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Quantifying entanglement in $\mathbb{C}^N \otimes \mathbb{C}^N$ by analyzing separability in $\mathbb{C}^2 \otimes \mathbb{C}^N$

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Quantifying entanglement in $\mathbb{C}^N \otimes \mathbb{C}^N$ by analyzing separability in $\mathbb{C}^2 \otimes \mathbb{C}^N$

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A fundamental challenge in quantum entanglement is determining whether a given bipartite quantum state is separable or entangled, a problem known to be computationally intractable in general. This thesis focuses on bipartite systems of the form $\mathbb{C}^2 \otimes \mathbb{C}^N$, consisting of a qubit and a qudit, which offer a rich yet tractable setting for studying entanglement.

The central objective of this thesis is to investigate the maximal Schmidt number that an entangled quantum state can attain in $\mathbb{C}^N \otimes \mathbb{C}^N$ systems. The Schmidt number is a *bona fide* measure of entanglement in bipartite systems. Here, we investigate how this measure of entanglement correlates with the structure of separable states in $\mathbb{C}^2 \otimes \mathbb{C}^N$.

To achieve this, the work combines analytical and numerical tools. Here, we examine structured quantum states, constructing families of states with computable or bounded Schmidt number, and apply criteria to assess their entanglement. In particular, we focus on the study of those entangled states that are positive under partial transposition (PPT), also denoted as bound entangled states. By integrating the above approaches, we provide a better characterization of entanglement in low-dimensional bipartite systems and we offer novel insights on how to classify quantum states according to their Schmidt number.

Overall, this study advances the characterization of quantum correlations in $\mathbb{C}^N \otimes \mathbb{C}^N$ systems for a particular family of states, but offers a foundation for future investigations into entanglement quantification and separability criteria in generic states.

Keywords: PPT, Entanglement, Separability, Schmidt Number, Entanglement Witnesses.

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1 Introduction

This master's thesis investigates the maximal Schmidt number of a given bipartite quantum state in $\mathbb{C}^N \otimes \mathbb{C}^N$, and its relationship to PPT constraints. The importance of our study comes from the fact that quantum entanglement is a fundamental resource in quantum information science, enabling applications in quantum communication, computing, and cryptography, among others. However, identifying whether a given quantum state is separable or not is, in general, a complex task.

A mixed state ρ_{AB} of a bipartite composite system acting in $\mathcal{H}_A \otimes \mathcal{H}_B$, is said to be **separable**, if it can be written as a convex combination of tensor products of density matrices $\rho_A^i \otimes \rho_B^i$. The state is called **entangled** if it cannot be written as a convex combination of tensor products of density matrices. Computationally, the separability problem has been classified as an NP-hard problem (1), thus it is at least as difficult as the hardest problems in the complexity class NP, meaning that it might not have a solution that can be verified in polynomial time. This computational intractability has motivated a wide range of partial results and criteria that attempt to characterize entanglement in specific settings or provide necessary or sufficient conditions for some restricted class of states.

In this thesis, we focus on bipartite quantum systems of the form $\mathbb{C}^2 \otimes \mathbb{C}^N$ - that is, systems consisting of a qubit and a qudit. This setting, despite its apparent simplicity, is both foundational and nontrivial: the structure of entanglement in several complex scenarios reduces to the analysis of separability/entanglement of the above form.

A key quantitative measure of entanglement in bipartite systems is the so-called Schmidt number of a mixed state. The Schmidt number generalizes the notion of the Schmidt rank of pure states to mixed states. The Schmidt rank of a pure bipartite state indicates how many degrees of freedom are entangled between subsystems. The Schmidt number captures how much entanglement is present in a mixed state by describing the minimal Schmidt rank required across all possible decompositions of the mixed state into pure states. The Schmidt number is, therefore, the smallest of the largest Schmidt ranks needed to achieve a given mixed state, computed over all possible decompositions. In this way, it represents the minimal Schmidt rank that is needed, no matter how the state is written as a mixture of pure states. Obviously, such min-max optimization is extremely difficult to compute, so generally speaking, it is not easy to determine the Schmidt number of a given bipartite system.

Thus, separable states are exactly those with Schmidt number one, but entangled states can have a range of all possible Schmidt numbers, from two up to the smallest local Hilbert space dimension in the bipartite setting.

Studying the Schmidt number, therefore, allows us to classify entangled states more finely, distinguishing, for example, those that are low-dimensional in their entanglement from those whose correlations genuinely span over the full dimension of the smallest associated Hilbert space. This distinction is not only mathematically natural, but it is also operationally relevant. Several quantum information protocols require entanglement of a certain type of Schmidt number to offer an advantage (2) (3)(4).

Understanding how the Schmidt number behaves under various constraints and structural assumptions is an important path in entanglement theory. In particular, a central objective of this thesis is to investigate how the maximal Schmidt number that a quantum state can possess in $\mathbb{C}^N \otimes \mathbb{C}^N$ correlates with the structure of separable and entangled states in $\mathbb{C}^2 \otimes \mathbb{C}^N$. While entangled states that are NPT, that is, not positive under partial transposition, can attain maximal Schmidt number, there is strong evidence that states that are PPT entangled cannot have maximal Schmidt number.

This investigation involves several complementary approaches. First, it examines structured quantum states, in particular, we focus on symmetric states. The symmetry embedded in such states involves specific coherence patterns or diagonal components, which simplifies the understanding of their entanglement properties. It also involves constructing and studying families of states for which the Schmidt number can be explicitly computed or bounded. In addition, the work develops or applies methods to determine whether a state is separable or possesses a high Schmidt number, making use of both analytic criteria and numerical algorithms.

This master's thesis is structured as follows. In the next section, we provide the mathematical preliminaries needed for this work. First, we introduce generic definitions concerning pure and mixed states, and some properties of matrices. Then, we focus on a set of theorems whose importance will become relevant when dealing with bipartite systems of the form $\mathbb{C}^2 \otimes \mathbb{C}^N$. We move then to the notions of completely positive maps, as well as the so-called k-positive maps. We end the mathematical section by introducing the Choi decomposition and the relation between the Choi decomposition of a map and the Schmidt number of a system. In Section 3, we apply some of the concepts we have introduced to analyze the Schmidt number of symmetric states in $C^4 \otimes C^4$. In Section 4, we present our conclusions and list some open questions for future research.

2 Mathematical preliminaries

Here, we introduce the mathematical framework and essential concepts that will be used throughout the thesis. Our goal is to establish the language and knowledge basis to analyze entanglement rigorously. Our work is focused on bipartite quantum systems in finite systems, with particular attention to linear algebraic and theoretical tools to support the study of quantum entanglement.

2.1 Quantum states and entanglement

In quantum theory, the state of an isolated physical system is represented by a normalized vector $|\psi\rangle$ which lives in a Hilbert space $\mathscr{H}$, that is, a complex vector space with an inner product $\langle\psi|\psi\rangle$ such that the norm defined by $|\psi| = \sqrt{\langle\psi|\psi\rangle}$ turns $\mathscr{H}$ into a complete metric space. For our purposes, we will focus on finite-dimensional complex Hilbert spaces $\mathbb{C}^m$, whose elements are complex-valued column vectors of size m.

When dealing with composite systems, which are systems made up of two or more parties, we describe each subsystem with its own Hilbert space. For example: if one party is described by the space $\mathscr{H}_A = \mathbb{C}^m$ and the other $\mathscr{H}_B = \mathbb{C}^n$, then the total system is described by the tensor product of these two spaces, $\mathscr{H}_{AB} = \mathscr{H}_A \otimes \mathscr{H}_B$. The space $\mathscr{H}_{AB}$ contains all possible states of the joint system and gives rise to certain quantum phenomena like entanglement, where the state of the whole system cannot be described as a product state.

In general, there exist two types of quantum states: **pure** and **mixed** states. A pure state is described by a single vector $|\psi\rangle$ in a Hilbert space. However, when we do not have complete information about the system, or when the system is part of a larger entangled system, we must use a more general object: a **mixed state**.

Definition 1. *A **mixed state** is a convex combination of pure states, represented as:*

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \tag{1}$$

where each $|\psi_i\rangle$ is a pure state, $p_i \geq 0$, and $\sum_i p_i = 1$.

A quantum state is generally represented by an operator called the density matrix or density operator, denoted by ρ. Mathematically, this is a linear operator acting on $\mathscr{H}$ that satisfies two properties:

1. It is positive semidefinite, that is, all its eigenvalues are non-negative.
2. It has unit trace: $\text{Tr}(\rho) = 1$.

Density operators, $\rho \in \mathcal{B}(\mathscr{H})$, are bounded operators acting on $\mathscr{H}$, and also mixed states are described by density matrices that are positive semidefinite and have unit trace. Notice that in a finite Hilbert space, all positive operators are necessarily Hermitian, so $\rho = \rho^\dagger$. Two important concepts that help us understand how an operator behaves are its range and kernel.

Definition 2. *The **kernel** of ρ, with ρ being hermitian, is defined as $K\{\rho\} = \{|\psi\rangle \in \mathscr{H} : \rho|\psi\rangle = 0\}$, meaning is the subspace spanned by the eigenvectors with zero eigenvalue.*

Definition 3. *The **range** of ρ is defined as $R\{\rho\} = \{|\psi\rangle \in \mathscr{H} : \exists |\phi\rangle ; \rho|\psi\rangle = |\phi\rangle\}$, if ρ is hermitian then the subspace of $\mathscr{H}$ is spanned by the eigenvectors of ρ with eigenvalue $\lambda > 0$.*

Having introduced the concepts of range and kernel of a matrix, which help describe the internal structure of a quantum state, we now turn our attention to bipartite systems. We formally define first what a separable/entangled state is and introduce one of the most important operations used in the study of entanglement: the partial transposition.

Definition 4. *Let ρ be a density matrix acting on the bipartite Hilbert space $\mathscr{H}_{AB}$. Then ρ is called **separable** when it can be written as a convex combination of product states:*

$$\rho = \sum_i p_i \rho_A^i \otimes \rho_B^i \tag{2}$$

where each $p_i \geq 0$, $\sum_i p_i = 1$ and, each ρ_A^i and ρ_B^i is a valid density matrix on the subsystems $\mathscr{H}_A$ and $\mathscr{H}_B$, respectively.

Definition 5. *A quantum state ρ is said to be **entangled** if it is not separable, that is, it cannot be written in the form:*

$$\rho \neq \sum_i p_i \rho_A^i \otimes \rho_B^i. \tag{3}$$

Let ρ be a bipartite quantum state acting on $\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B$, and let $\{|i\rangle\}$ and $\{|j\rangle\}$ be orthonormal bases for $\mathscr{H}_A$ and $\mathscr{H}_B$, respectively. Then ρ can be represented in this product basis as:

$$\rho = \sum_{ijkl} \rho_{ijkl} |i\rangle\langle k| \otimes |j\rangle\langle l| \,. \tag{4}$$

Definition 6. *The* ***partial tranpose*** *of ρ with respect to the first subsystem A, denoted ρ^{T_A}, is defined by tranposing only the indices associated with A:*

$$\rho^{T_A} = \sum_{ijkl} \rho_{ijkl} |k\rangle\langle i| \otimes |j\rangle\langle l| \,. \tag{5}$$

The same definition applies to partial tranposition concerning subsystem B, denoted ρ^{T_B}, where only the second factor is transposed.

Partial transposition plays a central role in the Peres-Horodecki criterion for separability. First, Peres stated the following:

Theorem 1. *(5) If ρ is separable the $\rho^{T_A} \geq 0$ and $\rho^{T_B} = (\rho^{T_A})^T \geq 0$.*

This works for arbitrary dimensions, though it is only valid in the given direction. Lately, the only if direction was proposed by Horodecki and is only valid in special cases:

Theorem 2. *(6) In $\mathbb{C}^2 \otimes \mathbb{C}^2$ or $\mathbb{C}^2 \otimes \mathbb{C}^3$ ρ is separable iff $\rho^{T_A} \geq 0$.*

The Peres-Horodecki criterion gives a powerful necessary and sufficient condition for detecting entanglement via the partial transposition. Thus, this criterion says that separability implies PPT, and that NPT implies entanglement. However, this criterion is not completely useful for higher dimensions; we know there exist entangled states with positive partial transposition, known as **bound entangled states**.

To get a better understanding of entanglement, it is helpful to first consider pure states, where a complete characterization of entanglement is done thanks to the **Schmidt decomposition**.

Definition 7. *Let $|\psi\rangle \in \mathscr{H}_A \otimes \mathscr{H}_B$ be a pure state. Then there exist orthonormal basis $\{|e_i\rangle\}$ for $\mathscr{H}_A$ and $\{|f_i\rangle\}$ for $\mathscr{H}_B$ such that*

$$|\psi\rangle = \sum_{i=1}^{r} \lambda_i |e_i\rangle \otimes |f_i\rangle \,, \tag{6}$$

where $\lambda_i > 0$, and r is the Schmidt rank of $|\psi\rangle$. The ***Schmidt rank*** *is a measure of entanglement; a value of $r = 1$ indicates that the state is separable, and for $r > 1$ the state is entangled.*

While the Schmidt decomposition is a complete tool for pure state entanglement detection, the situation for mixed states is more complex. In this case, one needs to analyze the structure of the support of the state, its kernel, and its partial transpose, often in terms of how they interact with product vectors. To extend the intuition of the Schmidt decomposition to mixed states, we need to introduce the notion of the Schmidt number.

