB})\ \wedge\ \forall w \in \mathcal{H}_A,\ X_w \in \mathcal{L}^+(\mathcal{H}_B). \tag{3.11}$$

The aim of the following sections is to present an algorithm, which determines if a given matrix X satisfies the conditions from (3.11). The algorithm is meant to answer the question for the system of lowest dimension, that is a system $\mathcal{H}^2 \otimes \mathcal{H}^2$ of two qubits. The rest of this section is dedicated to setting up the problem precisely.

Let $X_{ii',jj'}$ denote the elements of the matrix X, which in the considered case is 4×4. For X to be considered an entanglement witness, it has to be hermitian and not positive-semidefinite. Assuming that one knows the elements of X both of these conditions can be easily checked. The difficult part of the problem is checking if the matrix X_w is positive-semidefinite for all $w \in \mathcal{H}^2$. Setting $w_1 = x$ and $w_2 = y$, one obtains

$$X_w = \left[\begin{array}{cc} |x|^2 X_{11,11} + \overline{x}y X_{11,12} + & |x|^2 X_{11,21} + \overline{x}y X_{11,22} + \\ +\overline{y}x X_{12,11} + |y|^2 X_{12,12} & +\overline{y}x X_{12,21} + |y|^2 X_{12,22} \\ \hline |x|^2 X_{21,11} + \overline{x}y X_{21,12} + & |x|^2 X_{21,21} + \overline{x}y X_{21,22} + \\ +\overline{y}x X_{22,11} + |y|^2 X_{22,12} & +\overline{y}x X_{22,21} + |y|^2 X_{22,22} \end{array}\right], \tag{3.12}$$

which is a 2×2 hermitian matrix, as $\overline{X_{ij,i'j'}} = X_{i'j',ij}$ follows from hermicity of X. Now, one can pose the problem in a way that can be directly adressed by the algorithm.

Proposition 3.5. An operator $X \in \mathcal{L}(\mathcal{H}^2 \otimes \mathcal{H}^2)$ is an entanglement witness if and only if

i) X is a hermitian matrix;

ii) X is not positive semidefinite; and

iii) $\forall w \in \mathcal{H}^2,\ \mathrm{Tr}(X_w) \geq 0 \wedge \det(X_w) \geq 0$.

Proof. Condition iii) follows from the proposition 3.2 □

4. Detour on polynomials

4.1 Preliminaries

The purpose of this subsection is to familiarize the reader with some of the properties of polynomials, particularly focusing on their nonnegativity conditions. Although the detour might seem unnecessary at first, the theorems and methods presented here, make a comeback in the section 5.

Let f denote an univariate real polynomial of n-th degree. Each polynomial of this type can be expressed as

$$f(t) = \sum_{i=0}^{n} a_i t^i = g(t) \prod_{i}^{d} (t - \lambda_i)^{n_i}, \tag{4.1}$$

where g is a polynomial with no real roots, d is a number of real roots of f and n_i denotes multiplicity of i-th real root λ_i. One can find the greatest common divisor of any two polynomials by aplying the well known Euclidean algorithm.

Definition 4.1 (Euclidean algorithm for univariate polynomials [16])**.** Let f_0 and f_1 denote two real, univariate polynomials such that the degree of f_0 is greater or equal to the degree of f_1. Dividing f_0 by f_1 results in a remainder f_2 and a quotient q_1 satisfying

$$f_0(t) = f_1(t) q_1(t) + f_2(t). \tag{4.2}$$

Repating the step for f_1, f_2 and then subsequent remainders, results in sequences of quotients $\{q_i\}$ and remainders $\{f_i\}$. The elements of the sequences satisfy

$$f_k(t) = f_{k+1}(t)q_{k+1}(t) + f_{k+2}(t), \quad k = 0, 1, ..., p-1, \tag{4.3}$$

where f_p is the last non zero remainder in a sequence and hence, the greatest common divisor of f_0 and f_1, which is denoted as $f_p = \gcd(f_0, f_1)$.

Proposition 4.1. The gcd of a polynomial f from (4.1) and its derivative f' is given by

$$f_p(t) = \mathcal{N} \prod_i^d (t - \lambda_i)^{n_i - 1}, \tag{4.4}$$

where $\mathcal{N}$ is some proportionality constant.

