Leopold Franzens Universität Innsbruck

Bachelor's Thesis

Operator Systems and Separability of Quantum States

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1 Introduction

In quantum physics, a quantum state describes the properties of particles in the context of quantum mechanics. From a mathematical point of view, a quantum state is a positive semidefinite matrix $\rho \in \mathrm{Mat}_{d_1,d_1}(\mathbb{C}) \otimes \mathrm{Mat}_{d_2,d_2}(\mathbb{C}) \otimes ... \otimes \mathrm{Mat}_{d_n,d_n}(\mathbb{C})$ with $d_1, ..., d_n \in \mathbb{N}$. A quantum state can be either separable or entangled, which finds expression in different physical behaviors, but also affects it's mathematical properties (see definition 2.1). To determine whether a quantum state is separable or entangled is an important task in Quantum Information Theory. Gurvits demonstrated in 2003 that this problem is NP-hard [5]. Therefore, it is a large research field to look for easy-to-use criterions to determine if a quantum state is separable.

In this Bachelor's thesis, we look solely at bipartite quantum states, meaning that we only consider quantum states ρ with $\rho \in \mathrm{Mat}_{d_1,d_1}(\mathbb{C}) \otimes \mathrm{Mat}_{d_2,d_2}(\mathbb{C})$. Due to the definition of the tensor product of vector spaces, each such quantum state has a decomposition of the form $\rho = \sum_{i=1}^{m} P_i \otimes Q_i$, with $P_i \in \mathrm{Mat}_{d_1,d_1}(\mathbb{C}), Q_i \in \mathrm{Mat}_{d_2,d_2}(\mathbb{C})$. The minimum m that can be chosen for this decomposition is called the operator Schmidt rank of ρ.

The main theorem in this work states that every bipartite quantum state with operator Schmidt rank 2 is separable. This was first proven by Cariello in [1]. In this work, the proof formulated by Gemma De las Cuevas, Tom Drescher, and Tim Netzer in [3] is lined out and explained in detail. The original proof by Cariello is very direct and specific, while the proof by De las Cuevas, Drescher and Netzer uses the theory of operator systems and spectrahedra which originally comes from the field of Convex Algebraic Geometry.

After a short overview of the important properties of the tensor product and positive semidefinite matrices in Section 2, Section 3 introduces the spectrahedron and its generalization, the free spectrahedron. We then demonstrate that a free spectrahedron is an operator system. This is the motivation to investigate selected properties of operator systems, following the results of Tobias Fritz, Tim Netzer, and Andreas Thom [4]. Thereafter, we have all the necessary tools to put the proof of the main theorem together.

In Section 4 an example is provided to show that there are non-separable bipartite quantum states with operator Schmidt rank 3. In preparation, we introduce the PPT-criterion, a necessary condition for separability. This criterion was first mentioned by Peres and Horodecki [6], [8] and is also called the Peres-Horodecki criterion.

The first counterexample was found by Cariello in [2] and is presented in this work. This example is then generalized to find a set of non-separable quantum states. Cariello's counterexample is in $\mathrm{Mat}_{3,3}(\mathbb{C}) \otimes \mathrm{Mat}_{3,3}(\mathbb{C})$, but we show that it can be modified to a counterexample in $\mathrm{Mat}_{4,4}(\mathbb{C}) \otimes \mathrm{Mat}_{4,4}(\mathbb{C})$.

2 Notation

A positive semidefinite matrix $\rho \in \text{Mat}_{d_1,d_1}(\mathbb{C}) \otimes \text{Mat}_{d_2,d_2}(\mathbb{C}) \otimes ... \otimes \text{Mat}_{d_n,d_n}(\mathbb{C})$ with $d_1, ..., d_n \in \mathbb{N}$ is named quantum state [3]. It is often also required that $Trace(\rho) = 1$, but the condition is not relevant for this work and hence we drop it.
Also we look solely at quantum states $\rho \in \text{Mat}_{s,s}(\mathbb{C}) \otimes \text{Mat}_{t,t}(\mathbb{C})$.
Therefore ρ has a depiction as sum of monomial tensor products

$$\rho = \sum_{i=1}^{m} P_i \otimes Q_i$$

where $m \in \mathbb{N}$, $P_i \in \text{Mat}_{s,s}(\mathbb{C}),\ Q_i \in \text{Mat}_{t,t}(\mathbb{C})$ for all $i \in \{1, ..., m\}$.
The minimum m that can be chosen for this decomposition is called the operator Schmidt rank of ρ. It is shown in [3] Lemma 14 that, without loss of generality, we can assume P_i, Q_i to be hermitian matrices if ρ is hermitian.
The set of positive semidefinite $d \times d$ matrices over $\mathbb{C}$ is denoted by PSD_d

Upon review of the properties of these quantum states, it has been shown that the property of separability is relevant for applications in physics.

Definition 2.1 (Separability)**.** A quantum state $\rho \in \text{Mat}_{s,s}(\mathbb{C}) \otimes \text{Mat}_{t,t}(\mathbb{C})$, with ρ positive semidefinite, is separable if there exists a $\tilde{m} \in \mathbb{N}$ and matrices $\tilde{P}_i \in \text{PSD}_s, \tilde{Q}_i \in \text{PSD}_t$ for all $i \in \{1, ..., \tilde{m}\}$ such that

$$\rho = \sum_{i=1}^{\tilde{m}} \tilde{P}_i \otimes \tilde{Q}_i.$$

So a separable quantum state has a depiction consisting of positive semidefinite matrices, often referred to as separable decomposition.
To study quantum states and their behaviors, we first look at the basic concepts used in the definitions above.