The **Schmidt number** is a tool used to quantify the entanglement present in a quantum state. For bipartite systems is called the Schmidt rank, which applies to pure states. Specifically, for a bipartite quantum state ρ_{AB}, the Schmidt number, denoted as $\mathrm{SN}(\rho_{AB})$, is defined as the minimum, over all pure state ensembles that result in ρ_{AB} of the maximal Schmidt rank of the pure states in the ensembles. Formally,

Definition 8. $\mathrm{SN}(\rho_{AB}) = \inf_{\{p_i, |\psi_i\rangle\}} \max_i \mathrm{SR}(|\psi_i\rangle)$ *where* $\mathrm{SR}(|\psi_i\rangle)$ *denotes the Schmidt rank of the pure state* $|\psi_i\rangle$.

A mixed state ρ_{AB} is entangled if and only if its Schmidt number is greater than one. Beyond merely detecting entanglement, the Schmidt number also reflects the minimal local Hilbert space dimensions required to prepare the state using local operations and classical communication (LOCC)(7).

In practice, computing the Schmidt number of a state is highly nontrivial due to the need to minimize over an infinite number of possible decompositions of the state. Nonetheless, various mathematical techniques have been developed to estimate or bound the Schmidt number in specific cases. Among the most studied are bipartite systems of the form $\mathbb{C}^2 \otimes \mathbb{C}^N$, where the reduced dimensionality on one party makes it possible to derive explicit structural results. The following lemmas are built on this fact and provide essential tools for analyzing separability and entanglement in such systems.

Now, we consider positive partial transpose (PPT) states. The following lemma helps to construct product vectors orthogonal to given ones and reduce the rank while preserving the PPT property.

Lemma 1. *(8) Let* ρ *be a PPT state in* $\mathbb{C}^2 \otimes \mathbb{C}^N$ *such that* $\rho\,|e, f\rangle = 0$. *Then there exists a unit vector* $|\hat{e}\rangle \perp |e\rangle$ *such that*

$$\rho = \rho' + \Lambda\,|\hat{e}, f\rangle\langle\hat{e}, f|\,, \tag{7}$$

where

$$\rho' \geq 0, (\rho')^{T_A} \geq 0, \langle e|\hat{e}\rangle = 0 \tag{8}$$

and

$$r\{\rho'\} = r\{\rho\} - 1 \quad r\{(\rho')^{T_A}\} = r\{\rho^{T_A}\} - 1 \tag{9}$$

Lemma 2. *(8) Every 2-dimensional subspace of* $\mathbb{C}^2 \otimes \mathbb{C}^2$ *contains a product vector.*

Definition 9. *A bipartite quantum state* ρ *is called an* ***edge state*** *if:*

- ρ *is entangled and has positive partial transpose (PPT),*
- *there exists no product vector* $|e, f\rangle \in R(\rho)$ *such that* $|e^*, f\rangle \in R(\rho^{T_A})$.

Equivalently, an edge state is a PPT entangled state from which it is impossible to subtract any projector onto a product vector while preserving positivity and the PPT property. To clarify the explanation, figure 1 helps to visualize the concept of edge state.

In other words, edge states lie on the *boundary* of the set of PPT states: any infinitesimal subtraction of a product state results in a state that is no longer PPT. This makes them extreme examples of bound entanglement.

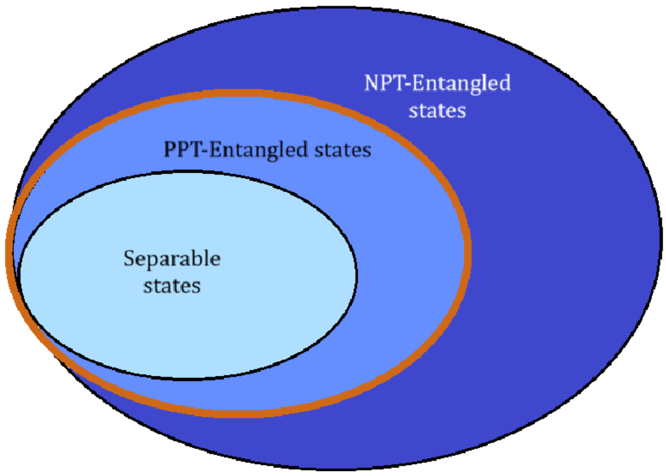

Figure 1: Representation of the quantum states differentiating those that are separable, PPT-entangled and NPT-entangled. Also notice that the orange line represents de edge states. Source: From the author.

Lemma 3. *(8) If ρ is a PPT state, i.e. $\rho^{T_A} \geq 0$, acting in $\mathbb{C}^2 \otimes \mathbb{C}^2$ and $r\{\rho\} = 2$ then ρ is separable.*

This last lemma may well suggest that the PPT states fulfilling that conditions are a mixture of product states; no bound entangled states exist with such low rank. As the rank increases, we need more conditions to prove separability.

2.2 Symmetric subspace

In the study of the separability problem, known to be NP-hard (9) in general, it is often advantageous to restrict attention to subspaces exhibiting additional structure. One particularly useful choice is the *symmetric subspace*, which arises naturally in the context of systems composed of indistinguishable bosonic particles.

Formally, let $\mathscr{H} = (\mathbb{C}^d)^{\otimes N}$ denote the Hilbert space of N d-dimensional subsystems.

Definition 10. *The **symmetric subspace** $Sym^N(\mathbb{C}^d)$ is defined as the subspace of $\mathscr{H}$ consisting of all vectors $|\psi\rangle$ that are invariant under the action of the symmetric group S_N, i.e.,*

$$Sym^N(\mathbb{C}^d) := \{|\psi\rangle \in \mathscr{H} | U_\pi |\psi\rangle = |\psi\rangle \quad \forall \pi \in S_N\} \tag{10}$$

where U_π is the unitary operator implementing the permutation π on tensor factors.

Working within the symmetric subspace offers two key advantages for the separability problem.

One is a dimensional reduction where the dimension of $Sym^N(\mathbb{C}^d)$ is

$$\dim \mathrm{Sym}^N(\mathbb{C}^d) = \binom{N+d-1}{d-1}, \tag{11}$$

which is significantly smaller than d^N for $N > 1$, thereby reducing the complexity of computations.

Moreover, an enhanced structure is achieved given that the states in $Sym^N(\mathbb{C}^d)$ admit a basis of what are the so-called *Dicke states* and can be described by a reduced set of parameters, enabling more systematic and partially analytic approaches to entanglement analysis.

Definition 11. *Dicke states define a complete orthonormal basis for the symmetric subspace. For the bipartite case they are defined as follows:*

$$|D_{ii}\rangle = |ii\rangle \quad \text{and} \quad |D_i\rangle = \frac{|ij\rangle + |ji\rangle}{\sqrt{2}}, \tag{12}$$

where $i \neq j = 0, 1, \cdots, n-1$. *From the definition we get that* $|D_{ij}\rangle = |D_{ji}\rangle$.

Another useful definition is the diagonal symmetric state.

Definition 12. *A diagonal symmetric state* ρ_{DS} *is defined as a state which is diagonal in the Dicke basis. For bipartite systems* ρ_{DS} *is expressed as*

$$\rho_{DS} = \sum_{i \leq j = 0}^{n} p_{ij} \, |D_{ij}\rangle\langle D_{ij}| \tag{13}$$

where p_{ij} *form a probability distribution.*

This class of states is particularly tractable because its high degree of symmetry allows a complete characterization of separability in low dimensions via the positive partial transpose (PPT) criterion. Specifically, it has been shown the following:

Theorem 3. *(10) Let* ρ *be a DS state acting on* $\mathbb{C}^d \otimes \mathbb{C}^d$, *with* $d \leq 4$.

$$\rho \text{ is separable} \iff \rho \text{ is PPT.} \tag{14}$$

For $d \geq 5$, the equivalence between separability and the PPT condition no longer holds: there exist PPT diagonal symmetric states that are entangled. Nevertheless, in the $d = 2, 3, 4$ cases, this equivalence provides an efficient separability check within the symmetric subspace, turning the otherwise NP-hard problem into a tractable one for this special class.

2.3 Quantum maps, k-positive maps and witnesses

Up to this point, we have focused on states within Hilbert spaces and operators that act on them. Now, we take a step further by introducing maps, also known as superoperators, which act on these operators themselves, transforming one operator into another within the Hilbert space framework.

The following are some formal definitions to characterize a map.

Definition 13. *A map* $\Lambda : \mathcal{B}(\mathscr{H}_A) \to \mathcal{B}(\mathscr{H}_B)$ *is called linear and self-adjoint if:*

- *It is linear, meaning that for any operators* O_1, O_2 *and scalasrs* $\alpha, \beta \in \mathbb{C}$,

$$\Lambda(\alpha O_1 + \beta O_2) = \alpha \Lambda(O_1) + \beta \Lambda(O_2). \tag{15}$$

- *It maps Hermitian operators to Hermitian operators, i.e., for any $O \in \mathcal{B}(\mathscr{H}_A)$,*

$$\Lambda(O^\dagger) = \Lambda(O)^\dagger \tag{16}$$

Definition 14. *A linear map Λ is called trace-preserving if for all operators $O \in \mathcal{B}(\mathscr{H}_A)$,*

$$\mathrm{Tr}(\Lambda(O)) = \mathrm{Tr}(O). \tag{17}$$

Definition 15. *A linear, self-adjoint map Λ is called positive if it maps positive semidefinite operators to positive semidefinite operators. That is, for any $\rho \in \mathcal{B}(\mathscr{H}_A)$ with $\rho \geq 0$,*

$$\Lambda(\rho) \geq 0. \tag{18}$$

Definition 16. *A positive linear map Λ is said to be completely positive if, for any auxiliary Hilbert space $\mathscr{H}_A$, the extended map*

$$\Lambda' = \mathbb{1}_A \otimes \Lambda : \mathcal{B}(\mathscr{H}_A \otimes \mathscr{H}_B) \to \mathcal{B}(\mathscr{H}_A \otimes \mathscr{H}_C) \tag{19}$$

is also a positive map.

Definition 17. *A map Λ is called k-positive if the extended map $\mathbb{1}_k \otimes \Lambda$, where $\mathbb{1}_k$ denotes the identity map on a k-dimensional Hilbert space,*

$$\Lambda' = \mathbb{1}_k \otimes \Lambda : \mathcal{B}(\mathbb{C}^k \otimes \mathscr{H}_B) \to \mathcal{B}(\mathbb{C}^k \otimes \mathscr{H}_C) \tag{20}$$

is positive, that is, it maps positive semidefinite operators to positive semidefinite operators.

Beyond these foundational definitions, we now turn the focus on one of the key uses of quantum maps: entanglement detection. In particular, positive but not completely positive maps play a crucial role in this context. In fact, if no k-positive map detects a given state ρ_{AB} it follows that $\mathrm{SN}(\rho_{AB}) \leq k$.

Definition 18. *A bipartite state $\rho_{AB} \in \mathcal{D}(\mathscr{H}_A \otimes \mathscr{H}_B)$ is entangled if and only if there exists a positive map $\Lambda : \mathcal{B}(\mathscr{H}_B \to \mathscr{H}_C)$ such that the extended map $\mathbb{1} \otimes \Lambda$ acts non-positively on ρ_{AB}, that is,*

$$(\mathbb{1} \otimes \Lambda)(\rho_{AB}) \not\geq 0. \tag{21}$$

This criterion generalizes when considering the Schmidt number of a quantum state. In particular, the concept of k-positivity allows for a hierarchy of entanglement detection. A state has a Schmidt number greater than k if and only if there exists a k-positive (but not completely positive) map capable of revealing this.

Theorem 4. *Let $\rho_{AB} \in \mathcal{D}(\mathscr{H}_A \otimes \mathscr{H}_B)$ be a quantum state and $\mathrm{SN}(\rho_{AB}) > k$ if and only if there exists a k-positive map $\Lambda : \mathcal{B}(\mathscr{H}_B \otimes \mathscr{H}_C)$ such that*

$$(\mathbb{1}_A \otimes \Lambda)(\rho_{AB}) \not\geq 0. \tag{22}$$

2.4 Characterizing entanglement in the PPT set via Schmidt Number

Given a mixed quantum state ρ, one fundamental question is whether the state is entangled or not. For pure states, this can be answered by examining the Schmidt decomposition; however, for mixed states, the situation is more subtle. One powerful approach to address this question involves the use of entanglement witnesses.

Definition 19. *An entanglement witness W is a Hermitian operator constructed such that:*

- $\mathrm{Tr}(W\sigma) \geq 0$ *for all separable states σ.*
- *there exists at least one entangled ρ such that* $\mathrm{Tr}(W\rho) < 0$*.*

Among these witnesses, a notable class is the set of decomposable witnesses, which can be expressed in the form:

$$W = aP + (1-a)Q^{T_B} \tag{23}$$

where $P, Q \geq 0$. However, decomposable witnesses cannot detect PPT entangled states. Such states are often referred to as bound entangled states and require more sophisticated tools for their detection. Also, witnesses who can detect PPT states are non-decomposable, meaning they can not be written as in equation (23).

Analogously to the construction of entanglement witnesses for the detection of entanglement, a new concept called k-Schmidt witnesses (k-SW) can be defined to detect whether a state has a Schmidt number greater than k. These witnesses are tailored to identify states that cannot be decomposed into mixtures of pure states with Schmidt rank at most k, thus providing a powerful tool for certifying high-dimensional entanglement.

These are generalizations of standard entanglement witnesses shaped to detect whether a state's Schmidt number exceeds a given threshold. Formally, a k-Schmidt witness is a Hermitian operator W_k satisfying:

- $\mathrm{Tr}(W_k\sigma) \geq 0$ for all states σ with Schmidt number less than k,
- but there exists at least one state ρ with $\mathrm{SN}(\rho) \geq k$ such that $\mathrm{Tr}(W_k\rho) < 0$.

Thus, k-SWs allows us to verify that a given state is not just entangled, but possesses a Schmidt number of at least k.