Proof. Follows straight from differentiating (4.1). □

The proposition 4.1 stems from the fact that the multiple roots of a polynomial are passed onto its derivative, with their multiplicities reduced by one. The roots of the polynomial (4.4) are the multiple roots of f with same multiplicities as in the derivative f'. For f with only single roots the $\gcd(f, f')$ is a zeroth degree polynomial.

Proposition 4.2. For a polynomial f with roots of any multiplicity, one can construct

$$\tilde{f}(t) = f(t)/\gcd(f(t), f'(t)) = \tilde{g}(x) \prod_i^d (x - \lambda_i), \tag{4.5}$$

which is a polynomial with all the roots of f reduced to single multiplicity.

Proof. Follows straight from poroposition 4.1. □

Definition 4.2 (Sturm sequence [16])**.** Let f_0 be a polynomial with only single roots and let f_1 be its derivative f_0'. A Sturm sequence is a chain of polynomials

$$S = \{p_i(t)\} = \{f_0(t), f_1(t), -f_2(t), -f_3(t), f_4(t), f_5(t), -f_6(t), -f_7(t), ...\}, \tag{4.6}$$

where f_i denote polynomials obtained from applying Euclidean algorithm to f_0 and f_1. The last element of the sequence is p_n, with n being the degree of polynomial f_0.

Theorem 4.1 (Sturm theorem [16])**.** *Let f be a real, univariate polynomial with only single roots, and let S be its Sturm sequence. Let $N(t)$ denote the number of variations, i.e. number of sign changes in the sequence S evaluated at point t. For any real numbers a, b, such that $a < b$, $f(a) \neq 0$ and $f(b) \neq 0$, the number of roots of f in the interval (a, b) is equal to $N(a) - N(b)$.*

4.2 Nonnegativity conditions for polynomials

One can determine whether a polynomial is nonnegative on some interval of its domain by investigating the number and multiplicities of its roots. Nonnegativity and positivity conditions for low degree polynomials were derived and consisely summarized in [12]. As it turns out, some of those criteria will be relevant for 2×2 entanglement witnesses. In most nonnegativity conditions presented here, unless stated otherwise, it is assumed that the polynomial is of even degree and has positive leading and free coefficients.

Of particular interest, are the nonnegativity conditions of quartic polynomials

$$g(t) = a_4t^4 + a_3t^3 + a_2t^2 + a_1t + a_0 \tag{4.7}$$

for all real t. For that purpose one can find

$$f(t) = t^4 + \alpha t^3 + \beta t^2 + \gamma t + 1 \tag{4.8}$$

with coefficients defined as

$$\alpha = a_3a_4^{-\frac{3}{4}}a_0^{-\frac{1}{4}},\ \beta = a_2a_4^{-\frac{1}{2}}a_0^{-\frac{1}{2}},\ \gamma = a_1a_4^{-\frac{1}{4}}a_0^{-\frac{3}{4}}. \tag{4.9}$$

The discriminant of such f is given by

$$\Delta(f) = 4[\beta^2 - 3\alpha\gamma + 12]^3 - [72\beta + 9\alpha\beta\gamma - 2\beta^3 - 27\alpha^2 - 27\gamma^2]^2. \tag{4.10}$$

Theorem 4.2 (Nonnegativity conditions of a quartic polynomial [12])**.** *Suppose that $g(t)$ is a quartic polynomial with real coefficients expressed as in (4.7), such that $a_4 > 0$ and $a_0 > 0$. Let the coresponding polynomial $f(t)$ be defined as in (4.8), (4.10) and (4.9). Then $g(t) \geq 0$ and $f(t) \geq 0$ for all real t iff $\Delta(f) \geq 0$, $|\alpha - \gamma| \leq 4\sqrt{\beta + 2}$ and either*

i) $-2 \leq \beta \leq 6$; or

ii) $\beta > 6$ and $|\alpha + \gamma| \leq 4\sqrt{\beta - 2}$.