2.1 Tensor product

A common depiction of the tensor product of two matrices is the Kronecker product, which we use in this work. It is defined in the following way:

Definition 2.2 (Tensor product)**.** Let $A \in \text{Mat}_{n,m}(\mathbb{C}),\ B \in \text{Mat}_{s,t}(\mathbb{C})$. The tensor product of A and B is given by

$$A \otimes B = \begin{pmatrix} A_{11}B & A_{12}B & \dots & A_{1m}B \\ A_{21}B & A_{22}B & \dots & A_{2m}B \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1}B & A_{n2}B & \dots & A_{nm}B \end{pmatrix}$$

Here, we basically multiply every entry of A with every entry of B and arrange them into a single, lager matrix. The Kronecker product satisfies all properties of a regular tensor product. In particular, it has the universal property of tensor products (see Definition 4.2), which will be useful in Chapter 4.

Lemma 2.3 (Properties of the Kronecker product). *For $A,\ C \in \mathrm{Mat}_{n,n}(\mathbb{C})$ and $B,\ D \in \mathrm{Mat}_{m,m}(\mathbb{C})$ it holds that*

$$(A \otimes B)(C \otimes D) = AC \otimes BD \tag{1}$$

and

$$(A \otimes B)^* = A^* \otimes B^* \tag{2}$$

Proof. A simple calculation shows that this lemma is true. □

2.2 Properties of positive semidefinite matrices

A matrix $A \in \mathrm{Her}_t(\mathbb{C})$ is said to be positive semidefinite, or short $A \geq 0$, if all eigenvalues of A are greater or equal zero. This is equivalent to the following condition:

$$\forall v \in \mathbb{C}^t : \ v^* A v \geq 0 \tag{3}$$

This follows from the fact, that a hermitian matrix can be orthogonally diagonalised.

Lemma 2.4. *The set of positive semidefinite matrices of dimension $t \times t$, short PSD_t, is closed under addition and multiplication with a non-negative factor.*

Proof. Let $A, B \in \mathrm{PSD}_t$, $a \in \mathbb{R}_{\geq 0}$ and $v \in \mathbb{C}^t$ be arbitrary. Then

$$v^*(A + aB)v = v^* A v + a v^* B v \geq 0.$$

□

3 The main theorem

Here we look at the main theorem this thesis is about and derive the proof in detail. This theorem is taken from [3], Corollary 10.

Theorem 3.1 (Main Theorem). *For any choice of $P_1, P_2 \in \mathrm{Her}_s(\mathbb{C})$ and $Q_1, Q_2 \in \mathrm{Her}_t(\mathbb{C})$ with*

$$\rho = P_1 \otimes Q_1 + P_2 \otimes Q_2 \geq 0$$

ρ is separable and admits a separable decomposition with at most two terms.

For the proof we must introduce the concept of convex cones and operator systems on such convex cones.

3.1 Convex cones

Definition 3.2 (Convex cone)**.** A subset C of a vector space V over $\mathbb{R}$ or $\mathbb{C}$ is called a convex cone, if $\forall a, b \in C$ and $\forall \alpha, \beta \in \mathbb{R}_{\geq 0}$ it holds that

$$\alpha a + \beta b \in C.$$

Definition 3.3 (Salient convex cone)**.** A convex cone C is said to be salient, if and only if $C \cap -C = \{0\}$.

A non-salient convex cone always contains not less than one linear subset of dimension at least one. A salient cone is always peaked at 0.
For example the half plain $C_1 = \{(x, y) \in \mathbb{R}^2 | x \geq 0\}$ is non-salient because it contains the linear subset $\{(0, y) | y \in \mathbb{R}\}$ which is also a contained in $-C_1 = \{(x, y) \in \mathbb{R}^2 | x \leq 0\}$. Conversely, the positive orthant

$$C_2 = \left\{ \sum_{i=1}^{n} a_i(1,0) + b_i(0,1) |\ n \in \mathbb{N},\ a_i, b_i \in \mathbb{R}_{\geq 0} \text{ for } i \in \{1, ..., n\} \right\}$$

is salient as no vector with a negative component is in the cone. Both cones are depicted in Figure 1.

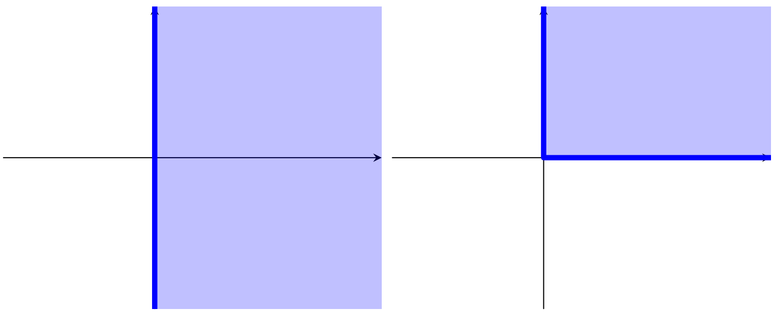


Figure 1: The half plain, non-salient, and the positive orthant, salient

The for the proof relevant convex cone is the spectrahedron of the matrices P_1, P_2 which is defined as follows:

Definition 3.4 (Spectrahedron)**.** The spectrahedron generated by the matrices $A_1, ..., A_m \in \mathrm{Her}_s(\mathbb{C})$ is given by

$$S(A_1, .., A_m) := \{(b_1, ..., b_m) \in \mathbb{R}^m | \sum_{i=1}^{m} b_1 A_1 \geq 0\}.$$

Generalizing the spectrahedron for the non-commutative case leads to the definition of the free spectrahedron.