Theorem 5. *A state $\rho \in \mathcal{D}(\mathscr{H}_A \otimes \mathscr{H}_B)$ has Schmidt number at least k, i.e.,* $\mathrm{SN}(\rho) \geq k$*, if and only if there exists a k-Schmidt witness W_k such that*

$$\mathrm{Tr}(W_k\rho) < 0. \tag{24}$$

2.5 Choi isomorphisim

Note the striking similarity between Theorem 5 and the earlier criterion involving k-positive maps. These two tools are not only analogous but mathematically interconnected. In particular, the Choi matrix of a k-positive map serves as a (k+1)-Schmidt witness. The Choi matrix associated with a map $\Lambda : \mathcal{B}(\mathscr{H}_A \otimes \mathscr{H}_B)$ is defined as:

$$\mathrm{J}_\Lambda = \sum_{i,j=0}^{d_A-1} |i\rangle\langle j| \otimes \Lambda(|i\rangle\langle j|), \tag{25}$$

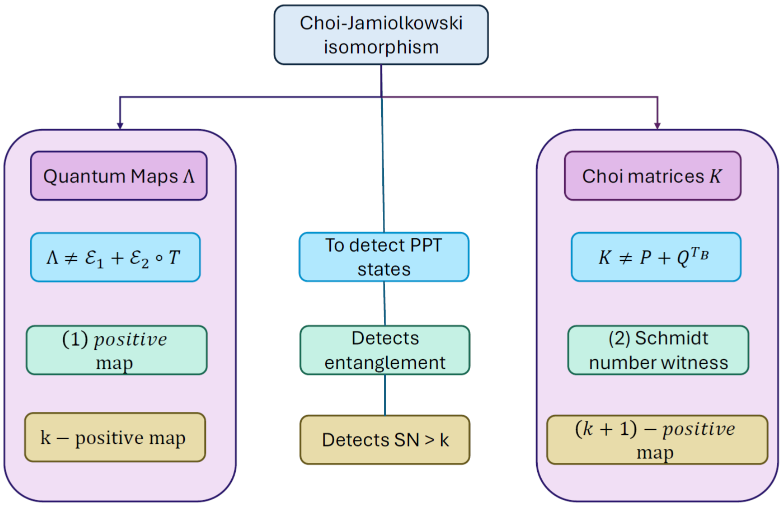

Figure 2: Schematic overview of the Choi-Jamiołkowski isomorphism and its applications in entanglement detection. Source: From the author.

where $\{|i\rangle\}$ is an orthonormal basis for $\mathscr{H}_A$. This matrix encodes the action of Λ and provides a bridge between the algebraic structure of positive maps and the geometric characterization of entanglement via Schmidt number witnesses. A visualization of this can be seen in figure 2.

We are particularly interested in analyzing the Schmidt number of PPT entangled states. Recall that if a bipartite quantum state has a negative partial transpose, the state is NPT, it is necessarily entangled. However, detecting entanglement in PPT states is a much more delicate task, as no efficient general method exists for certifying entanglement in such cases.

Despite this difficulty, the tools introduced earlier, namely k-positive maps and k-Schmidt witnesses, can still be employed to bound the Schmidt number of PPT states. Nevertheless, for these methods to be effective in the PPT region, they must satisfy an additional structural condition: they must be non-decomposable.

In the context of quantum maps, a map Λ is said to be non-decomposable if it cannot be written as

$$\Lambda \neq \mathcal{E}_1 + \mathcal{E}_2 \circ T \tag{26}$$

where $\mathcal{E}_1$ and $\mathcal{E}_2$ are completely positive maps, and T denotes the transposition map. Only such non-decomposable maps are capable of detecting the entanglement of PPT states.

Similarly, for a k-Schmidt witness W_k to detect a PPT entangled state, it must also be non-decomposable. That is, it must not be expressed in the form:

$$W_k \neq P + Q^{T_B} \tag{27}$$

where $PQ \geq 0$, as we have seen in the previous section.

2.6 The Choi decomposition

Now we turn to the question of whether it is possible to find bounds on the Schmidt number (SN) of PPT states by analyzing the structure of k-postivie maps. First, we introduce the concept of the trivial lifting of a linear map.

Definition 20. *Let $\Lambda : \mathcal{B}(\mathbb{C}^n) \to \mathcal{B}(\mathbb{C}^m)$ be a linear map and let $I \subset \{0, 1, \cdots, n-1\}$ be a set with $|I| = p$. The I-trivial lifting of Λ, denoted $\Lambda_I : \mathcal{B}(\mathbb{C}^{n+p}) \to \mathcal{B}(\mathbb{C}^m)$, is defined by:*

$$\Lambda_I(|i\rangle\langle j|) = 0 \tag{28}$$

whenever $i \in I$ or $j \in I$.

Intuitively, a trivial lifting increases the input dimension of the original map Λ, but acts trivially (i.e., vanishes) on specific indices in the set I. This action is also reflected in the Choi matrix J_{Λ_I}, which can be obtained from the Choi matrix J_Λ by inserting blocks of zero rows and columns corresponding to indices in I. Explicitly, $\langle ij| J_{\Lambda_I} |kl\rangle = 0$ whenever $j \in I$ or $l \in I$. As an important remark, the trivial lifting is not unique, giving freedom to choose which indices to add or eliminate depending on the desired final dimensions, this lets us tackle the problems from the simplest cases.

A crucial feature of this construction is that the k-positivity and decomposability of the original map Λ are preserved under the action of the trivial lifting.

This notion leads to a powerful result known as the Choi decomposition, which provides a way to decompose any k-positive map into a sum involving a completely positive map and a trivial lifting of a positive map:

Theorem 6. *(11) Let $2 \leq k \leq n$ and $n \leq m$. Then any k-positive map $\Lambda : \mathcal{B}(\mathbb{C}^n) \to \mathcal{B}(\mathbb{C}^m)$ can be written as:*

$$\Lambda = \mathcal{E} + \Phi_I, \tag{29}$$

where $\mathcal{E}$ is a completely positive map and Φ_I is the I-trivial lifting of a positive map $\Phi : \mathcal{B}(\mathbb{C}^{n-k+1}) \to \mathcal{B}(\mathbb{C}^m)$, for any subset $I \subset \{0, 1, \cdots, n-1\}$ with $|I| = k-1$.

Consequently, such a decomposition exists for any choice of the index set I of the appropriate size; this non-uniqueness gives substantial flexibility when applying the decomposition. While it was previously known that at least one suitable index set I always exists, it has now been shown that Choi decompositions are possible for all such sets, providing greater freedom in structural analysis.

This decomposition plays a key role in studying the decomposability of k-positive maps by reducing the question to the decomposability of positive maps in lower dimensions. For example, consider a 2-positive map $\Lambda : \mathcal{B}(\mathbb{C}^3) \to \mathcal{B}(\mathbb{C}^3)$. Applying the Choi decomposition yields:

$$\Lambda = \mathcal{E} + \Phi_I, \tag{30}$$

where Φ_I is a trivial lifting of a positive map $\Phi : \mathcal{B}(\mathbb{C}^2) \to \mathcal{B}(\mathbb{C}^3)$. It is known that all positive maps from $\mathcal{B}(\mathbb{C}^2)$ to $\mathcal{B}(\mathbb{C}^3)$ are decomposable, implying that Φ_I and hence Λ are also decomposable. As a result, all 2-positive maps $\Lambda : \mathcal{B}(\mathbb{C}^3) \to \mathcal{B}(\mathbb{C}^3)$ are decomposable. This, in turn, implies that all PPT states of two qutrits($\mathbb{C}^3 \otimes \mathbb{C}^3$) have Schmidt number strictly less than three.

A similar conclusion was previously established for two-qubit PPT states, where the maximal Schmidt number(which is 2 in this case) cannot be attained, meaning all two-qubit PPT states are separable. These results naturally lead to the broader question:

Can PPT states in $\mathbb{C}^d \otimes \mathbb{C}^d$ ever achieve the maximal Schmidt number d?

To approach this question, one strategy is to investigate whether all (d-1)-positive maps from $\mathcal{B}(\mathbb{C}^d) \to \mathcal{B}(\mathbb{C}^d)$ are decomposable.

Focusing on the next open case, let us consider $d = 4$, i.e., PPT states in $\mathbb{C}^4 \otimes \mathbb{C}^4$. The question now becomes: Are all 3-positive maps $\Lambda : \mathcal{B}(\mathbb{C}^4) \to \mathcal{B}(\mathbb{C}^4)$ decomposable?
Applying the Choi decomposition, we obtain $\Lambda = \mathcal{E} + \Phi_I$, where Φ_I is a trivial lifting of a positive map $\Phi : \mathcal{B}(\mathbb{C}^2) \to \mathcal{B}(\mathbb{C}^4)$. However, in this case, there exists positive maps Φ on these dimensions that are non-decomposable. Consequently, no general conclusion can be drawn about the decomposability of Λ, and therefore, the question of whether all PPT states in $\mathbb{C}^4 \otimes \mathbb{C}^4$ have Schmidt number less than 4 remains open.

Thanks to the duality between k-positive maps and k-SW, an analogue of the Choi decomposition can also be formulated for the latter:

Theorem 7. *(12) Let $3 \leq k \leq n$, and $n \leq m$. Then any k-Schmidt witness $W_k \in \mathcal{B}(\mathbb{C}^n \otimes \mathbb{C}^m)$ can be decomposed as:*

$$W_k = P + W_I, \tag{31}$$

where $P \geq 0$ is a positive semidefinite operator, and W_I is an I-trivial lifting of an entanglement witness $W \in \mathcal{B}(\mathbb{C}^{n-k+2} \otimes \mathbb{C}^m)$, for any subset $I \subset \{0, 1, \cdots, n-1\}$ with $|I| = k - 2$.

This decomposition mirrors the structure of theorem 6 for k-positive maps, and provides an effective technique to analyze k-SW in terms of lower-dimensional entanglement witnesses extended via trivial lifting.

2.6.1 Limits of detection using Choi-type decompositions

For further understanding of Schmidt number detection, especially in the context of PPT states, it becomes necessary to develop a stronger criterion with more restrictive conditions than previously discussed. The key insight underlying this refinement is that the Choi decomposition of a k-positive map (and by duality, of a k-Schmidt witness) is not unique.

Theorem 8. *Let $W_k \in \mathcal{B}(\mathbb{C}^n \otimes \mathbb{C}^m)$ with $n \leq m$ be a k-Schmidt witness, $2 \leq k \leq n$, and let $\rho \in \mathcal{D}(\mathbb{C}^n \otimes \mathbb{C}^m)$. If there exists a Choi-type decomposition*

$$W_k = P + W_I, \tag{32}$$

where $P \geq 0$ and W_I is an I-trivial lifting, such that

$$\mathrm{Tr}(W_I \rho) \geq 0. \tag{33}$$

*then ρ is **not detected** by W_k; i.e.,*

$$\mathrm{Tr}(W_k \rho) \geq 0. \tag{34}$$

This result has an important consequence: to show that a state ρ is not detected by any n-Schmidt witness (i.e., it does not have maximal Schmidt number), it is sufficient to exhibit one Choi decomposition such that the corresponding lifted operator W_I fails to detect ρ. In particular, detection by W_k requires that $\mathrm{Tr}(W_I \rho) < 0$ for all such decompositions, but this condition alone is necessary but not sufficient for detection.

To make this criterion more explicit, consider a state $\rho \in \mathcal{D}(\mathbb{C}^n \otimes \mathbb{C}^m)$, with $n \leq m$, represented in block form as:

$$\rho = \sum_{i,j=0}^{n-1} |i\rangle\langle j| \otimes X_{ij}, \qquad X_{ij} \in \mathcal{B}(\mathbb{C}^m). \tag{35}$$

Let W_n be an n-Schmidt witness with a Choi-type decomposition $W_n = P + W_I$, where $|I| = n-2$. Then, there exists exactly two indices $\{r_0, r_1\} \subset \{0, \cdots, n-1\}$ such that the nonzero part of the trivial lifting W_I acts only on the subspace spanned by $\{|r_0\rangle, |r_1\rangle\}$. In this case, we can write:

$$W_I = \sum_{i,j=0}^{1} |i\rangle\langle j| \otimes A_{r_i,r_j}, \tag{36}$$

and the expectation value becomes:

$$\mathrm{Tr}(W_I\rho) = \mathrm{Tr}(W_I Y) \tag{37}$$

where $Y \in \mathcal{B}(\mathbb{C}^2 \otimes \mathbb{C}^m)$ is the principal submatrix:

$$Y = \sum_{i,j=0}^{1} |i\rangle\langle j| \otimes X_{r_i,r_j}. \tag{38}$$

Thus, to conclude that ρ is not detected by any n-Schmidt witness (and hence $\mathrm{SN}(\rho) < n$), it suffices to find a pair of indices $\{r_0, r_1\}$ such that the corresponding submatrix Y is separable in $\mathbb{C}^2 \otimes \mathbb{C}^m$.

This provides a practical and geometrically intuitive method: If at least one of the 2x2 principal submatrices is separable, then the original state cannot have maximal Schmidt number. Moreover, all of these submatrices will be PPT if the intial state is also PPT.

3 Results: Applications in the symmetric subspace $\mathbb{C}^d \otimes \mathbb{C}^d$

Here in this section we focus on how the different techniques we have presented in the previous sections can allow us to bound the Schmidt number of PPT-Entangled states in the symmetric subspace; i.e., determine whether PPT-bound states in the symmetric subspace can have maximal Schmidt Number.

3.1 Case $\mathcal{S}(\mathbb{C}^3 \otimes \mathbb{C}^3)$

In $\mathcal{S}(\mathbb{C}^d \otimes \mathbb{C}^d)$ for $d \leq 4$, coherences give rise to PPT bound states.