Proposition 4.3. Suppose that $g(t)$ is a quartic polynomial satisfying

$$a_3 = -a_1 \quad \text{and} \quad a_4 = a_0 > 0, \tag{4.11}$$

that is $g(t) = a_4t^4 + a_3t^3 + a_2t^2 - a_3t + a_4$ and $f(t) = t^4 + \alpha t^3 + \beta t^2 - \alpha t + 1$. For such a polynomial, conditions in theorem 4.2 simplify to $f(t) \geq 0$ for all real t iff

$$|\alpha| \leq 2\sqrt{\beta + 2} \ \wedge \ -2 \leq \beta. \tag{4.12}$$

Proof. Assuming that $g(t)$ satisfies requirements considered in the proposition, one obtains the discriminant

$$\Delta(f) = 27\frac{(4a_3^3 - 4a_0a_2 - 8a_0^2)^2((2a_0 - a_2)^2 + 4a_3^2)}{a_0^6}, \tag{4.13}$$

which is always nonnegative. Condition $|\alpha + \gamma| \leq 4\sqrt{\beta + 2}$ simplifies to $0 \leq 4\sqrt{\beta + 2}$ and is always satisfied when $\beta > 6$. □

For polynomials of higher degree than 4-th, one can determinine if $f(t) \geq 0$ for a given interval (a, b) with the help of Sturm sequences. The first and obvious requirement is that the polynomial has to be nonnegative at the ends of the interval i.e. $f(a) \geq 0$ and $f(b) \geq 0$. One can find the number of roots d_1 of a polynomial $f(t)$ on a given interval, by applying the Sturm theorem to the corresponding $\tilde{f}(t)$ defined in proposition 4.2. If $d_1 = 0$ then $f(t) \geq 0$ for $t \in (a, b)$. Otherwise, the question comes down to finding multiplicities of the roots of $f(t)$ in (a, b). Polynomial satisfies $f(t) \geq 0$, if considered roots are of even multiplicity. By setting $f_2 = \gcd(f, f')$ one can again find the number of its roots d_2, by applying Sturm theorem to $\tilde{f}_2$. Following the proposition 4.1, f_2 has only multiple roots of f, with their multiplicities reduced by one. Hence, d_2 is the number of multiple roots of f. Repeating the procedure for $f_k = \gcd(f_{k-1}, f'_{k-1})$ until $d_k = 0$, results in a sequence of numbers

$$d = \{d_1, d_2, ...\}. \tag{4.14}$$

Proposition 4.4. Suppose that f is a real, univariate polynomial and d is a p-element sequence constructed as in (4.14). Then $f(t) \geq 0$ for $t \in (a, b)$ if and only if $f(a) \geq 0$, $f(b) \geq 0$ and for all even $k \leq p$, the elements of the sequence d satisfy $d_k = d_{k-1}$. In particular, $f(t) \geq 0$ for all $t \in \mathbb{R}$ iff the degree n of f is even, the leading coefficient $a_n > 0$ and $d_k = d_{k-1}$ for all even $k \leq p$.

An element d_i of the sequence d corresponds to the number of roots of polynomials f_i and $\tilde{f}_i$, with the latter having only roots of single multiplicity. If $d_k = d_{k+1}$ then $\tilde{f}_k$ and $\tilde{f}_{k+1}$ have the same roots. If $d_k > d_{k+1}$, then the polynomial f has some roots of multiplicity k, that are single roots of f_k and no longer appear in f_{k+1}. Hence, one can construct polynomials

$$\delta f_k = \frac{\tilde{f}_k}{\tilde{f}_{k+1}}, \quad k = 1, 2, ..., \tag{4.15}$$

with only single roots, corresponding to the roots of f with multiplicity k. From this follows another polynomial of the form

$$\sigma_f = \prod_{k=0} \delta f_{2k+1}, \tag{4.16}$$

which comprises all odd multiplicity roots of f. Polynomial (4.16) should have only single roots and hence can be checked by a single run of Sturm theorem.

4.3 Logical formulas on polynomials

Being able to evaluate statements such as

$$f(t) \geq 0, \quad t \in (a, b) \tag{4.17}$$

allows one to check more complicated logical formulas of the form

$$\Theta(g_1(t) \geq 0, g_2(t) \geq 0, ..., g_n(t) \geq 0),\ t \in (a, b), \tag{4.18}$$

where g_i are univariate real polynomials. Operations such as negation

$$\neg(g(t) \geq 0), \quad t \in (a, b) \Leftrightarrow -g(t) > 0, \quad t \in (a, b) \tag{4.19}$$

and conjuntion

$$g_1(t) \geq 0 \ \wedge \ g_2(t) \geq 0, \quad t \in (a, b) \tag{4.20}$$

are easy to check as the former requires only a single application of Sturm theorem and the latter comes down to checking individual statements separately. In order to evaluate the alternative

$$g_1(t) \geq 0 \ \vee \ g_2(t) \geq 0, \quad t \in (a, b), \tag{4.21}$$

one needs to apply a slightly different approach.