Definition 3.5 (Free spectrahedron)**.** The r-level of the free spectrahedron defined by $A_1, ..., A_m \in \text{Her}_s(\mathbb{C})$ with $r \in \mathbb{N}$ is given by

$$FS_r(A_1, ..., A_m) := \left\{ (B_1, ..., B_m) \in \text{Her}_r(\mathbb{C})^m | \sum_{i=1}^{m} A_i \otimes B_i \geq 0 \right\}$$

The free spectrahedron defined by $A_1, ..., A_m$ is the collection of the above:

$$FS(A_1, ..., A_m) := (FS_r(A_1, ..., A_m))_{r \in \mathbb{N}}$$

Note that the 1-level of the free spectrahedron equals the spectrahedron.

Lemma 3.6. *For $r \in \mathbb{N}$ and linear independent $A_1, ..., A_m \in \text{Her}_s(\mathbb{C})$, the r-level of the free spectrahedron defined by $A_1, ..., A_m$ is a closed salient convex cone.*

Proof. Short calculation shows that $FS_r(A_1, ..., A_m)$ is a convex cone.
Let $(B_1, ..., B_m) \in FS_r(A_1, ..., A_m) \backslash \{0\}$, then $\sum_{i=1}^m A_i \otimes B_i \geq 0$. Due to the linearity of the tensor product it follows that $\sum_{i=1}^m A_i \otimes (-B_i) = -\sum_{i=1}^m A_i \otimes B_i$ is negative semidefinite. If $\sum_{i=1}^m A_i \otimes B_i = 0$ the linear independence of the A_i induces that $B_1 = ... = B_m = 0$ which contradicts our choice of the B_i. Therefore $-(B_1, ..., B_m) \notin FS_r(A_1, ..., A_m)$.
It is known that the r-level of the free spectrahedron is closed, as the property of being positive semidefinite is a closed condition. For each vector v, $v^*Av \geq 0$ is already a closed condition. □

3.2 Operator system

Generally, an operator system is a complex construction (see [4]), but in our case it suffices to use a slightly simplified but less general definition.

Definition 3.7 (Operator system)**.** An operator system is a set of non-empty closed salient convex cones $(C_r)_{r \geq 1}$ with

1) $C_1 \subset \text{Her}_1(\mathbb{C})^m \simeq \mathbb{R}^m$
   $C_2 \subset \text{Her}_2(\mathbb{C})^m = \{(A_1, ..., A_m) |\ A_i \in \text{Her}_2(\mathbb{C})\ ,\ i = 1, ..., m\}$
   $C_3 \subset \text{Her}_3(\mathbb{C})^m$
   $\vdots$
2) $\forall r, s \in \mathbb{N}\ \forall V \in \text{Mat}_{r,s}(\mathbb{C})\ \forall (A_1, ..., A_m) \in C_r :\ (V^*A_1V, ..., V^*A_mV) \in C_s$

Lemma 3.8 (Free spectrahedron is operator system)**.** *If $C_r = FS_r(A_1, ..., A_m)$ for $A_1, ..., A_m \in \text{Her}_s(\mathbb{C})$ and $r \in \mathbb{N}$ then $(C_r)_{r \geq 1}$ is an operator system.*

Proof. Per definition ($FS_r(A_1, ..., A_m) := \{(B_1, ..., B_m) \in \text{Her}_r(\mathbb{C})^m | \sum_{i=1}^m A_i \otimes B_i \geq 0\}$, see 3.5) it holds that for $r \in \mathbb{N}:\ C_r \subset \text{Her}_r(\mathbb{C})^m$.

Let $r, s \in \mathbb{N},\ V \in \mathrm{Mat}_{r,s}(\mathbb{C})$ and $(B_1, ..., B_m) \in C_r$ be arbitrary. With the help of Lemma 2.3 we can show that

$$\sum_{i=1}^{m} A_i \otimes V^* B_i V = (Id \otimes V)^* \left(\sum_{i=1}^{m} A_i \otimes B_i \right) (Id \otimes V).$$

If a matrix $A \in \mathrm{Her}_r(\mathbb{C})$ is positive semidefinite, then V^*AV is positive semidefinite as well for any $V \in \mathrm{Mat}_{r,s}(\mathbb{C})$. If $x \in \mathbb{C}^s$ then $x^*V^*AVx = (Vx)^*A(Vx) \geq 0$.
Combining these two results we get $(V^*B_1V, ..., V^*B_mV) \in C_s$. □

The following two definitions are taken from [4] Section 3.