Recently, it has been found that the only edge states that exist in $\mathcal{S}(\mathbb{C}^3 \otimes \mathbb{C}^3)$ belong to the following family of states:

$$\rho = \rho_{DS} + \alpha\, |D_{00}\rangle\langle D_{12}| + \beta\, |D_{11}\rangle\langle D_{02}| + \gamma\, |D_{22}\rangle\langle D_{01}| \tag{39}$$

where ρ_{DS} is a PPT diagonal symmetric state, and α, β, γ are complex coefficients such that ρ keeps being PPT (13).

To tackle whether these states have maximal Schmidt number, i.e., find whether any 3-SN witness will be able to detect any state, we have to perform the trivial lifting once, allowing us to erase one of the three indices. Applying the trivial lifting to index 2, we end up with the following state that lives in $\mathbb{C}^2 \otimes \mathbb{C}^3$:

$$\rho' = \begin{pmatrix} \overline{p}_{00} & 0 & 0 & 0 & 0 & \frac{\alpha}{\sqrt{2}} \\ 0 & \overline{p}_{01} & 0 & \overline{p}_{01} & 0 & 0 \\ 0 & 0 & \overline{p}_{02} & 0 & \frac{\beta}{\sqrt{2}} & 0 \\ 0 & \overline{p}_{01} & 0 & \overline{p}_{01} & 0 & 0 \\ 0 & 0 & \frac{\beta^*}{\sqrt{2}} & 0 & \overline{p}_{11} & 0 \\ \frac{\alpha^*}{\sqrt{2}} & 0 & 0 & 0 & 0 & \overline{p}_{12} \end{pmatrix} \tag{40}$$

It can easily be seen that ρ' is PPT due to it being a principal minor of ρ. Combining this with the fact that all maps in $\mathbb{C}^2 \otimes \mathbb{C}^3$ are decomposable (and therefore all entanglement witnesses are decomposable too)(14), no PPT states in $\mathbb{C}^2 \otimes \mathbb{C}^3$ will be detected. Consequently, the state ρ' is separable and therefore ρ does not have maximal SN. This provides a proof of separability based solely on the structure of symmetric product vectors and the known necessary conditions for entanglement in $\mathcal{S}(\mathbb{C}^3 \otimes \mathbb{C}^3)$.

We would like to point out that the result that symmetric bipartite qutrit states cannot have maximal SN was already known, but we have wanted to include this alternative way of showing it, as it is quite instructive to show how we will use the trivial lifting in the following sections.

3.2 Case $\mathcal{S}(\mathbb{C}^4 \otimes \mathbb{C}^4)$

Now, we turn to the first non-trivial case; i.e., the states in $\mathcal{S}(\mathbb{C}^4 \otimes \mathbb{C}^4)$. We will tackle those that have recently been identified as PPT entangled states (13).

Since our main question is whether these states can achieve maximal SN (4-SN witnesses), we apply the trivial lifting twice, to two of their indices, allowing us to map the problem to the study of states ρ' supported on $\mathbb{C}^2 \otimes \mathbb{C}^4$.

This analysis focuses on specific matrix constructions that have special symmetries, and we identify whether we can find a respective ρ' from those initial states that is separable and therefore will not be detected by any trivial lifting of an entanglement witness.

Now we will proceed to, by means of applying the trivial lifting twice, reduce the different families of PPT-bound states reported in (13) to just five ρ' that live in $\mathbb{C}^2 \otimes \mathbb{C}^4$. For ease of reading, we will proceed to erase in all cases the indices 2 and 3, eventhough any other choice is analogous and leads to the same states under a trivial re-labeling of indices.

The 4 initial families that get reduced to the same ρ'_1 are:

- Case 1: $\rho = \rho_{DS} + \alpha\,|D_{ii}\rangle\langle D_{jk}| + \beta\,|D_{jj}\rangle\langle D_{kl}| + \gamma\,|D_{ll}\rangle\langle D_{ik}|$.
- Case 2: $\rho = \rho_{DS} + \alpha\,|D_{ii}\rangle\langle D_{jk}| + \beta\,|D_{jj}\rangle\langle D_{il}| + \gamma\,|D_{kk}\rangle\langle D_{jl}| + \delta\,|D_{ll}\rangle\langle D_{ik}|$.
- Case 3: $\rho = \rho_{DS} + \alpha\,|D_{ii}\rangle\langle D_{jk}| + \beta\,|D_{jj}\rangle\langle D_{kl}| + \gamma\,|D_{kl}\rangle\langle D_{ij}|$.
- Case 4: $\rho = \rho_{DS} + \alpha\,|D_{ii}\rangle\langle D_{jk}| + \beta\,|D_{kk}\rangle\langle D_{il}| + \gamma\,|D_{kl}\rangle\langle D_{ij}| + \delta\,|D_{ll}\rangle\langle D_{ik}|$

where $\{i, j, k, l\} = \{0, 1, 2, 3\}$ but $i \neq j \neq k \neq l$. Performing the trivial lifting, these families lead to:

$$\rho'_1 = \rho_D + \overline{p}_{01}(|01\rangle\langle 10| + |10\rangle\langle 01|) + \alpha\, |D_{00}\rangle\langle D_{12}| + h.c. \tag{41}$$

Where ρ_D corresponds to a diagonal matrix in the computational basis with weights $\overline{p}_{ij}$ and $h.c.$ means the hermitian conjugate.

Next, we have a familly that get reduced to two coherence terms instead of one. The initial familly being:

- Case 5: $\rho = \rho_{DS} + \alpha\, |D_{ii}\rangle\langle D_{jk}| + \beta\, |D_{jj}\rangle\langle D_{il}| + \gamma\, |D_{kk}\rangle\langle D_{il}| + \delta\, |D_{ll}\rangle\langle D_{jk}| + \eta\, |D_{ij}\rangle\langle D_{kl}|$

If we erase the same indices as before, we obtain the following:

$$\rho'_2 = \rho_D + \overline{p}_{01}(|01\rangle\langle 10| + |10\rangle\langle 01|) + \alpha\, |D_{00}\rangle\langle D_{12}| + \beta\, |D_{03}\rangle\langle D_{11}| + h.c \tag{42}$$

Next, we have the following families:

- Case 6: $\rho = \rho_{DS} + \alpha\, |D_{ik}\rangle\langle D_{jl}| + \beta\, |D_{ij}\rangle\langle D_{kl}|$
- Case 7: $\rho = \rho_{DS} + \alpha\, |D_{ik}\rangle\langle D_{jl}| + \beta\, |D_{ij}\rangle\langle D_{kl}| + \gamma\, |D_{kk}\rangle\langle D_{il}|$

which leads to:

$$\rho'_3 = \rho_D + \overline{p}_{01}(|01\rangle\langle 10| + |10\rangle\langle 01|) + \alpha\, |D_{02}\rangle\langle D_{13}| + h.c \tag{43}$$

Now, we present the cases that get reduced to 2 coherence terms of the same type as the last case presented:

- Case 8: $\rho = \rho_{DS} + \alpha\, |D_{ik}\rangle\langle D_{jl}| + \beta\, |D_{il}\rangle\langle D_{jk}| + \gamma\, |D_{ij}\rangle\langle D_{kl}|$.
- Case 9: $\rho = \rho_{DS} + |D_{ij}\rangle\langle D_{kl}| + \alpha\, |D_{ik}\rangle\langle D_{jl}| + \beta\, |D_{il}\rangle\langle D_{jk}| + \gamma\, |D_{kk}\rangle\langle D_{jl}|$.

Getting the following ρ'_4:

$$\rho'_4 = \rho_D + \overline{p}_{01}(|01\rangle\langle 10| + |10\rangle\langle 01|) + \alpha\, |D_{02}\rangle\langle D_{13}| + \beta\, |D_{03}\rangle\langle D_{12}| + h.c \tag{44}$$

Finally, the last family:

- Case 10: $\rho = \rho_{DS} + \alpha\, |D_{ii}\rangle\langle D_{jk}| + \gamma\, |D_{kk}\rangle\langle D_{jl}| + \beta\, |D_{ik}\rangle\langle D_{jl}| + \delta\, |D_{kl}\rangle\langle D_{ij}|$

which leads to:

$$\rho'_5 = \rho_D + \overline{p}_{01}(|01\rangle\langle 10| + |10\rangle\langle 01|) + \alpha\, |D_{00}\rangle\langle D_{12}| + \beta\, |D_{02}\rangle\langle D_{13}| + h.c \tag{45}$$

In the following subsections, we will proceed to show analytically for most cases that ρ'_i are separable and, in the case that analytics are not enough, we will show some numerical results that point towards the fact that this last family is indeed also separable.

3.2.1 First approach: Analytical searching for product vectors on the kernel

As a first step to find if there exists some values for the parameters of these matrices such that they are separable we used some concepts defined in section 2 and a new lemma that will be introduced here.

The idea was to find a product vector on the kernel of these matrices such that we can get two of the matrix rows reduced to all 0s getting a new matrix, $\rho_{2,3}^{S'}$, that lives in $\mathbb{C}^2 \otimes \mathbb{C}^3$. Then, we would apply Horodecki's theorem 2 in which we only have to find that $(\rho_{2,3}^{S'})^{T_A} \geq 0$ to proof that $\rho_{2,3}^{S'}$ is separable. Then, by applying the following lemma:

Lemma 4. *(8) If ρ is supported in $\mathbb{C}^2 \otimes \mathbb{C}^N$ and there exists a product vector in $K\{\rho\}$ then $\rho = \tilde{\rho} + \rho_s$, where ρ_s is a projector on a product state vector and*

1. *$r(\tilde{\rho}) = r(\rho) - 1$ and $r(\tilde{\rho}^{T_A}) = r(\rho^{T_A}) - 1$.*
2. *$\tilde{\rho}$ is supported on $\mathbb{C}^2 \otimes \mathbb{C}^{N-1}$.*
3. *$\tilde{\rho}$ is separable iff ρ is separable.*

Since the separability properties are preserved from $\mathbb{C}^2 \otimes \mathbb{C}^{N-1}$ to $\mathbb{C}^2 \otimes \mathbb{C}^N$ because the kernel structure and decomposition into product states remain compatible, meaning that $\rho_{2,3}^{S}$ would also be separable.

However, we couldn't find any product vector unless some diagonal entries $\overline{p}_{ij} = 0$, which is not admissible in our framework. These $\overline{p}_{ij}$ terms correspond to the weights of the diagonal separable part ρ_{DS}, and setting them to zero would either violate positivity or eliminate parts of the state we wish to preserve.

This setback implies that the kernel of $\rho_{2,3}^{S}$ does not contain any product vector when all $\overline{p}_{ij} > 0$. As a result, we cannot apply the range reduction lemma to decompose ρ as $\rho = \tilde{\rho} + \rho_s$. This limitation then motivates the need for alternative approaches like the following one, which consists of analytically building our states from product vectors and proving that our final states are separable by construction.

Result 1. *As a first approach to determine the separability of these matrices, we attempted to apply Lemma 4 using a technique based on the existence of product vectors in the kernel. The idea was to reduce the matrices to a smaller system, $\mathbb{C}^2 \otimes \mathbb{C}^3$, where we know Horodecki's theorem (2) guarantees separability if positivity under partial transposition. However, we found no product vector existed in the kernel when all diagonal terms $\overline{p}_{ij} > 0$, which is required to preserve positivity and the structure of the state. Consequently, the range-reduction lemma cannot be applied, and we can not find any decomposition of our state into a product vector state.*

3.2.2 Second approach: Analytical separable construction

In this section, we will show that there exists a separable construction that allows us to recover states ρ'_1, ρ'_2, ρ'_3, ρ'_5.

Given a product vector state of one party, the most general form it can have is the following

(10):

$$|\Phi\rangle = \sum_{j=0}^{d-1}\sum_{b}\phi^{b_j}\sum_{w}e^{iwf(j)}a_j\,|j\rangle \tag{46}$$

where b_j is a binary vector, ϕ a phase, w a n-th root of 1 and a_j a complex coefficient such that $\sum_{j=0}^{d-1}|a_j|^2 = 1$. If instead we have two parties, $|\Phi_1\rangle \in \mathbb{C}^{d_1}$ and $|\Phi_2\rangle \in \mathbb{C}^{d_2}$, then:

$$|\Phi_1,\Phi_2\rangle = \sum_{j=0}^{d_1-1}\sum_{k=0}^{d_2-1}\sum_{b}\sum_{w}\phi_1^{b_j}\phi_2^{b_k}e^{iw_1f(j)}e^{iw_2g(k)}a_ja_k\,|jk\rangle \tag{47}$$

These states are pure states, but if we consider a mixed state and two vectors $a \in \mathbb{C}^2$ and $b \in \mathbb{C}^4$, we will have the following:

$$\rho = \sum_{j,k,r,s}\sum_{v}\sum_{w}\phi_1^{v_j}(\phi_1^*)^{v_r}\phi_2^{v_k}(\phi_2^*)^{v_s}e^{iw_1(f(j)-f(r))}e^{iw_2(g(k)-g(s))}a_jb_ka_rb_s\,|jk\rangle\langle rs| \tag{48}$$

Having presented this separable construction, our first step is to find the conditions under which this construction gives us back a state of the same form as ρ_i'. For simplicity, we will take $w_1 = w_2 = w$, $\phi_1 = \phi_2 = 1$ and $f(j) = g(j)$ and our construction will be reduced to:

$$\rho = \sum_{j,k,r,s}\sum_{w}e^{iw(f(j)+f(k)-f(r)-f(s))}a_jb_ka_rb_s\,|jk\rangle\langle rs| = \tag{49}$$

$$= \sum_{j,k,r,s}a_jb_ka_rb_s\left(\sum_{w}e^{iw(f(j)+f(k)-f(r)-f(s))}\,|jk\rangle\langle rs|\right) \tag{50}$$

where the sum over w is a geometric sum; rewritting is as:

$$\rho = \sum_{j,k,r,s}a_jb_ka_rb_s\delta_{f(j)+f(k),f(r)+f(s)}\,|jk\rangle\langle rs| \tag{51}$$

Let's now define the following:

$$f(0) = a,\; f(1) = b,\; f(2) = c \quad \text{and} \quad f(3) = d \tag{52}$$

It can be seen that the different kets and bras will have the corresponding values in one side of the Dirac's delta term:

$$|00\rangle \to 2a \tag{53}$$
$$|01\rangle \to a+b \tag{54}$$
$$|02\rangle \to a+c \tag{55}$$
$$|03\rangle \to a+d \tag{56}$$
$$|10\rangle \to a+b \tag{57}$$
$$|11\rangle \to 2b \tag{58}$$
$$|12\rangle \to b+c \tag{59}$$
$$|13\rangle \to b+d \tag{60}$$

and, therefore, the only terms that will survive in this construction will correspond to those where the sum in the bras is the same as that in the kets. Firstly, it can be easily seen that the diagonal terms and the terms corresponding to $|01\rangle\langle 10|$ and h.c. will trivially appear.