First, assume that the interval (a, b) is divided into smaller intervals by a set of l ordered points $t_1 < t_2 < ... < t_l$, such that in each interval (t_i, t_{i+1}) there is at most one sign flip for each polynomial g. The method for finding a suitable set of such points is presented in algorithm 1. One can now evaluate the statement (4.21) by checking signs of g_1 and g_2 at the ends of each interval (t_i, t_{i+1}). All possible combinations of endpoint signs on a interval, are presented in table 1. In cases 1-7, either $\mathrm{sgn}(g_1(t_i)) = \mathrm{sgn}(g_1(t_{i+1}))$ or $\mathrm{sgn}(g_2(t_i)) = \mathrm{sgn}(g_2(t_{i+1}))$ are positive. This means that the interval is valid and the procedure moves on to checking the next one. Cases 10-16 are not valid so condition (4.21) doesn't hold, as for at least one of the boundaries both g_1 and g_2 are negative.

Case	$g_1\,(t_i)$	$g_2\,(t_i)$	$g_1\,(t_{i+1})$	$g_2\,(t_{i+1})$
1	+	+	+	+
2	+	+	+	−
3	+	+	−	+
4	+	−	+	+
5	−	+	+	+
6	−	+	−	+
7	+	−	+	−
8	**+**	**−**	**−**	**+**
9	**−**	**+**	**+**	**−**
10	+	+	−	−
11	−	−	+	+
12	+	−	−	−
13	−	+	−	−
14	−	−	+	−
15	−	−	−	+
16	−	−	−	−

Table 1: Possible sign combinations of polynomials g_1 and g_2 at the endpoints of the interval (t_i, t_{i+1}), when there is at most one sign change for each polynomial.

In cases 8 and 9 the outcome depends on which of the polynomials changes its sign first, so they require more investigation. In order to answer this question one can start with finding the number of roots of

$$\gcd(\sigma_{g_1}, \sigma_{g_2}) \tag{4.22}$$

in the interval (t_i, t_{i+1}), where olynomials σ_{g_i} are defined as in (4.16). This can be done using Sturm theorem. If the outcome is one, then g_1 and g_2 have a common root and the

Algorithm 1 Algorithm in *Mathematica* returning a mesh of l points $\{t_1, ..., t_l\}$, such that on each interval (t_i, t_{i+1}) polynomials g_1 and g_2 have at most one root.

Input:

- g_1, g_2 - real, nonzero, univariate polynomials.
- a, b - real numbers, such that $a < b$ and g_1 and g_2 have no roots on $(-\infty, a]$ and $[b, +\infty)$.

Output:

- $\{t_1, t_2, ..., t_l\}$ - mesh of points, such that g_1, g_2 have no roots for $t < t_1$ or $t > t_l$, none of t_i's is a root of g_1 or g_2, and on each interval (t_i, t_{i+1}) there is at most one root of g_1 or g_2.

```
In[1]:= (*Recursive function generating the mesh of points for polynomials
         g1, g2 expressed in terms of variable var. Points a and b
         are such that neither g1 nor g2 has roots for var<a or var>b*)
        generateMesh[g1_, g2_, var_, a_, b_] :=
        Module[{rootsG1, rootsG2, mid, leftMesh, rightMesh,
                    reducedG1, reducedG2, offset},
        (*Function reduceRootMultiplicities returns a reduced version
         of the input polynomial of the form from proposition 4.2*)
          reducedG1 = reduceRootMultiplicities[g1, var];
          reducedG2 = reduceRootMultiplicities[g2, var];
        (*Function countRealRootsInInterval returns the number
         of roots of a polynomial on (a,b)*)
          rootsG1 = countRealRootsInInterval[reducedG1, var, a, b];
          rootsG2 = countRealRootsInInterval[reducedG2, var, a, b];
        (*If both polynomials have at most one root in the interval,
        return the endpoints*)
          If[rootsG1 <= 1 && rootsG2 <= 1,
                Return[{a, b}]];
        (*Otherwise, bisect the interval*)
          mid = (a + b)/2;
        (*If mid is a root of either g1 or g2, offset mid*)
        (*Function IsRoot returns T/F*)
          While[Or[IsRoot[g1, var, mid], IsRoot[g2, var, mid]],
                offset = (mid + b)/2;
                mid += offset];
        (*Recursively generate meshes for the left and right subintervals*)
          leftMesh = GenerateMesh[g1, g2, var, a, mid];
          rightMesh = GenerateMesh[g1, g2, var, mid, b];
        (*Combine the meshes, removing the duplicate midpoint*)
          Return[Join[Most[leftMesh], rightMesh]]]
```