Definition 3.9 (Minimal operator system)**.** Let $C \subset \mathbb{R}^m$ be a closed salient convex cone. We define the minimal operator system containing C as $C^{\min} = (C_s^{\min})_{s\geq 1}$ with

$$C_s^{\min} := \left\{ \sum_i c_i \otimes P_i |\ c_i \in C,\ P_i \in \mathrm{PSD}_s \right\}$$

Lemma 3.10. *The minimal operator system is minimal in the sense that for all operator systems $(D_s)_{s\geq 1}$ with $D_1 = C$ it follows that $\forall s \in \mathbb{N}:\ C_s^{min} \subseteq D_s$.*

Proof. Let $(D_s)_{s\geq 1}$ be an operator system with $D_1 = C$. Part 2) in the definition of operator systems (3.7) yields that for each matrix $V \in \mathrm{Mat}_{1,s}(\mathbb{C})$ and for every $(c_1, ..., c_m) \in C = D_1$, it holds that $(V^*c_1V, ..., V^*c_mV) \in D_s$ for an arbitrary $s \in \mathbb{N}$. Because $c_i \in \mathbb{R}$ we get $V^*c_iV = c_i(V^*V) = c_i \otimes (V^*V)$. Now $\forall x \in \mathbb{C}^s:\ x^*V^*Vx = (Vx)^*(Vx) = \langle Vx, Vx\rangle \geq 0$. Therefore $V^*V \in \mathrm{PSD}_s$.
On the other hand each positive semidefinite matrix A can be factorized, such that $A = \sum_i v_i v_i^*$ for some column vectors $v_i \in \mathbb{C}^s$. Then we can write $A = \sum_i V_i^* V_i$ with $V_i = v_i^*$.
Therefore an element $\sum_i c_i \otimes P_i \in C_s^{\min}$ can be written as

$$\begin{aligned}\sum_i c_i \otimes P_i &= \sum_i c_i \otimes \sum_j V_{i,j}^* V_{i,j} \\ &= \sum_i \sum_j V_{i,j}^* c_i V_{i,j} \in D_s \end{aligned} \tag{4}$$

That (4) holds follows from the fact that $V_{i,j} \in \mathrm{Mat}_{1,s}$ and from using part 2) in the definition of operator systems. □

Definition 3.11 (Maximal operator system)**.** Let $C \subset \mathbb{R}^m$ be a closed salient convex cone. Then the maximal operator system containing C is given by:

$$C_s^{\max} = \{(B_1, ..., B_m) \in \mathrm{Her}_s(\mathbb{C})^m |\ \forall v \in \mathbb{C}^s\ (v^*B_1v, ..., v^*B_m) \in C\}.$$

We write $C^{\max}$ as short form for the family $(C_s^{\max})_{s\geq 1}$

Lemma 3.12. *C^{max} is the maximal operator system, where maximal in this context means that for any operator system $(D_r)_{r\geq 1}$ with $D_1 \subseteq C$ it holds that $D_s \subseteq C_s^{max}$.*

Proof. Let $(D_r)_{r\geq 1}$ be an operator system with $D_1 \subseteq C$. If $(B_1, ..., B_m) \in D_s$ then Definition 3.7 2) shows us that $\forall v \in \mathbb{C}^s : \ (v^*B_1v, ..., v^*B_mv) \in D_1 \subseteq C$. Therefore $(B_1, ..., B_m) \in C_s^{\max}$. □

Definition 3.13 (Simplex cone)**.** A cone $C \subseteq \mathbb{R}^d$ is said to be a simplex cone if it is generated by d linear independent elements, i.e.
there exist $c_1, ..., c_d \in C$ linear independent, such that

$$C = \left\{ \sum_{i=1}^{d} \lambda_i c_i | \ \lambda_i \in \mathbb{R}_{\geq 0} \right\}$$

Lemma 3.14 (Max = Min for simplex cone)**.** *If $C \subseteq \mathbb{R}^d$ is a simplex cone, then it is isomorphic to the positive orthant $\mathbb{R}^d_{\geq 0}$. Moreover, $C^{min} = C^{max}$ if C is a simplex cone. [[4], Thm. 4.7]*

Proof. Let $C \subseteq \mathbb{R}^d$ be a simplex cone. There exist $c_1, ..., c_d \in C$ linear independent vectors generating C. Mapping the c_i to the standard basis vectors gives us the isomorphism:

$$\begin{aligned} \varphi : \ & C \to \mathbb{R}^d_{\geq 0} \text{ which is linear, with} \\ & c_i \mapsto e_i := (0, ..., 0, 1, 0, ..., 0) \text{ where the } i\text{-th entry is 1 and the rest 0. } i \in 1, ..., d. \end{aligned}$$

Therefore we can now assume that $C = \mathbb{R}^d_{\geq 0}$. Let $s \in \mathbb{N}$ be arbitrary.
Then, using the characterization of positive semidefinite (see (3)), we obtain

$$\begin{aligned} C_s^{\max} &= \left\{ (A_1, ..., A_d) \in \mathrm{Her}_s(\mathbb{C})^d | \ \forall v \in \mathbb{C}^s \ (v^*A_1v, ..., v^*A_dv) \in C \right\} \\ &= \left\{ (A_1, ..., A_d) \in \mathrm{Her}_s(\mathbb{C})^d | \ \forall v \in \mathbb{C}^s \ (v^*A_1v, ..., v^*A_dv) \in \mathbb{R}^d_{\geq 0} \right\} \\ &= \left\{ (A_1, ..., A_d) \in \mathrm{Her}_s(\mathbb{C})^d | \ A_i \geq 0, \ i \in \{1, ..., d\} \right\}. \end{aligned}$$