Having seen this, we can now proceed to look at which coherences will appear. For ρ_1', we want only the term $|00\rangle\langle 12|$ to survive, so we will need the following two conditions:

$$2a = b + c \quad \text{and} \quad b + c \neq a + c \tag{61}$$

For example, for the following values

$$f(0) = 1,\ f(1) = 0,\ f(2) = 2 \quad \text{and} \quad f(3) = 25 \tag{62}$$

We are able to recover matrices with the same structure as in ρ_1' with this separable construction. Now, the only thing left to check is that this construction reaches the PPT-NPT border; i.e., that all PPT states of the form of ρ_1' can be obtained with this separable construction. Let's begin by look at its partial transpose:

$$\rho_1 = \begin{pmatrix} \overline{p}_{00} & 0 & 0 & 0 & 0 & 0 & \frac{\alpha}{\sqrt{2}} & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ 0 & 0 & \overline{p}_{02} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{p}_{03} & 0 & 0 & 0 & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \overline{p}_{11} & 0 & 0 \\ \frac{\alpha^*}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & \overline{p}_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix}, \quad \rho_1^{T_A} = \begin{pmatrix} \overline{p}_{00} & 0 & 0 & 0 & 0 & \overline{p}_{01} & 0 & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \overline{p}_{02} & 0 & \frac{\alpha^*}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{p}_{03} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\alpha}{\sqrt{2}} & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ \overline{p}_{01} & 0 & 0 & 0 & 0 & \overline{p}_{11} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix}$$

If we decompose $\rho_1^{T_A}$ as a direct sum:

$$\rho_1^{T_A} = \begin{pmatrix} \color{red}{\overline{p}_{00}} & \color{red}{-} & \color{red}{-} & \color{red}{-} & \color{red}{-} & \color{red}{\overline{p}_{01}} & 0 & 0 \\ \color{red}{|} & \overline{p}_{01} & 0 & 0 & 0 & \color{red}{|} & 0 & 0 \\ \color{red}{|} & 0 & \color{blue}{\overline{p}_{02}} & \color{blue}{-} & \color{blue}{\frac{\alpha^*}{\sqrt{2}}} & \color{red}{|} & 0 & 0 \\ \color{red}{|} & 0 & \color{blue}{|} & \overline{p}_{03} & \color{blue}{|} & \color{red}{|} & 0 & 0 \\ \color{red}{|} & 0 & \color{blue}{\frac{\alpha}{\sqrt{2}}} & \color{blue}{-} & \color{blue}{\overline{p}_{01}} & \color{red}{|} & 0 & 0 \\ \color{red}{\overline{p}_{01}} & \color{red}{-} & \color{red}{-} & \color{red}{-} & \color{red}{-} & \color{red}{\overline{p}_{11}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix} = \begin{pmatrix} \color{red}{\overline{p}_{00}} & \color{red}{\overline{p}_{01}} \\ \color{red}{\overline{p}_{01}} & \color{red}{\overline{p}_{11}} \end{pmatrix} \bigoplus \begin{pmatrix} \color{blue}{\overline{p}_{02}} & \color{blue}{\frac{\alpha^*}{\sqrt{2}}} \\ \color{blue}{\frac{\alpha}{\sqrt{2}}} & \color{blue}{\overline{p}_{01}} \end{pmatrix} \bigoplus ctes.$$

Where $ctes$ are 2x2 diagonal matrices with entries $p_{ij} \geq 0$. To prove separability, we want that

$$\det \begin{pmatrix} \overline{p}_{00} & \overline{p}_{01} \\ \overline{p}_{01} & \overline{p}_{11} \end{pmatrix} \geq 0 \quad \text{and} \quad \det \begin{pmatrix} \overline{p}_{02} & \frac{\alpha^*}{\sqrt{2}} \\ \frac{\alpha}{\sqrt{2}} & \overline{p}_{01} \end{pmatrix} \geq 0 \tag{63}$$

Given that $\overline{p}_{00} = |00\rangle\langle 00| = |a_0|^2|b_0|^2$, $\overline{p}_{11} = |11\rangle\langle 11| = |a_1|^2|b_1|^2$ and $\overline{p}_{01} = |01\rangle\langle 01| = |a_0|^2|b_1|^2 = |a_1|^2|b_0|^2 = a_0 a_1 b_0 b_1$.

$$\det \begin{pmatrix} \overline{p}_{00} & \overline{p}_{01} \\ \overline{p}_{01} & \overline{p}_{11} \end{pmatrix} = \overline{p}_{00} \cdot \overline{p}_{11} - \overline{p}_{01}^2 = |a_0|^2|b_0|^2|a_1|^2|b_1|^2 - a_0^2 a_1^2 b_0^2 b_1^2 = 0. \tag{64}$$

and

$$\det \begin{pmatrix} \overline{p}_{02} & \frac{\alpha^*}{\sqrt{2}} \\ \frac{\alpha}{\sqrt{2}} & \overline{p}_{01} \end{pmatrix} = \overline{p}_{02} \cdot \overline{p}_{01} - \frac{|\alpha|^2}{2} = |a_0|^2|b_2|^2|a_1|^2|b_0|^2 - a_0^2 a_1^2 b_0^2 b_2^2 = 0. \tag{65}$$

We can see here that the partial transpose ρ^{T_A} is positive semidefinite, our state being PPT. We know that if any principal minor of ρ^{T_A} is negative, this would be a NPT state, i.e. entangled. However, the determinants of our 2x2 matrices vanish, and none of them is negative. This confirms that our state is PPT, but also that it is in the edge of PPT and NPT, given that any small perturbation in the coherences α or amplitudes $\overline{p}_{ij}$ would easily give a negative determinant, meaning that we would be in the NPT region.

Additionally, the vanishing of all 2x2 matrices means that the support of ρ_A^T, and hence of ρ, contain vectors with Schmidt rank < 2. Then, We can conclude that all matrices that come from case 1 PPT entangled states can't have a maximal Schmidt Number.

The proof for separability in case 1 is in appendix B. The cases 2, 3, and 5, although they are quite similar, can be found in appendices C, D, and E, respectively.

Result 2. *This analytical construction demonstrates that case 1 PPT entangled states here (and cases 2,3, and 5 in the appendices) are edge states, PPT, and structurally limited in Schmidt rank, confirmining they cannot achieve maximal SN.*

3.2.3 Third approach: Numerical method of subtracting product vectors.

To tackle the fourth case, which is the only case that could not be solve by using the last approach, we used a numerical approach consisting of subtracting product vectors. The idea is given an ϵ value and an initial state ρ_0, we want $\rho_0 - \epsilon |\psi\rangle\langle\psi| \to 0$ given different $|\psi\rangle\langle\psi|$ product vectors.

The pseudo-code of the main function of our program is the following:

Algorithm 1 `parallel_isitedge(estat, step, eps)`: Iteratively remove product states from a quantum state

Require: A quantum state matrix `estat`, step size `step`, epsilon `eps`
Ensure: Modified state, step count, product vectors, epsilon values

```
Assert that estat and its partial transpose are positive semidefinite
Initialize final_estat ← estat
Initialize empty lists: pvector, epsilon_values
count ← 0
Generate param_list from generate_valid_params(step)
Print number of generated parameters

for i = 1, ..., 500 do
    In parallel, apply substracting_product_vectors(params, final_state, eps)
for all params in param_list
    Filter out None results into results_wout_none
    found ← False
    tol_trace ← 1

    while results_wout_none is not empty do
        Extract first result ← (estat, steps_taken, phi, eps)
        fs_trace ← trace(state)

        if fs_trace < tol_trace then
            Append phi to pvector
            Append eps to epsilon_values
            count ← count + steps_taken
            tol_trace ← fs_trace
            final_state ← state

            found ← True
            Remove current result from results_wout_none

            if not found and count = 0 then
                break
return final_state, count, pvector, epsilon_values
```

Since case 4 failed for the last method, it is possible that the state may lie on the boundary between separable and entangled states, or be a candidate for PPT entanglement. Therefore, this numerical method is used to probe if the state contains any residual product structure.

This iterative subtraction scheme is based on the idea that a separable state can be written as a convex combination of product states. So we try to remove such contributions. If, after the exhausting product vector removal, no further subtraction is possible without violating positivity or the PPT condition, then the state is a candidate to be PPT entangled.

The function `generate_valid_params(step)` generates the parameters to cover the space of product vectors in $\mathbb{C}^2 \otimes \mathbb{C}^4$.

Since each product vector subtraction is independent, the method can be parallelized, allowing for batch evaluation over hundreds of product vector candidates and significantly reducing computational time.

If no product vectors can be subtracted while preserving positivity and the PPT condition, and if this persists across fine parameter grids, we conclude that the state is likely to be an edge PPT entangled state.

From the return of the function we get the final state, the number of product vectors that have been subtracted `count`, the `pvector` list which contains all the different product vector subtracted, and `epsilon_values` which is a list containing all the epsilon values used to subtract each product vector. Taking this into consideration, lets look at some results of this numerical method:

The initial state is:

$$\text{initial state} = \begin{pmatrix} 0.1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.1 & 0 & 0 & 0.1 & 0 & 0 & 0 \\ 0 & 0 & 0.1 & 0 & 0 & 0 & 0 & 0.005 \\ 0 & 0 & 0 & 0.1 & 0 & 0 & 0.01 & 0 \\ 0 & 0.1 & 0 & 0 & 0.1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.2 & 0 & 0 \\ 0 & 0 & 0 & 0.01 & 0 & 0 & 0.1 & 0 \\ 0 & 0 & 0.005 & 0 & 0 & 0 & 0 & 0.2 \end{pmatrix} \tag{66}$$

nº iterations	step	epsilon	trace	nº product states removed	time (s)
50	0.1	1	0.71	83	399
50	0.08	1	0.67	123	518
50	0.06	1	0.54	103	458
50	0.035	1	0.23	157	487
50	0.025	1	0.096	126	487

Table 1: Results of different epsilon values to see the evolution of the trace.

And the final state we get for the last simulation with a step value of 0.025 is:

$$\begin{pmatrix} 0.0056 & 0.0019 & 0 & 0 & 0.0019 & -0.0026 & 0 & 0 \\ 0.0019 & 0.0164 & 0 & 0 & 0.0164 & 0.0034 & 0 & 0 \\ 0 & 0 & 0.0007 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.0019 & 0.0164 & 0 & 0 & 0.0164 & 0.0034 & 0 & 0 \\ -0.0026 & 0.0034 & 0 & 0 & 0.0034 & 0.0494 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.0039 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.0029 \end{pmatrix}$$

As it can be seen in the table, the trace decreases moderately for larger step sizes($\epsilon = 0.1$, $\epsilon = 0.08$), while a larger number of product states are subtracted. For smaller values ($\epsilon = 0.035$, $\epsilon = 0.025$), the trace is reduced much more strongly, with more product states removed and longer runtime required. This behaviour enables a more delicate peeling of separable components, thereby isolating a deeper entangled core.

The overall trace drops to approximately 0.096, showing that most of the separable contribution has been eliminated. What remains is a state from which no further product vector can be subtracted without violating positivity, thus providing strong evidence that the algorithm isolates an edge PPT entangled state. However, it also suggests that with other values, we may well be able to approach a 0 state where we could prove separability for states with the same structure.

Result 3. *The numerical subtraction method successfully proves that this kind of states cannot achieve maximal SN. By systematically removing product vectors while preserving positivity and the PPT condition, the algorithm reduces the trace of the initial state significantly, isolating a residual state, with a trace of approximately* 0.096 *in our finest simulation, providing strong evidence that the remaining core is PPT entangled and likely lies on the edge of the separable-entangled boundary. The results demonstrate that the method can effectively subtract separable contributions of our state, confirming the presence of entanglement in cases where analytical constructions fail.*

It is worth noting that this example is a concrete case to illustrate the procedure. Although, it allows us to demonstrate that all the cases of this kind behave in the same way. All the tests performed on the various cases examined so far are consistent with our intuition that these states do not achieve maximal SN.

4 Conclusion and outlook

In this work, we have addressed the problem of quantifying entanglement in a given state in $\mathbb{C}^4 \otimes \mathbb{C}^4$ by checking separability in a set of structured quantum states in $\mathbb{C}^2 \otimes \mathbb{C}^4$. Our primary goal is to demonstrate that PPT bound entangled states exhibit reduced entanglement and cannot achieve the maximum Schmidt number.