flip occurs at the same spot. In such a case the interval is valid. The result of this run of Sturm theorem should not be grater than one, as the interval is assumed to have at most one root of each polynomial. Hence, the only outcome left is zero, in which case, g_1 and g_2 have no common roots in (t_i, t_{i+1}). Then one can determine the precedence of the sign flips using bisection method illustrated in algorithm 2. In case 8 of table 1, the precedence in favour of g_2 implies a valid interval, while precedence in favour of g_1 implies that there exists $t \in (t_i, t_{i+1})$ in which both g_1 and g_2 are negative. One can apply a similiar logic in order to investigate the outcomes of case 9.

Algorithm 2 Algorithm in *Mathematica* checking the precedence of a sign change between two polynomials g_1 and g_2 on the interval (a, b).

Input:

- g_1, g_2 - real, nonzero, univariate polynomials having no common roots on interval (a, b).
- a, b - real numbers, such that $a < b$ and sings of g_1 and g_2 at points a, b satisfy either case 8 or case 9 from table 1.

Output:

- True/False - truth value of the statement: sign change of g_1 preceeds the sign change of g_2.

```
In[2]:= precedence[g1_, g2_, var_, a_, b_] :=
        Module[{s1, s2, mid},
        (*Bisection of the interval (a,b)*)
          mid = (a + b)/2;
        (*s1 = g1(mid)g1(a), s2 = g2(mid)g2(a)
        variables s1,s2 are positive as long as there is no sign change
        between a and mid*)
          s1 = (g1 /. var -> mid)*(g1 /. var -> a);
          s2 = (g2 /. var -> mid)*(g2 /. var -> a);
        (*sing of g1 flips before sign of g2*)
          If[And[s1 <= 0, s2 > 0], Return[True]];
        (*sing of g2 flips before sign of g1*)
          If[And[s1 > 0, s2 <= 0], Return[False]];
        (*Inconclusive - neither g1 nor g2 flipped on interval (a,mid)
        -> apply bisection to the interval (mid,b)*)
          If[And[s1 > 0, s2 > 0],
           Return[PolynomialPrecedence[g1, g2, var, mid, b]]];
        (*Inconclusive - both g1 and g2 flipped on interval (a,mid)
        -> apply bisection to the interval (a,mid)*)
          PolynomialPrecedence[g1, g2, var, a, mid]]
```

5. Criteria for entanglement witnesses in $\mathcal{H}^2 \otimes \mathcal{H}^2$

5.1 Trace of X_w

Being equipped with tools from section 4, it is now possible to check if a given operator $X \in \mathcal{L}(\mathcal{H}^2 \otimes \mathcal{H}^2)$ is an entanlgement witness. The task here, is to present an algorithm determining if an operator satisfies condition iii) of proposition 3.5. That is, checking if a corresponding matrix X_w from (3.12) satisfies

A) $\mathrm{Tr}(X_w) \geq 0$; and

B) $\det(X_w) \geq 0$,

for all $w \in \mathcal{H}^2$. It turns out, that condition A) can be expressed explicitly in terms of elements of matrix X. Taking the trace of the matrix expressed in (3.12) evaluates to

$$\begin{aligned}\mathrm{Tr}\{X_w\} = |x|^2 (X_{11,11} + X_{21,21}) + |y|^2 (X_{12,12} + X_{22,22}) + \\ + \overline{x}y (X_{11,12} + X_{21,22}) + x\overline{y} (X_{12,11} + X_{22,21}). \quad (5.1)\end{aligned}$$