Similarly, we get

$$C_s^{\min} = \left\{ \sum_i c_i \otimes P_i | \ c_i \in C = \mathbb{R}^d_{\geq 0}, \ P_i \in \mathrm{Her}_s(\mathbb{C}), \ P_i \geq 0 \right\}.$$

The tensor product used here is again the Kronecker product, where c_i can be treated as a $1 \times d$ matrix.
Therefore,

$$\sum_i c_i \otimes P_i = \left(\sum_i (c_i)_1 P_i, ..., \sum_i (c_i)_d P_i \right)$$

As $C^{\max}$ is the maximal operator system containing C, we already get the inclusion $C_s^{\min} \subseteq C_s^{\max}$ for every $s \in \mathbb{N}$.
To show the other inclusion, let $(A_1, ..., A_d) \in C_s^{\max}$, in particular $A_i \geq 0$.
Set $c_i = e_i \in \mathbb{R}^d_{\geq 0}$. Then

$$(A_1, ..., A_d) = \sum_{i=1}^{d} c_i \otimes A_i \in C_s^{\min}$$
$$\Rightarrow C_s^{\min} = C_s^{\max}$$

□

3.3 Proof

Now it is time to bring together all the above results to prove the main theorem of this thesis:

Theorem 3.1 (Main Theorem)**.** *For any choice of* $P_1, P_2 \in \mathrm{Her}_s(\mathbb{C})$ *and* $Q_1, Q_2 \in \mathrm{Her}_t(\mathbb{C})$ *with*

$$\rho = P_1 \otimes Q_1 + P_2 \otimes Q_2 \geq 0$$

ρ *is separable and admits a separable decomposition with at most two terms.*

Proof. Let $P_1, P_2 \in \mathrm{Her}_s(\mathbb{C})$, $Q_1, Q_2 \in \mathrm{Her}_t(\mathbb{C})$ and $\rho = P_1 \otimes Q_1 + P_2 \otimes Q_2$ be positive semidefinite.
Note that if P_1, P_2 are linear dependent there exists a $\lambda \in \mathbb{C}$ such that $P_2 = \lambda P_1$ and

$$\begin{aligned} \rho &= P_1 \otimes Q_1 + (\lambda P_1 \otimes Q_2) \\ &= P_1 \otimes Q_1 + P_1 \otimes (\lambda Q_2) \\ &= P_1 \otimes (Q_1 + \lambda Q_2) \\ &= P_1 \otimes \tilde{Q} \end{aligned}$$

with $\tilde{Q} = Q_1 + \lambda Q_2 \in \mathrm{Her}_t(\mathbb{C})$. Here, we can use the same argument as in the second case below to show that ρ is separable.
From now on we will therefore assume that P_1, P_2 are linear independent.
There are three possible cases for $C := FS_1(P_1, P_2) \in \mathbb{R}^2$:

1. $C = \{0\}$
2. C contains a vector different from 0, with all other elements being generated by the first, thus C is a single ray.
3. C contains two linear independent elements. Then C is generated by two linear independent vectors $v_1, v_2 \in C$, i.e. $\forall w \in C \ \exists a, b \in \mathbb{R}_{\geq 0}: \ w = av_1 + bv_2$. Hence C is a simplex cone.

We will now look at the three cases separately and prove the statement of the theorem, namely that ρ is separable, for each case.

First case

Assume that $C = FS_1(P_1, P_2) = \{(b_1, b_2) \in \mathbb{R}^2 | \, b_1P_1 + b_2P_2 \geq 0\} = \{0\}$. Since $\rho \geq 0$ it holds for every $v \in \mathbb{C}^s$ and every $w \in \mathbb{C}^t$ that

$$
\begin{aligned}
0 \leq & (v \otimes w)^* \rho (v \otimes w) \\
= & v^* P_1 v \otimes w^* Q_1 w + v^* P_2 v \otimes w^* Q_2 w \qquad (5)\\
= & v^* P_1 v \cdot w^* Q_1 w + v^* P_2 v \cdot w^* Q_2 w \qquad (6)\\
= & v^* (w^* Q_1 w P_1 + w^* Q_2 w P_2) v
\end{aligned}
$$

To get from line (5) to line (6) we use that $w^* Q_i w$ is a scalar and therefore the tensor product simplifies to the scalar product.
As the inequality holds for every $v \in \mathbb{C}^s$, $w^* Q_1 w P_1 + w^* Q_2 w P_2$ is positive semidefinite and therefore $(w^* Q_1 w, w^* Q_2 w) \in C$. But then $w^* Q_1 w = 0$ and $w^* Q_2 w = 0$ for all $w \in \mathbb{C}^t$, which yields that $Q_1 = Q_2 = 0$. In total, we have that $\rho = 0$ and therefor ρ is separable, with the separable decomposition being the tensor product of the zero matrix of dimension s with the zero matrix of dimension t.