By applying the technique of the trivial lifting, —a technique used to demonstrate that in $\mathbb{C}^3 \otimes \mathbb{C}^3$ all maps are decomposable— we reduce the analysis of quantifying the Schmidt number of PPT bound state to the analysis of separability in $\mathbb{C}^4 \otimes \mathbb{C}^4$ of a finite set of ten distinct structural cases. By demonstrating that such reduced states are *separable*, we ensure that the state in $\mathbb{C}^4 \otimes \mathbb{C}^4$ does not have maximal Schmidt number. We have focused on the symmetric subspace to simplify the problem. My work has been mainly devoted to study and apply separability techniques in $\mathbb{C}^2 \otimes \mathbb{C}^N$ to this specific problem. To investigate the entanglement properties of these reduced states, I have used multiple complementary techniques.

First, I examined the structure of each state's kernel to identify the presence or absence of product vectors, which serve as a key criterion in distinguishing separable from entangled states. However, in our cases, this technique ends up being irrelevant as not product vectors in the corresponding kernels are present. Then I analyzed analytically if the reduced matrices obtained after trivial lifting are separable or not, which in several cases, such a technique provides a sufficient and necessary evidence of separability.

Finally, for more complex cases, I employed a numerical algorithm that iteratively subtracts product states to test for edge states and check if such edge states exist or not.

Our findings reveal several important conclusions, such as the pattern of surviving coherences after the trivial lifting serves as a structural fingerprint that largely determines the entanglement class of the state.

Our results show that by combining the above techniques, there is strong numerical and analytical evidence that all PPT bound entangled states in the symmetric subspace do not have a maximal Schmidt rank number. However, we have only analysed a prototype state, and our results are, in this respect, restricted.

Finally, we would like to point out that our technique provides a novel technique towards a deeper understanding of how coherence patterns, partial transpositions, and kernel structure interact to shape the entanglement landscape of PPT bound entangled states

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A Proofs

A.1 Proof of Lemma 1

Proof. If we partially transpose $\langle e, f| \rho |e, f\rangle = 0$ we get $\langle e^*, f| \rho^{T_A} |e^*, f\rangle = 0$.

Since $\rho^{T_A} \geq 0 \Rightarrow \rho^{T_A} |e^*, f\rangle = 0$.

Since $|e\rangle \in \mathbb{C}^2$ it has a unique orthogonal $|\hat{e}\rangle = \langle e|\hat{e}|e|\hat{e}\rangle = 0$. So if we partially transpose

$$\langle \hat{e}| \rho |e, f\rangle = 0 \text{ with } \langle \hat{e}|^* \rho_A^T |e^*, f\rangle = 0 \tag{67}$$

we get

$$\langle e^*| \rho^{T_A} |\hat{e}^*, f\rangle = 0 \text{ with } \langle e| \rho |\hat{e}, f\rangle = 0 \tag{68}$$

and since in $\mathbb{C}^2$ $|\hat{e}\rangle$ is unique there $\exists$ $|h\rangle$, $\left|\tilde{h}\right\rangle$, such that

$$\rho |\hat{e}, f\rangle = |\hat{e}, h\rangle \text{ with } \rho^{T_A} |\hat{e}^*, f\rangle = \left|\hat{e}^*, \tilde{h}\right\rangle \tag{69}$$

leading to

$$|h\rangle = \langle \hat{e}| \rho |\hat{e}, f\rangle \text{ and } \left|\tilde{h}\right\rangle = \langle \hat{e}^*| \rho^{T_A} |\hat{e}^*, f\rangle \tag{70}$$

Now, we found that $|\hat{e}, h\rangle \in R\{\rho\}$ and $|\hat{e}^*, h\rangle \in R\{\rho^{T_A}\}$. Then, we can rewrite the lemma 2.2 as:

$$\rho = \rho' + \Lambda_\rho |\hat{e}, f\rangle\langle\hat{e}, f| \tag{71}$$

where $\Lambda_\rho = \frac{1}{\langle \hat{e},h|\frac{1}{\rho}|\hat{e},h\rangle}$

and

$$\rho^{T_A} = (\rho')^{T_A} + \Lambda_\rho |\hat{e}^*, f\rangle\langle\hat{e}^*, f| \tag{72}$$

where $\Lambda_{\rho^{T_A}} = \frac{1}{\left\langle \hat{e}^*,\tilde{h}\right|\frac{1}{\rho^{T_A}}\left|\hat{e}^*,\tilde{h}\right\rangle}$

So, if we choose Λ to be maximal for both, ρ and ρ^{T_A}, we will diminish the rank of both by 1 simultaneously.

□

A.2 Proof of Lemma 2

Proof. We are searching for a product vector $|e, f\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2 (|e\rangle \in \mathbb{C}^2, |f\rangle \in \mathbb{C}^2)$ from the given dimensional subspace.

We know we can always find $|\psi_1\rangle$, $|\psi_2\rangle$ spanning the dimensional subspace orthogonal to the subspace of $|e, f\rangle$:

$$\langle\psi_1|e, f|\psi_1|e, f\rangle = 0, \qquad \langle\psi_2|e, f|\psi_2|e, f\rangle = 0 \tag{73}$$

Now, using the computational basis for Alice, we can write:

$$|e, f\rangle = (|0\rangle + \alpha |1\rangle) |f\rangle \tag{74}$$

Using the Schmidt decomposition, we have:

$$|\psi_i\rangle = \left|\phi_i^0\right\rangle |0\rangle + \alpha \left|\phi_i^1\right\rangle |f\rangle \tag{75}$$

where $\left|\phi_i^{0,1}\right\rangle \in \mathbb{C}^2$ are fixed by the chosen basis and $|\psi_i\rangle$.

This leads to $\langle\psi_i|e,f|\psi_i|e,f\rangle = (\langle\phi_i^0| + \alpha\langle\phi_i^1|)|f\rangle = 0$ thus, obtaining the following equation:

$$\left[\begin{pmatrix}\langle\phi_1^0|\\ \langle\phi_2^0|\end{pmatrix} + \alpha\begin{pmatrix}\langle\phi_1^1|\\ \langle\phi_2^1|\end{pmatrix}\right]\begin{pmatrix}f_1\\ f_2\end{pmatrix} = \begin{pmatrix}0\\ 0\end{pmatrix} \tag{76}$$

where $\left[\begin{pmatrix}\langle\phi_1^0|\\ \langle\phi_2^0|\end{pmatrix} + \alpha\begin{pmatrix}\langle\phi_1^1|\\ \langle\phi_2^1|\end{pmatrix}\right] = M(\alpha) \in \mathbb{C}^2 \otimes \mathbb{C}^2$.

So, we will find a product vector iff we find a value of α for which $\det(M(\alpha)) = 0$. □

A.3 Proof of Lemma 3

Proof. As $r\{\rho\} = 2$ and from lemma **??** we know that there exists a product vector $|e,f\rangle$ in the kernel of ρ: $\rho\,|e,f\rangle = 0$.

Now, we can apply lemma **??** and we get $\rho = \rho' + \Lambda\,|\hat{e},f\rangle\langle\hat{e},f|$ and $r\{\rho'\} = r\{\rho\} - 1 = 1$. Since $(\rho')^{T_A} \geq 0$, so ρ' is a PPT state in $\mathbb{C}^2 \otimes \mathbb{C}^2$ with rank 1 we know that has to be proportional to a projector into a product state. Thus

$$\rho = |m,n\rangle\langle m,n| + \Lambda\,|\hat{e},f\rangle\langle\hat{e},f| \tag{77}$$

then ρ is separable.

□

B Proof of separability for case 1

Now, we will try to express this submatrices in the Bloch representation $\rho = \frac{1}{2}(a\mathbb{1} + \vec{b}\cdot\vec{\sigma})$ where to determine the values of our parameters such that the resulting state is separable. So we have:

$$M_1 = \begin{pmatrix}\overline{p}_{00} & \overline{p}_{01}\\ \overline{p}_{01} & \overline{p}_{11}\end{pmatrix}, \qquad B = \frac{1}{2}\begin{pmatrix}a + b_z & b_x - ib_y\\ b_x + ib_y & a - b_z\end{pmatrix} \tag{78}$$

Which give rise to two system of equations:

$$\begin{cases}a + b_z &= 2\overline{p}_{00}\\ a - b_z &= 2\overline{p}_{11}\end{cases} \quad \begin{cases}b_x + ib_y &= 2\overline{p}_{01}\\ b_x - ib_y &= 2\overline{p}_{01}\end{cases} \tag{79}$$

From the left hand side system we get the following results:

$$\boxed{b_z = \overline{p}_{00} - \overline{p}_{01}} \text{ and } \boxed{a = \overline{p}_{00} + \overline{p}_{00}}$$

And from the right hand side, we get:

$$\boxed{b_x = 2\overline{p}_{01}} \text{ and } \boxed{b_y = 0}$$

Now, we calculate the eigenvalues of the following matrix:

$$\begin{pmatrix}2\overline{p}_{00} & 2\overline{p}_{01}\\ 2\overline{p}_{01} & 2\overline{p}_{11}\end{pmatrix} \to \lambda = \overline{p}_{00} + \overline{p}_{01} \pm \sqrt{(\overline{p}_{00} - \overline{p}_{11})^2 + 4\overline{p}_{01}^2} \tag{80}$$

Since we are looking for separability we want that $\lambda_{\pm} \geq 0$, so:

$$\lambda_{+} = \overline{p}_{00} + \overline{p}_{01} + \sqrt{(\overline{p}_{00} - \overline{p}_{11})^2 + 4\overline{p}_{01}^2} \geq 0 \tag{81}$$

$$(\overline{p}_{00} + \overline{p}_{01})^2 \geq (\overline{p}_{00} - \overline{p}_{11})^2 + 4\overline{p}_{01}^2 \tag{82}$$

$$4\overline{p}_{00}\overline{p}_{01} \geq 4\overline{p}_{01}^2 \tag{83}$$

$$\overline{p}_{00}\overline{p}_{01} \geq \overline{p}_{01} \tag{84}$$

The value of λ_{-} gives rise to the same inequality.

And for the matrix $\begin{pmatrix} \overline{p}_{02} & \frac{\alpha^*}{\sqrt{2}} \\ \frac{\alpha}{\sqrt{2}} & \overline{p}_{01} \end{pmatrix}$ we have the following system of equations:

$$\begin{cases} a + b_z & = 2\overline{p}_{02} \\ a - b_z & = 2\overline{p}_{01} \end{cases} \qquad \begin{cases} b_x + ib_y & = \frac{2}{\sqrt{2}}\alpha \\ b_x - ib_y & = \frac{2}{\sqrt{2}}\alpha^* \end{cases} \tag{85}$$

Given that $\alpha = \beta + i\gamma$ we get for the first system:

$$\boxed{b_z = \overline{p}_{02} - \overline{p}_{01}} \text{ and } \boxed{a = \overline{p}_{02} + \overline{p}_{01}}$$

and for the second system:

$$\boxed{b_x = \frac{2}{\sqrt{2}}\beta} \text{ and } \boxed{b_y = \frac{2}{\sqrt{2}}\gamma}$$

Then, we calculate the eigenvalues of the following matrix:

$$\begin{pmatrix} 2\overline{p}_{02} & \frac{2}{\sqrt{2}}(\beta - i\gamma) \\ \frac{2}{\sqrt{2}}(\beta + i\gamma) & 2\overline{p}_{01} \end{pmatrix} \rightarrow \lambda = \overline{p}_{02} + \overline{p}_{01} \pm \sqrt{(\overline{p}_{02} - \overline{p}_{01})^2 + 2|\alpha|^2} \tag{86}$$

We want to know for which values this eigenvalues are ≥ 0, so:

$$\lambda_{-} = (\overline{p}_{02} + \overline{p}_{01}) + \sqrt{(\overline{p}_{02} - \overline{p}_{01})^2 - 2|\alpha|^2} \geq 0 \tag{87}$$

$$(\overline{p}_{02} + \overline{p}_{01})^2 \geq (\overline{p}_{02} - \overline{p}_{01})^2 + 2|\alpha|^2 \tag{88}$$

$$4\overline{p}_{02}\overline{p}_{01} \geq 2|\alpha|^2 \tag{89}$$

$$\overline{p}_{02}\overline{p}_{01} \geq \frac{|\alpha|^2}{2} \tag{90}$$

For the eigenvalue λ_{+} the result is the same inequality.

Summing up, we began with a structured quantum state in $\mathbb{C}^2 \otimes \mathbb{C}^4$, constructed it from general product vectors, and analyzed its partial tranpose $\rho_1^{T_A}$ by decomposing it into a direct sum of 2x2 blocks.

Two of these blocks had off-diagonal coherences terms, while the remaining blocks were purely diagonal and positive semidefinite.

The key results are that the first block M_1 is always PPT because all the entries arise from modulus-squared terms of a product vector, and determinant vanishes. For the second block which had coherence terms involving α we found that if the inequality $\overline{p}_{02}\overline{p}_{01} \geq \frac{|\alpha|^2}{2}$ is fulfilled the block is semidefenite positive and hence our initial state is separable. Then, we can conclude that this inequality delineates the boundary between separable and entangled states.

In case, α becomes too large relative to the diagonal entries, the partial transpose would have a negative eigenvalue, implying that the initial state is NPT and hence entangled. In case, the equality holds, the state lies on the edge of separability and any small perturbation in the coherence terms would push the state into the entangled region.