Since X_w is hermitian, its trace has to be a real number. After substituting

$$\tau_1 = X_{11,11} + X_{21,21}, \quad \tau_2 = X_{12,12} + X_{22,22} \quad \text{and} \quad \rho = X_{11,12} + X_{21,22}, \tag{5.2}$$

into the expression (5.1), one obtains

$$\mathrm{Tr}(X_w) = |x|^2 \tau_1 + |y|^2 \tau_2 + 2\,\mathrm{Re}\,(\overline{x}y\rho). \tag{5.3}$$

From (5.2) it should be clear that τ_i are real numbers while ρ is complex. Setting

$$w = \begin{pmatrix} x \\ y \end{pmatrix} = R \begin{pmatrix} \cos\theta \\ \sin\theta e^{i\varphi} \end{pmatrix}, \tag{5.4}$$

results in

$$\mathrm{Tr}(X_w) = |R|^2 \left(\cos^2\theta\tau_1 + \sin^2\theta\tau_2 + \sin 2\theta\,(\cos\varphi\,\mathrm{Re}(\rho) - \sin\varphi\,\mathrm{Im}(\rho))\right). \tag{5.5}$$

The factor R is a complex number which does not affect positivity of the expression, even if w is not normalized. The expression (5.5) can now be minized with respect to θ and φ. One obtains that $\mathrm{Tr}\{X_w\}$ has a minimum value for

$$\cos\varphi = -\frac{\mathrm{Re}\,(\rho)}{|\rho|}, \quad \sin\varphi = \frac{\mathrm{Im}\,(\rho)}{|\rho|} \tag{5.6}$$

and

$$\cos 2\theta = \frac{(\tau_2 - \tau_1)}{\sqrt{(\tau_2 - \tau_1)^2 + 4|\rho|^2}}, \quad \sin 2\theta = \frac{2|\rho|}{\sqrt{(\tau_2 - \tau_1)^2 + 4|\rho|^2}}. \tag{5.7}$$

From the latter it is easy to find that

$$\cos^2\theta = \frac{1}{2}\left(\frac{(\tau_2 - \tau_1)}{\sqrt{(\tau_2 - \tau_1)^2 + 4|\rho|^2}} + 1\right) \tag{5.8}$$

and

$$\sin^2\theta = \frac{1}{2}\left(1 - \frac{(\tau_2-\tau_1)}{\sqrt{(\tau_2-\tau_1)^2+4|\rho|^2}}\right). \tag{5.9}$$

Proposition 5.1. The matrix X_w from (3.12) satisfies $\mathrm{Tr}\{X_w\} \geq 0$ for all $w \in \mathcal{H}^2$ if and only if

$$\mathrm{Tr}\{X\} = \tau_1 + \tau_2 \geq 0 \ \wedge \ \tau_1\tau_2 \geq |\rho|^2, \tag{5.10}$$

where τ_1, τ_2 and ρ are defined as in (5.2).

Proof. Substituting (5.6), (5.7), (5.8) and (5.9) into (5.5) and requiring that the result has to be greater or equal to zero results in conditions (5.10). This gives requirements for $\min \mathrm{Tr}\{X_w\} \geq 0$ and hence $\mathrm{Tr}\{X_w\} \geq 0$ for all $w \in \mathcal{H}^2$. □

5.2 Determinant of X_w

In order to determine if $\det\{X_w\} \geq 0$ one can employ a similar substitution to (5.4). For $x = 0$ the condition comes down to

$$|y|^4\left(X_{12,12}X_{22,22} - |X_{12,22}|^2\right) \geq 0. \tag{5.11}$$

Otherwise one can substitute

$$w = R\begin{pmatrix} 1 \\ re^{i\varphi}\end{pmatrix}, \tag{5.12}$$

where $r \in \mathbb{R}$. Same as before, the factor R does not affect the sign of the expression so for the purpose of the discussion one can safely set it to 1. With this substitution

$$\begin{aligned}\det\{X_w\} = c_1 r^4 + \left(c_2 e^{i\varphi} + \overline{c}_2 e^{-i\varphi}\right) r^3 + \left(c_3 e^{2i\varphi} + \overline{c}_3 e^{-2i\varphi} + c_4\right) r^2 + \\ + \left(c_5 e^{i\varphi} + \overline{c}_5 e^{-i\varphi}\right) r + c_6,\end{aligned} \tag{5.13}$$