Second case

Let C be a single ray, meaning that there exists one element $b = (b_1, b_2) \in C$ such that for each element $c \in C$ there exists a scalar $\lambda \in \mathbb{R}$ with $c = \lambda b$.
Now, without loss of generality, we can assume that $(b_1, b_2) = (1, 0)$, using the isomorphism defined by mapping (b_1, b_2) to $(1, 0)$.
Using the same argument as in case one, we see that for any $w \in \mathbb{C}^t : \, (w^* Q_1 w, w^* Q_2 w) \in C = \{\lambda(1, 0) | \, \lambda \in \mathbb{R}\}$. Therefore $Q_2 = 0$ has to hold, so $\rho = P_1 \otimes Q_1$.
As ρ is positive semidefinite we get for every $v \in \mathbb{C}^s$ and every $w \in \mathbb{C}^t$:

$$
\begin{aligned}
0 \leq & (v \otimes w)^* \rho (v \otimes w) \\
= & v^* P_1 v \otimes w^* Q_1 w \\
= & v^* P_1 v \cdot w^* Q_1 w
\end{aligned}
$$

This shows that either P_1, Q_1 are both positive semidefinite or both negative semidefinite. In the first case $\rho = P_1 \otimes Q_1$ is already a separable decomposition and ρ is separable. In the second case $-P_1, -Q_1$ are positive semidefinite and $(-P_1) \otimes (-Q_1) = P_1 \otimes Q_1 = \rho$. Hence in this case ρ is also separable.

Third case

Let C be a simplex cone.
From Lemma 3.14 we know that in this case the minimal operator system containing C equals the maximal operator system containing C. Hence all operator systems containing C must be the same.
Additionally, we have already shown in Lemma 3.8 that the free spectrahedron is an operator system and therefore equal to $C^{\min}$.

Recalling the Definition 3.5 of the free spectrahedron and adapting it to this case, we get $FS_t(P_1, P_2) = \{(B_1, B_2) \in \text{Her}_t(\mathbb{C})^2 |\ P_1 \otimes B_1 + P_2 \otimes B_2 \geq 0\}$. As $\rho = P_1 \otimes Q_1 + P_2 \otimes Q_2$ is positive semidefinite it follows that $(Q_1, Q_2) \in FS_t(P_1, P_2) = C_t^{\min} = \{\sum_i v_i \otimes H_i |\ v_i \in C,\ H_i \in \text{PSD}_t\}$. Hence there exist $v_1, ..., v_n \in C$ and $H_1, ..., H_n \in \text{PSD}_t$ such that $(Q_1, Q_2) = \sum_{j=1}^n v_j \otimes H_j$.
Due to the fact that C is a simplex cone, we can choose two generating elements $a = (a_1, a_2) \in C$ and $b = (b_1, b_2) \in C$ and find positive scalars $\lambda_j, \beta_j \in \mathbb{R}_{\geq 0}$ such that $v_j = \lambda_j a + \beta_j b$ for all j. This motivates the following transformation:

$$\begin{aligned}
\sum_{j=1}^n v_j \otimes H_j =& \sum_{j=1}^n (\lambda_j a + \beta_j b) \otimes H_j \\
=& \sum_{j=1}^n a \otimes \lambda_j H_j + \sum_{j=1}^n b \otimes \beta_j H_j \\
=& a \otimes \left(\sum_{j=1}^n \lambda_j H_j \right) + b \otimes \left(\sum_{j=1}^n \beta_j H_j \right) \\
=& (a_1 \tilde{H}_1 + b_1 \tilde{H}_2, a_2 \tilde{H}_1 + b_2 \tilde{H}_2)
\end{aligned}$$

Here $\tilde{H}_1 := \sum_{j=1}^n \lambda_j H_j$ and $\tilde{H}_2 := \sum_{j=1}^n \beta_j H_j$, both matrices being positive semidefinite.
Therefore, we get that $Q_i = a_i \tilde{H}_1 + b_i \tilde{H}_2$ for $i = 1, 2$. Substituting this in the representation of ρ yields:

$$\begin{aligned}
\rho =& P_1 \otimes (a_1 \tilde{H}_1 + b_1 \tilde{H}_2) + P_2 \otimes (a_2 \tilde{H}_1 + b_2 \tilde{H}_2) \\
=& (a_1 P_1 + a_2 P_2) \otimes \tilde{H}_1 + (b_1 P_1 + b_2 P_2) \otimes \tilde{H}_2 \qquad (7)
\end{aligned}$$

Now $a_1 P_1 + a_2 P_2$ and $b_1 P_1 + b_2 P_2$ are positive semidefinite, because $a, b \in C = FS_1(P_1, P_2)$. Therefore (7) gives us a separable decomposition of ρ, proving that ρ is separable. □

While cases one and two are quite straightforward, all the results from Chapter 2 and 3 were used to prove the theorem in the third case. The concept for the proof in the third case was taken from [3].

4 Counterexample

So far we have proven that each quantum state of the form $\rho = P_1 \otimes Q_1 + P_2 \otimes Q_2$ is separable. This naturally leads to the question whether a quantum state with operator Schmidt rank 3 is still always separable. In the proof of the operator Schmidt rank 2 scenario, we have used that there are only three possible cases for the cone $C = FS_1(P_1, P_2) \subseteq \mathbb{R}^2$. When looking at a quantum state $\rho = P_1 \otimes Q_1 + P_2 \otimes Q_2 + P_3 \otimes Q_3$, the relevant cone C would be $C := FS_1(P_1, P_2, P_3) \subseteq \mathbb{R}^3$. But in $\mathbb{R}^3$ a salient convex

cone might need infinitely many generators, for example if it is round, like the cone $\left\{(x,y,z) \in \mathbb{R}^3 | z \geq \sqrt{x^2+y^2}\right\}$. Its boundary can be seen in Figure 2.
Thus we can not directly adapt the proof from the operator Schmidt rank 2 case to the