C Case 2

Recall that we were looking at a mixed state and two vectors $a \in \mathbb{C}^2$ and $b \in \mathbb{C}^4$:

$$\rho = \sum_{j,k,r,s} \sum_{v} \sum_{w} \phi_1^{v_j} (\phi_1^*)^{v_r} \phi_2^{v_k} (\phi_2^*)^{v_s} e^{iw_1(f(j)-f(r))} e^{iw_2(g(k)-g(s))} a_j b_k a_r b_s |jk\rangle\langle rs| \tag{91}$$

Next, we want to find the conditions under which this construction gives us back a state of the same form as ρ_i'. For simplicity, we will take $w_1 = w_2 = w$, $\phi_1 = \phi_2 = 1$, and $f(j) = g(j)$ as before, and our construction will be reduced to:

$$\rho = \sum_{j,k,r,s} \sum_{w} e^{iw(f(j)+f(k)-f(r)-f(s))} a_j b_k a_r b_s |jk\rangle\langle rs| = \tag{92}$$

$$= \sum_{j,k,r,s} a_j b_k a_r b_s \left(\sum_{w} e^{iw(f(j)+f(k)-f(r)-f(s))} |jk\rangle\langle rs| \right) \tag{93}$$

where the sum over w is a geometric sum; rewritting is as:

$$\rho = \sum_{j,k,r,s} a_j b_k a_r b_s \delta_{f(j)+f(k),f(r)+f(s)} |jk\rangle\langle rs| \tag{94}$$

Let's now define the following:

$$f(0) = a,\ f(1) = b,\ f(2) = c \quad \text{and} \quad f(3) = d \tag{95}$$

It can be seen that the different kets and bras will have the corresponding values in one side of the Dirac's delta term:

$$|00\rangle \to 2a \tag{96}$$
$$|01\rangle \to a + b \tag{97}$$
$$|02\rangle \to a + c \tag{98}$$
$$|03\rangle \to a + d \tag{99}$$
$$|10\rangle \to a + b \tag{100}$$
$$|11\rangle \to 2b \tag{101}$$
$$|12\rangle \to b + c \tag{102}$$
$$|13\rangle \to b + d \tag{103}$$

In this case we want the terms $|00\rangle\langle 12|$ and $|11\rangle\langle 03|$ survive because is the one containing the coherence term. So we will need the following two conditions:

$$2a = b + c \quad \text{and} \quad 2b = a + d \tag{104}$$

For example, for the following values:

$$f(0) = 2,\ f(1) = 1,\ f(2) = 3 \quad \text{and} \quad f(3) = 0 \tag{105}$$

We are able to recover matrices with the same structure as in the case 2 with this separable construction.Then, we perform its partial transpose:

$$\rho_2 = \begin{pmatrix} \overline{p}_{00} & 0 & 0 & 0 & 0 & 0 & \frac{\alpha}{\sqrt{2}} & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ 0 & 0 & \overline{p}_{02} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{p}_{03} & 0 & \frac{\beta}{\sqrt{2}} & 0 & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\beta^*}{\sqrt{2}} & 0 & \overline{p}_{11} & 0 & 0 \\ \frac{\alpha^*}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & \overline{p}_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix}, \quad \rho_2^{T_A} = \begin{pmatrix} \overline{p}_{00} & 0 & 0 & 0 & 0 & \overline{p}_{01} & 0 & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & 0 & 0 & 0 & \frac{\alpha^*}{\sqrt{2}} \\ 0 & 0 & \overline{p}_{02} & 0 & \frac{\alpha^*}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{p}_{03} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\alpha}{\sqrt{2}} & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ \overline{p}_{01} & 0 & 0 & 0 & 0 & \overline{p}_{11} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{12} & 0 \\ 0 & \frac{\beta}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix}$$

If we decompose $\rho_2^{T_A}$ as a direct sum:

$$\rho_2^{T_A} = \begin{pmatrix} \overline{p}_{00} & - & - & - & - & \overline{p}_{01} & 0 & 0 \\ | & \overline{p}_{01} & - & - & - & | & - & \frac{\beta^*}{\sqrt{2}} \\ | & | & \overline{p}_{02} & - & \frac{\alpha^*}{\sqrt{2}} & | & 0 & | \\ | & | & | & \overline{p}_{03} & | & | & 0 & | \\ | & | & \frac{\alpha}{\sqrt{2}} & - & \overline{p}_{01} & | & 0 & | \\ \overline{p}_{01} & - & - & - & - & \overline{p}_{11} & 0 & | \\ 0 & | & 0 & 0 & 0 & 0 & \overline{p}_{12} & | \\ 0 & \frac{\beta}{\sqrt{2}} & - & - & - & - & - & \overline{p}_{13} \end{pmatrix} = \begin{pmatrix} \overline{p}_{00} & \overline{p}_{01} \\ \overline{p}_{01} & \overline{p}_{11} \end{pmatrix} \bigoplus \begin{pmatrix} \overline{p}_{02} & \frac{\alpha^*}{\sqrt{2}} \\ \frac{\alpha}{\sqrt{2}} & \overline{p}_{01} \end{pmatrix} \bigoplus \begin{pmatrix} \overline{p}_{01} & \frac{\beta^*}{\sqrt{2}} \\ \frac{\beta}{\sqrt{2}} & \overline{p}_{13} \end{pmatrix} \bigoplus ctes.$$

Where *ctes* are 2x2 diagonal matrices with entries $p_{ij} \geq 0$ and from case 1, we already know that the first two matrices have a determinant ≥ 0. So, for the third matrix, we want the same: To prove separability, we want that

$$\det \begin{pmatrix} \overline{p}_{01} & \frac{\beta^*}{\sqrt{2}} \\ \frac{\beta}{\sqrt{2}} & \overline{p}_{13} \end{pmatrix} \geq 0 \tag{106}$$

Given that $\overline{p}_{13} = |13\rangle\langle 13| = |a_1|^2|b_3|^2$, $\overline{p}_{01} = |01\rangle\langle 01| = |a_0|^2|b_1|^2 = |a_1|^2|b_0|^2 = a_0a_1b_0b_1$, and $\beta = |01\rangle\langle 13| = |a_0||b_1||a_1||b_3|$.

$$\det \begin{pmatrix} \overline{p}_{01} & \frac{\beta^*}{\sqrt{2}} \\ \frac{\beta}{\sqrt{2}} & \overline{p}_{13} \end{pmatrix} = \overline{p}_{01} \cdot \overline{p}_{13} - \frac{|\beta|^2}{2} = |a_0|^2|b_1|^2|a_1|^2|b_3|^2 - \frac{1}{2}a_0^2a_1^2b_1^2b_3^2 \geq 0. \tag{107}$$

$$|a_0|^2|b_1|^2|a_1|^2|b_3|^2 > \frac{1}{2}a_0^2a_1^2b_1^2b_3^2 \tag{108}$$

We can see here that the partial transpose ρ^{T_A} is positive semidefinite, our state being PPT. We know that if any principal minor of ρ^{T_A} is negative, this would be a NPT state,i.e. entangled. However, the determinants of our 2x2 matrices vanish or are greater than 0, and none of them is negative. This confirms that our state is PPT, but also that it is in the edge of PPT and NPT, given that any small perturbation in the coherences α or amplitudes $\overline{p}_{ij}$ would easily give a negative determinant, meaning that we would be in the NPT region.

Now, we will try to express this third matrix in the Bloch representation $\rho = \frac{1}{2}(a\mathbb{1} + \vec{b}\cdot\vec{\sigma})$ to determine the values of our parameters such that the resulting state is separable. So we have:

$$M_1 = \begin{pmatrix} \overline{p}_{01} & \frac{\beta^*}{\sqrt{2}} \\ \frac{\beta}{\sqrt{2}} & \overline{p}_{13} \end{pmatrix}, \qquad B = \frac{1}{2}\begin{pmatrix} a + b_z & b_x - ib_y \\ b_x + ib_y & a - b_z \end{pmatrix} \tag{109}$$

Which give rise to two systems of equations:

$$\begin{cases} a + b_z & = 2\overline{p}_{01} \\ a - b_z & = 2\overline{p}_{13} \end{cases} \quad \begin{cases} b_x - ib_y & = \frac{2}{\sqrt{2}}\beta^* \\ b_x + ib_y & = \frac{2}{\sqrt{2}}\beta \end{cases} \tag{110}$$

From the left hand side system we get the following results:

$$\boxed{b_z = \overline{p}_{01} - \overline{p}_{13}} \text{ and } \boxed{a = \overline{p}_{01} + \overline{p}_{13}}$$

And from the right hand side and considering $\alpha = \delta_1 + i\gamma_1$ $\beta = \delta_2 + i\gamma_2$, we get:

$$\boxed{b_x = \frac{2}{\sqrt{2}}\delta_2} \text{ and } \boxed{b_y = \frac{2}{\sqrt{2}}\gamma_2}$$

Now, we calculate the eigenvalues of the following matrix:

$$\begin{pmatrix} 2\overline{p}_{01} & \frac{2}{\sqrt{2}}\beta^* \\ \frac{2}{\sqrt{2}}\beta & 2\overline{p}_{13} \end{pmatrix} \to \lambda = (\overline{p}_{01} + \overline{p}_{13}) \pm \sqrt{(\overline{p}_{01} - \overline{p}_{13})^2 - 2|\beta|^2} \tag{111}$$

Since we are looking for separability, we want $\lambda_\pm \geq 0$, so:

$$\lambda_+ = (\overline{p}_{01} + \overline{p}_{13}) + \sqrt{(\overline{p}_{01} - \overline{p}_{13})^2 - 2|\beta|^2} \geq 0 \tag{112}$$

$$(\overline{p}_{01} + \overline{p}_{13})^2 \geq (\overline{p}_{01} - \overline{p}_{13})^2 + 2|\beta|^2 \tag{113}$$

$$4\overline{p}_{01}\overline{p}_{13} \geq 2|\beta|^2 \tag{114}$$

$$\overline{p}_{01}\overline{p}_{13} \geq \frac{|\beta|^2}{2} \tag{115}$$

We don't calculate the λ_- because it gives rise to the same inequality.

Summing up, we began with a structured quantum state in $\mathbb{C}^2 \otimes \mathbb{C}^4$, constructed it from general product vectors, and analyzed its partial tranpose $\rho_1^{T_A}$ by decomposing it into a direct sum of 2x2 blocks.

Three of these blocks had off-diagonal coherence terms, while the remaining blocks were purely diagonal and positive semidefinite.

The key results are that the first block M_1 is always PPT because all the entries arise from modulus-squared terms of a product vector, and the determinant vanishes. For the second block which had coherence terms involving α we found that if the inequality $\overline{p}_{02}\overline{p}_{01} \geq \frac{|\alpha|^2}{2}$ is fulfilled, the block is semidefenite positive and hence our initial state is separable. Finally, for the third block we found that if $\overline{p}_{01}\overline{p}_{13} \geq \frac{|\beta|^2}{2}$ is satisfied then our state is separable. Hence, we can conclude that this inequality delineates the boundary between separable and entangled states.

In case α or β becomes too large relative to the diagonal entries, the partial transpose would have a negative eigenvalue, implying that the initial state is NPT and hence entangled. In case the equality holds, the state lies on the edge of separability, and any small perturbation in the coherence terms would push the state into the entangled region.

D Case 3

Recall that we were looking at a mixed state and two vectors $a \in \mathbb{C}^2$ and $b \in \mathbb{C}^4$:

$$\rho = \sum_{j,k,r,s} \sum_{v} \sum_{w} \phi_1^{v_j} (\phi_1^*)^{v_r} \phi_2^{v_k} (\phi_2^*)^{v_s} e^{iw_1(f(j)-f(r))} e^{iw_2(g(k)-g(s))} a_j b_k a_r b_s \,|jk\rangle\langle rs| \tag{116}$$

Now, we need to find the conditions under which this construction gives us a state of the same form as ρ_i'. For simplicity, we will take $w_1 = w_2 = w$, $\phi_1 = \phi_2 = 1$ and $f(j) = g(j)$ and our construction will be reduced to:

$$\rho = \sum_{j,k,r,s} \sum_{w} e^{iw(f(j)+f(k)-f(r)-f(s))} a_j b_k a_r b_s \,|jk\rangle\langle rs| = \tag{117}$$

$$= \sum_{j,k,r,s} a_j b_k a_r b_s \left(\sum_{w} e^{iw(f(j)+f(k)-f(r)-f(s))} \,|jk\rangle\langle rs| \right) \tag{118}$$

where the sum over w is a geometric sum; rewritting is as:

$$\rho = \sum_{j,k,r,s} a_j b_k a_r b_s \delta_{f(j)+f(k),f(r)+f(s)} \,|jk\rangle\langle rs| \tag{119}$$

Let's now define the following:

$$f(0) = a,\ f(1) = b,\ f(2) = c \ \text{ and } \ f(3) = d \tag{120}$$

It can be seen that the different kets and bras will have the corresponding values in one side of the Dirac's delta term:

$$|00\rangle \rightarrow 2a \tag{121}$$
$$|01\rangle \rightarrow a + b \tag{122}$$
$$|02\rangle \rightarrow a + c \tag{123}$$
$$|03\rangle \rightarrow a + d \tag{124}$$
$$|10\rangle \rightarrow a + b \tag{125}$$
$$|11\rangle \rightarrow 2b \tag{126}$$
$$|12\rangle \rightarrow b + c \tag{127}$$
$$|13\rangle \rightarrow b + d \tag{128}$$