where

$$\begin{aligned}
c_1 &= X_{12,12}X_{22,22} - |X_{12,22}|^2 \in \mathbb{R},\\
c_2 &= X_{22,22}X_{11,12} + X_{12,12}X_{21,22} - X_{12,22}\overline{X}_{12,21} - \overline{X}_{12,22}X_{11,22} \in \mathbb{C},\\
c_3 &= X_{11,12}X_{21,22} - X_{11,22}\overline{X}_{12,21} \in \mathbb{C},\\
c_4 &= X_{11,12}\overline{X}_{21,22} - X_{12,22}\overline{X}_{11,21} + \overline{X}_{11,12}X_{21,22} - \overline{X}_{12,22}X_{11,21} + \\
&\quad + |X_{11,22}|^2 + |X_{12,21}|^2 + X_{11,11}X_{22,22} + X_{12,12}X_{21,21} \in \mathbb{R},\\
c_5 &= X_{11,11}X_{21,22} + X_{21,21}X_{11,12} - \overline{X}_{11,21}X_{11,22} - X_{11,21}\overline{X}_{12,21} \in \mathbb{C},\\
c_6 &= X_{11,11}X_{21,21} - |X_{11,21}|^2 \in \mathbb{R}.
\end{aligned} \tag{5.14}$$

The expression (5.13) can be rearranged into

$$\begin{aligned}
\det\{X_w\} = & \ c_1 r^4 + 2\left(\mathrm{Re}\,(c_2)\cos\varphi - \mathrm{Im}\,(c_2)\sin\varphi\right) r^3 + \\
& + \left(2\,\mathrm{Re}\,(c_3)\left(2\cos^2\varphi - 1\right) - 4\,\mathrm{Im}\,(c_3)\sin\varphi\cos\varphi + c_4\right) r^2 \\
& + 2\left(\mathrm{Re}\,(c_5)\cos\varphi - \mathrm{Im}\,(c_5)\sin\varphi\right) r + c_6,
\end{aligned} \tag{5.15}$$

where trigonometric functions can be expressed as

$$\cos\varphi = \frac{1-t^2}{1+t^2}, \quad \sin\varphi = \frac{2t}{1+t^2} \tag{5.16}$$

in terms of $t \in \mathbb{R}$ using stereographic projection. Subbing (5.16) into (5.15) and multiplying the expression by an always positive factor $(t^2+1)^2$, results in

$$\begin{aligned} W(r,t) = c_1(t^2+1)^2 r^4 - 2(t^2+1)\Lambda\left(t, c_2\right) r^3 + \\ + \chi\left(c_3, c_4, t\right) r^2 - 2(t^2+1)\Lambda\left(t, c_5\right) r + c_6(t^2+1)^2, \end{aligned} \tag{5.17}$$

where

$$\begin{aligned} \Lambda(t, c_i) = & \quad \mathrm{Re}\,(c_i)t^2 + 2\,\mathrm{Im}\,(c_i)t - \mathrm{Re}\,(c_i) \\ \chi\left(t, c_3, c_4\right) = & \quad (c_4 + 2\,\mathrm{Re}\,(c_3))t^4 + 8\,\mathrm{Im}\,(c_3)t^3 + 2(c_4 - 6\,\mathrm{Re}\,(c_3))t^2 - \\ & -8\,\mathrm{Im}\,(c_3)t + (c_4 + 2\,\mathrm{Re}\,(c_3)) \end{aligned} \tag{5.18}$$

were introduced just for the sake of clarity. The expression $W(r,t)$ is a bivariate, real polynomial of 4-th degree in both r and t. The condition $\det\{X_w\} \geq 0$ for all $w \in \mathcal{H}^2$ now comes down to checking if

$$W(r,t) \geq 0, \quad \forall t \in \mathbb{R},\ \forall r \in \mathbb{R}. \tag{5.19}$$