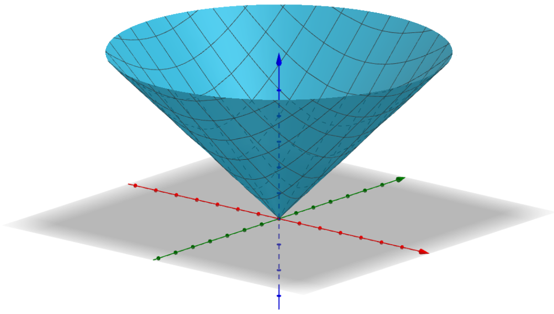


Figure 2: Boundary of a convex cone with infinite amount of generators

operator Schmidt rank 3 case. Therefore, it seems more likely to find a counterexample for this case. Specifically, we search for a quantum state $\rho = P_1 \otimes Q_1 + P_2 \otimes Q_2 + P_3 \otimes Q_3$ which is not separable, i.e. entangled.
To show that a quantum state is not separable using the definition of separability, we would have to go through all possible representations of ρ and show that none consists of positive semidefinite matrices only.
Therefore the first part of this section (4.1) presents an easy-to-test criterion for entanglement, the PPT-criterion. In the second part (4.2) we will see an explicit counterexample and analyze it.

4.1 PPT-criterion

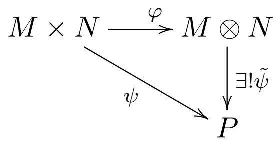
Definition 4.1 (Partial transposition)**.** The partial transposition (in the second component) of a quantum state $\rho = \sum_{j=1}^{m} P_j \otimes Q_j \in \mathrm{Mat}_{s,s}(\mathbb{C}) \otimes \mathrm{Mat}_{t,t}(\mathbb{C})$ is defined as

$$\rho^{t_2} := \sum_{j=1}^{m} P_j \otimes Q_j^{\mathrm{T}}.$$

At first it might seem that this definition depends on the representation of ρ and is therefore not well defined. It would be difficult to prove that the definition is well-defined using direct computation. However, it can be shown using the universal property of the tensor product:

Definition 4.2 (Universal property of the tensor product)**.** For vector spaces M, N, P over a field K and the tensor product $\varphi : M \times N \to M \otimes N$ it holds that
for all K-bilinear maps $\psi : M \times N \to P$ exists a unique linear map $\tilde{\psi} : M \otimes N \to P$ such that $\psi = \tilde{\psi} \circ \varphi$.

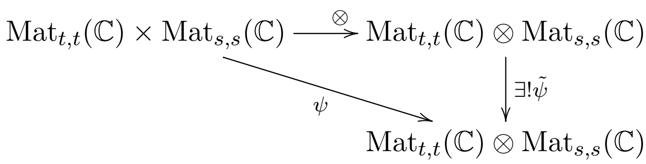
In other words, the universal property says, that the diagram below has to be commutative.



In the case of the partial transpose, we have that $M = \mathrm{Mat}_{s,s}(\mathbb{C})$, $N = \mathrm{Mat}_{t,t}(\mathbb{C})$, $P = \mathrm{Mat}_{s,s}(\mathbb{C}) \otimes \mathrm{Mat}_{t,t}(\mathbb{C})$,

$$\begin{aligned} \psi : \mathrm{Mat}_{t,t}(\mathbb{C}) \times \mathrm{Mat}_{s,s}(\mathbb{C}) &\to \mathrm{Mat}_{t,t}(\mathbb{C}) \otimes \mathrm{Mat}_{s,s}(\mathbb{C}) \\ (A, B) \mapsto (A, B^{\mathrm{T}}) &\mapsto A \otimes B^{\mathrm{T}}. \end{aligned}$$

In this case, the commutative diagram looks the following way:



ψ is the composition of transposing the second element of a tuple of matrices, which is bilinear, and forming the tensor product of these two matrices, which also is bilinear. Therefore, ψ is a bilinear map and the universal property tells us that there exists a unique map $\tilde{\psi} : \mathrm{Mat}_{t,t}(\mathbb{C}) \otimes \mathrm{Mat}_{s,s}(\mathbb{C}) \to \mathrm{Mat}_{t,t}(\mathbb{C}) \otimes \mathrm{Mat}_{s,s}(\mathbb{C})$ with:

$$\tilde{\psi}\left(\sum_{i=1}^{m} P_i \otimes Q_i\right) = \sum_{i=1}^{m} \psi((P_i, Q_i)) = \sum_{i=1}^{m} P_i \otimes Q_i^{\mathrm{T}}$$

This proves that the partial transpose is well-defined and independent of the representation of a quantum state.
Now we can use this tool to create the PPT-criterion needed to prove entanglement of a quantum state.

Definition 4.3 (PPT-Criterion)**.** A quantum state $\rho \in \mathrm{Mat}_{t,t}(\mathbb{C}) \otimes \mathrm{Mat}_{s,s}(\mathbb{C})$ is said to be positive under partial transposition (PPT), if its partial transpose ρ^{t_2} is positive semidefinite.