In this case we want the term $|02\rangle\langle 13|$ survives because is the one containing the coherence term. So we will need the following condition:

$$a + c = b + d \tag{129}$$

For example, for the following values:

$$f(0) = 5,\ f(1) = 12,\ f(2) = 8 \quad \text{and} \quad f(3) = 1 \tag{130}$$

We are able to recover matrices with the same structure as in the case 3 with this separable construction.Then, we perform its partial transpose:

$$\rho_3 = \begin{pmatrix} \overline{p}_{00} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ 0 & 0 & \overline{p}_{02} & 0 & 0 & 0 & 0 & \frac{\alpha}{2} \\ 0 & 0 & 0 & \overline{p}_{03} & 0 & 0 & 0 & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \overline{p}_{11} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{12} & 0 \\ 0 & 0 & \frac{\alpha^*}{2} & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix}, \quad \rho_3^{T_A} = \begin{pmatrix} \overline{p}_{00} & 0 & 0 & 0 & 0 & \overline{p}_{01} & 0 & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \overline{p}_{02} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{p}_{03} & 0 & 0 & \frac{\alpha^*}{2} & 0 \\ 0 & 0 & 0 & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ \overline{p}_{01} & 0 & 0 & 0 & 0 & \overline{p}_{11} & 0 & 0 \\ 0 & 0 & 0 & \frac{\alpha}{2} & 0 & 0 & \overline{p}_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix}$$

If we decompose $\rho_3^{T_A}$ as a direct sum:

$$\rho_3^{T_A} = \begin{pmatrix} \overline{p}_{00} & - & - & - & - & \overline{p}_{01} & 0 & 0 \\ | & \overline{p}_{01} & 0 & 0 & 0 & | & 0 & 0 \\ | & 0 & \overline{p}_{02} & 0 & 0 & | & 0 & 0 \\ | & 0 & 0 & \overline{p}_{03} & - & | & \frac{\alpha^*}{2} & 0 \\ | & 0 & 0 & | & \overline{p}_{01} & | & | & 0 \\ \overline{p}_{01} & - & - & - & - & \overline{p}_{11} & | & 0 \\ 0 & 0 & 0 & \frac{\alpha}{2} & - & - & \overline{p}_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix} = \begin{pmatrix} \overline{p}_{00} & \overline{p}_{01} \\ \overline{p}_{01} & \overline{p}_{11} \end{pmatrix} \bigoplus \begin{pmatrix} \overline{p}_{03} & \frac{\alpha^*}{2} \\ \frac{\alpha}{2} & \overline{p}_{12} \end{pmatrix} \bigoplus ctes.$$

Where *ctes* are 2x2 diagonal matrices with entries $p_{ij} \geq 0$, and from case 1, we already know that the first matrix has a determinant ≥ 0. So, for the second one, we want the same: To prove separability,

$$\det \begin{pmatrix} \overline{p}_{03} & \frac{\alpha^*}{2} \\ \frac{\alpha}{2} & \overline{p}_{12} \end{pmatrix} \geq 0 \tag{131}$$

Given that $\overline{p}_{12} = |12\rangle\langle 12| = |a_1|^2|b_2|^2$, $\overline{p}_{03} = |03\rangle\langle 03| = |a_0|^2|b_3|^2$, and $\alpha = |02\rangle\langle 13| = |a_0||b_2||a_1||b_3|$.

$$\det \begin{pmatrix} \overline{p}_{03} & \frac{\alpha^*}{2} \\ \frac{\alpha}{2} & \overline{p}_{12} \end{pmatrix} = \overline{p}_{03} \cdot \overline{p}_{12} - \frac{|\alpha|^2}{4} = |a_1|^2|b_2|^2|a_0|^2|b_3|^2 - \frac{1}{4}|a_0|^2|b_2|^2|a_1|^2|b_3|^2 \geq 0. \tag{132}$$

$$|a_0|^2|b_1|^2|a_1|^2|b_3|^2 - \frac{1}{4}|a_0|^2|b_2|^2|a_1|^2|b_3|^2 > 0 \tag{133}$$

We can see here that the partial transpose ρ^{T_A} is positive semidefinite, our state being PPT. We know that if any principal minor of ρ^{T_A} is negative, this would be a NPT state,i.e. entangled. However, the determinants of our 2x2 matrices vanish or are greater than 0, and none of them is negative. This confirms that our state is PPT, but also that it is on the edge of PPT and NPT, given that any small perturbation in the coherences α or amplitudes $\overline{p}_{ij}$ would easily give a negative determinant, meaning that we would be in the NPT region.

Now, we will try to express this matrix in the Bloch representation $\rho = \frac{1}{2}(a\mathbb{1} + \vec{b} \cdot \vec{\sigma})$ to determine the values of our parameters such that the resulting state is separable. So we have:

$$M_1 = \begin{pmatrix} \overline{p}_{03} & \frac{\alpha^*}{2} \\ \frac{\alpha}{2} & \overline{p}_{12} \end{pmatrix}, \qquad B = \frac{1}{2}\begin{pmatrix} a+b_z & b_x - ib_y \\ b_x + ib_y & a - b_z \end{pmatrix} \tag{134}$$

Which gives rise to two systems of equations:

$$\begin{cases} a + b_z &= 2\overline{p}_{03} \\ a - b_z &= 2\overline{p}_{12} \end{cases} \qquad \begin{cases} b_x - ib_y &= \alpha^* \\ b_x + ib_y &= \alpha \end{cases} \tag{135}$$

From the left-hand side system, we get the following results:

$$\boxed{b_z = \overline{p}_{03} - \overline{p}_{12}} \text{ and } \boxed{a = \overline{p}_{03} + \overline{p}_{12}}$$

And from the right hand side and considering $\alpha = \delta_1 + i\gamma_1$, we get:

$$\boxed{b_x = \delta_1} \text{ and } \boxed{b_y = \gamma_1}$$

Now, we calculate the eigenvalues of the following matrix:

$$\begin{pmatrix} 2\overline{p}_{03} & \alpha^* \\ \alpha & 2\overline{p}_{12} \end{pmatrix} \rightarrow \lambda = (\overline{p}_{03} + \overline{p}_{12}) \pm \sqrt{(\overline{p}_{03} - \overline{p}_{12})^2 - |\alpha|^2} \tag{136}$$

Since we are looking for separability, we want $\lambda_{\pm} \geq 0$, so:

$$\lambda_+ = (\overline{p}_{03} + \overline{p}_{12}) \pm \sqrt{(\overline{p}_{03} - \overline{p}_{12})^2 - |\alpha|^2} \geq 0 \tag{137}$$

$$(\overline{p}_{03} + \overline{p}_{12})^2 \geq (\overline{p}_{03} - \overline{p}_{12})^2 - |\alpha|^2 \tag{138}$$

$$\overline{p}_{03}\overline{p}_{12} \geq \frac{|\alpha|^2}{4} \tag{139}$$

We don't calculate the λ_- because it gives rise to the same inequality.

Summing up, we began with a structured quantum state in $\mathbb{C}^2 \otimes \mathbb{C}^4$, constructed it from general product vectors, and analyzed its partial tranpose $\rho_1^{T_A}$ by decomposing it into a direct sum of 2x2 blocks.

Two of these blocks had off-diagonal coherences terms, while the remaining blocks were purely diagonal and positive semidefinite.

The key results are that the first block M_1 is always PPT because all the entries arise from modulus-squared terms of a product vector, and the determinant vanishes. For the second block which had coherence terms involving α we found that if the inequality $\overline{p}_{03}\overline{p}_{12} \geq \frac{|\alpha|^2}{4}$ is fulfilled the block is semidefenite positive and hence our initial state is separable. Then, we can conclude that this inequality delineates the boundary between separable and entangled states.

In case, α becomes too large relative to the diagonal entries, the partial transpose would have a negative eigenvalue, implying that the initial state is NPT and hence entangled. In case, the equality holds, the state lies on the edge of separability and any small perturbation in the coherence terms would push the state into the entangled region.

E Case 5

Recall that we were looking at a mixed state and two vectors $a \in \mathbb{C}^2$ and $b \in \mathbb{C}^4$:

$$\rho = \sum_{j,k,r,s} \sum_{v} \sum_{w} \phi_1^{v_j} (\phi_1^*)^{v_r} \phi_2^{v_k} (\phi_2^*)^{v_s} e^{iw_1(f(j)-f(r))} e^{iw_2(g(k)-g(s))} a_j b_k a_r b_s |jk\rangle\langle rs| \tag{140}$$

Then, we need to find the conditions under which this construction gives us back a state of the same form as ρ_i'. For simplicity, we will take $w_1 = w_2 = w$, $\phi_1 = \phi_2 = 1$ and $f(j) = g(j)$ and our construction will be reduced to:

$$\rho = \sum_{j,k,r,s} \sum_{w} e^{iw(f(j)+f(k)-f(r)-f(s))} a_j b_k a_r b_s |jk\rangle\langle rs| = \tag{141}$$

$$= \sum_{j,k,r,s} a_j b_k a_r b_s \left(\sum_{w} e^{iw(f(j)+f(k)-f(r)-f(s))} |jk\rangle\langle rs| \right) \tag{142}$$

where the sum over w is a geometric sum; rewritting is as:

$$\rho = \sum_{j,k,r,s} a_j b_k a_r b_s \delta_{f(j)+f(k),f(r)+f(s)} |jk\rangle\langle rs| \tag{143}$$

Let's now define the following:

$$f(0) = a,\ f(1) = b,\ f(2) = c \quad \text{and} \quad f(3) = d \tag{144}$$

It can be seen that the different kets and bras will have the corresponding values in one side of the Dirac's delta term:

$$|00\rangle \to 2a \tag{145}$$
$$|01\rangle \to a + b \tag{146}$$
$$|02\rangle \to a + c \tag{147}$$
$$|03\rangle \to a + d \tag{148}$$
$$|10\rangle \to a + b \tag{149}$$
$$|11\rangle \to 2b \tag{150}$$
$$|12\rangle \to b + c \tag{151}$$
$$|13\rangle \to b + d \tag{152}$$

In this case we want that the terms $|00\rangle\langle 12|$ and $|02\rangle\langle 13|$ survive because is the one containing the coherence term. So we will need the following two conditions:

$$2a = b + c \quad \text{and} \quad b + d = a + c \tag{153}$$

For example, for the following values:

$$f(0) = 5,\ f(1) = 2,\ f(2) = 8 \quad \text{and} \quad f(3) = 11 \tag{154}$$

We are able to recover matrices with the same structure as in the case 2 with this separable construction.Then, we perform its partial transpose:

$$\rho_5 = \begin{pmatrix} \overline{p}_{00} & 0 & 0 & 0 & 0 & 0 & \frac{\alpha}{2} & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ 0 & 0 & \overline{p}_{02} & 0 & 0 & 0 & 0 & \frac{\beta}{2} \\ 0 & 0 & 0 & \overline{p}_{03} & 0 & 0 & 0 & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \overline{p}_{11} & 0 & 0 \\ \frac{\alpha^*}{2} & 0 & 0 & 0 & 0 & 0 & \overline{p}_{12} & 0 \\ 0 & 0 & \frac{\beta^*}{2} & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix}, \quad \rho_3^{T_A} = \begin{pmatrix} \overline{p}_{00} & 0 & 0 & 0 & 0 & \overline{p}_{01} & 0 & 0 \\ 0 & \overline{p}_{01} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \overline{p}_{02} & 0 & \frac{\alpha^*}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{p}_{03} & 0 & 0 & \frac{\beta^*}{2} & 0 \\ 0 & 0 & \frac{\alpha}{2} & 0 & \overline{p}_{01} & 0 & 0 & 0 \\ \overline{p}_{01} & 0 & 0 & 0 & 0 & \overline{p}_{11} & 0 & 0 \\ 0 & 0 & 0 & \frac{\beta}{2} & 0 & 0 & \overline{p}_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix}$$

If we decompose $\rho_3^{T_A}$ as a direct sum:

$$\rho_3^{T_A} = \begin{pmatrix} \overline{p}_{00} & - & - & - & - & \overline{p}_{01} & 0 & 0 \\ | & \overline{p}_{01} & 0 & 0 & 0 & | & 0 & 0 \\ | & 0 & \overline{p}_{02} & - & \frac{\alpha^*}{2} & | & 0 & 0 \\ | & 0 & | & \overline{p}_{03} & - & | & \frac{\beta^*}{2} & 0 \\ | & 0 & \frac{\alpha}{2} & | & \overline{p}_{01} & | & | & 0 \\ \overline{p}_{01} & - & - & - & - & \overline{p}_{11} & | & 0 \\ 0 & 0 & 0 & \frac{\beta}{2} & - & - & \overline{p}_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{p}_{13} \end{pmatrix} = \begin{pmatrix} \overline{p}_{00} & \overline{p}_{01} \\ \overline{p}_{01} & \overline{p}_{11} \end{pmatrix} \bigoplus \begin{pmatrix} \overline{p}_{03} & \frac{\alpha^*}{2} \\ \frac{\alpha}{2} & \overline{p}_{12} \end{pmatrix} \bigoplus \begin{pmatrix} \overline{p}_{02} & \frac{\alpha^*}{2} \\ \frac{\alpha}{2} & \overline{p}_{01} \end{pmatrix} \bigoplus ctes.$$

Where $ctes$ are 2x2 diagonal matrices with entries $p_{ij} \geq 0$ and from case 3, we already know that the first and second matrix has a determinant ≥ 0 and also from case 2 we already know that the third has a determinant ≥ 0.

So, for this case we have that the key results are that all matrices are PPT, in the case of the second and third matrices, for this to be true, these following inequalities have to be satisfied:

$$\overline{p}_{03}\overline{p}_{12} \geq \frac{|\alpha|^2}{4} \quad \text{and} \quad \overline{p}_{02}\overline{p}_{01} \geq \frac{|\beta|^2}{2} \tag{155}$$

Two of these blocks had off-diagonal coherences terms, while the remaining blocks were purely diagonal and positive semidefinite.

Then, we can conclude that this inequality delineates the boundary between separable and entangled states.

In case, α or β become too large relative to the diagonal entries, the partial transpose would have a negative eigenvalue, implying that the initial state is NPT and hence entangled. In case, the equality holds, the state lies on the edge of separability and any small perturbation in the coherence terms would push the state into the entangled region.