From (5.11) it is clear that the first requirement shoud be $c_1 \geq 0$. When $c_1 > 0$, $W(r,t)$ is a 4-th degree polynomial in r. Assuming $c_6 > 0$, the strategy is to apply the nonnegativity conditions for all $r \in \mathbb{R}$ from theorem 4.2. This in itself is not as straightforward, because the coefficients of $W(r,t)$ are themselves be polynomials in t. For that purpose let

$$f_W(t,r) = r^4 + \alpha_W r^3 + \beta_W r^2 + \gamma_W r + 1, \tag{5.20}$$

where

$$\alpha_W = \frac{-2\Lambda(t,c_2)}{\sqrt[4]{c_1^3 c_6}(t^2+1)}, \quad \beta_W = \frac{\chi\left(t, c_3, c_4\right)}{\sqrt{c_1 c_6}(t^2+1)^2} \quad \text{and} \quad \gamma_W = \frac{-2\Lambda(t,c_5)}{\sqrt[4]{c_1 c_6^3}(t^2+1)} \tag{5.21}$$

were defined in (4.9). Recalling theorem 4.2 one now needs to check if

$$\begin{aligned} \Delta(f_W) \geq 0 \ \wedge\ |\alpha_W - \gamma_W| \leq \sqrt{\beta_W + 2} \ \wedge \\ \wedge \left(-2 \leq \beta_W \leq 6 \ \vee\ \left(\beta_W > 0 \ \wedge\ |\alpha_W + \gamma_W| \leq \sqrt{\beta_W - 2}\right)\right). \end{aligned} \tag{5.22}$$

The condition on the discriminant of f_W evaluates to checking if its numerator, a 16-th degree polynomial polynomial $g_\Delta(t)$ is nonnegative for all real t. This can be achieved by applying the strategy presented in proposition 4.4. The full expressions for coefficients of g_Δ is included in appendix A. The polynomial itself can be found by requiring that (4.10) is greater or equal to zero, and inserting (5.21). The rest of (5.22) can also be rephrased as conditions on polynomials in t by simply pluging in expressions for α_W, β_W, γ_W and rearranging the inequalities. Introducing

$$g_1(t) = 4c_1c_6\chi(t, c_3, c_4 + 2\sqrt{c_1c_6}) - \Lambda^2(t, \sqrt{c_1}c_5 - \sqrt{c_6}c_2), \tag{5.23}$$

$$g_2(t) = \chi\left(t, c_3, c_4 + 2\sqrt{c_1c_6}\right), \tag{5.24}$$

$$g_3(t) = \chi\left(t, -c_3, 6\sqrt{c_1c_6} - c_4\right), \tag{5.25}$$

$$g_4(t) = 4c_1c_6\chi(t, c_3, c_4 - 2\sqrt{c_1c_6}) - \Lambda^2(t, \sqrt{c_1}c_5 + \sqrt{c_6}c_2), \tag{5.26}$$

one can prove that

$$|\alpha_W - \gamma_W| \le \sqrt{\beta_W + 2} \Leftrightarrow g_1(t) \ge 0 \tag{5.27}$$

and

$$-2 \le \beta_W \le 6 \ \vee \ \left(\beta_W > 0 \ \wedge \ |\alpha_W + \gamma_W| \le \sqrt{\beta_W - 2}\right) \tag{5.28}$$

is equivalent to

$$g_2(t) \ge 0 \ \wedge \ (g_3(t) \ge 0 \vee g_4(t) \ge 0)\,. \tag{5.29}$$

Expressions g_1, g_2, g_3 and g_4 are 4-th degree polynomials in t. Their explicit form is included in appendix A. All of the requirements can be summarized by the following.

Proposition 5.2. Bivariate polynomial $W(r,t)$ from (5.17), with $c_1 > 0$ and $c_6 > 0$ is nonnegative for all $t \in \mathbb{R}$ and all $r \in \mathbb{R}$ iff for all real t i) $g_\Delta(t) \ge 0$, ii) $g_1(t) \ge 0$ and iii) $g_2(t) \ge 0 \ \wedge \ (g_3(t) \ge 0 \vee g_4(t) \ge 0)$.

Proposition 5.3. (Approach) Conditions presented in proposition 5.2 can be checked using following approaches:

1. In condition i) one can apply proposition 4.4.

2. In condition ii) one can apply proposition 4.3.

3. In condition iii) one can apply the algorithm from section 4.3.

A. Polynomials

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