Lemma 4.4 (Separable implies PPT)**.** *Every separable quantum state is PPT.*

Proof. Let $\rho = \sum_{i=1}^{m} P_i \otimes Q_i$ be a separable quantum state, with $P_i, Q_i \geq 0$ for all i. We must show that ρ^{t_2} is positive semidefinite, which we do by showing that

1. If $A \geq 0$ then $A^{\mathrm{T}} \geq 0$.
2. If $A, B \geq 0$ then $A \otimes B \geq 0$.

To prove 1. we look at the characteristic polynomial of a matrix $A \geq 0$:

$$\begin{aligned}\chi_A(\lambda) &= \det(\lambda Id - A) \\ &= \det\left((\lambda Id - A)^{\mathrm{T}}\right) \\ &= \det\left(\lambda Id - A^{\mathrm{T}}\right) \\ &= \chi_{A^{\mathrm{T}}}(\lambda)\end{aligned}$$

So A and its transpose have the same characteristic polynomial. The eigenvalues of A are the roots of the characteristic polynomial. Therefore A and A^{T} have the same eigenvalues and hence A^{T} is positive semidefinite if and only if A is positive semidefinite.
To prove 2. let $A \in \mathrm{PSD}_t$ with eigenvalues $\lambda_1, ..., \lambda_t$ and corresponding eigenvectors $v_1, ..., v_t \in \mathbb{C}^t$, $B \in \mathrm{PSD}_s$ with eigenvalues $\gamma_1, ..., \gamma_s$ and corresponding eigenvectors $w_1, ..., w_s \in \mathbb{C}^s$. Then for any $i \in \{1, ..., t\}$ and $j \in \{1, ..., s\}$

$$\begin{aligned}(A \otimes B)(v_i \otimes w_j) =& Av_i \otimes Bw_j \qquad (8) \\ =& \lambda_i v_i \otimes \gamma_j w_j \\ =& \lambda_i \gamma_j (v_i \otimes w_j)\end{aligned}$$

In line 8 we use Lemma 2.3.
This shows that for each $i \in \{1, ..., t\}$ and $j \in \{1, ..., s\}$ $\lambda_i \gamma_j$ is an eigenvalue of $A \otimes B$ corresponding to the eigenvector $v_i \otimes w_j$ giving a total of $t \cdot s$ eigenvalues. As $A \otimes B \in \mathrm{Mat}_{ts,ts}(\mathbb{C})$, we already found all possible eigenvalues.
If A and B have only non-negative eigenvalues then so does $A \otimes B$.
Combining these two parts completes the proof. □

We have shown that every separable quantum state is PPT. Therefore, if a state is not PPT it is not separable.
As the PPT criterion is easy to test, we can now start looking for an entangled quantum state with operator Schmidt rank 3.

4.2 Example

Cariello discovered an example for an entangled quantum state with operator Schmidt rank 3 in [2], which we present and analyse.
In this example, we first define two matrices, $D \in \mathrm{Mat}_{3,3}(\mathbb{C})$ being a diagonal matrix and $A \in \mathrm{Mat}_{3,3}(\mathbb{C})$ being an antisymmetric matrix.

$$D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -10 \end{pmatrix} \; ; \quad A = \begin{pmatrix} 0 & 1 & 1 \\ -1 & 0 & 1 \\ -1 & -1 & 0 \end{pmatrix}$$

Let m_q be the smallest eigenvalue of $D \otimes D - A \otimes A$. Then we set the matrix C to be:

$$\begin{aligned} C &:= |m_q| Id \otimes Id + D \otimes D - A \otimes A \\ &= |m_q| Id \otimes Id + D \otimes D + (\mathrm{i}A) \otimes (\mathrm{i}A) \end{aligned} \tag{9}$$

Per construction, C is positive semidefinite. In (9), C has the usual form of a quantum state as a sum of tensor products of each two hermitian matrices. It is easy to see, that Id, D, A are linear independent, thus C cannot be expressed with less addends and has operator Schmidt rank 3.
Now, to show that C is not separable, we check whether C is PPT.

$$\begin{aligned} C^{t_2} &= |m_q| Id \otimes Id + D \otimes D + (\mathrm{i}A) \otimes (-\mathrm{i}A) \\ &= |m_q| Id \otimes Id + D \otimes D + A \otimes A \end{aligned}$$

The simplest way to show that C is not PPT is to use a Computer Algebra System (CAS), calculate the eigenvalues of C^{t_2} and see that at least one of them is negative. Mathematica [7] gives a value of approximately -31.08315516 for m_q. Continuing the calculation with the exact value in Mathematica yields the following eigenvalues of C^{t_2}:

$$131.1, 40.29, 35.19, 33.17, 32.02, 22.05, 19.95, 2.006, -0.05639$$

As shown above, the last eigenvalue is negative and this by a significant amount, with the second decimal being different from zero. If the true eigenvalue would be positive, this result is unlikely to be gained by numerical computation errors.
Therefore C is not PPT and hence it is not separable.

In addition to performing numerical computations we can also show this analytically. We do this by proving that the smallest eigenvalue of $D \otimes D + A \otimes A$ is negative and smaller than the smallest eigenvalue of $D \otimes D - A \otimes A$, which is also negative (see [2], Lemma 5.1).
Using a CAS we get the characteristic polynomial of $D \otimes D + A \otimes A$

$$\begin{aligned} p(x) = &- x^9 + 36x^8 + 5420x^7 + 104400x^6 - 427924x^5 - 14134608x^4 + 11251344x^3 \\ &+ 415328832x^2 - 1106058240x + 671846400 \end{aligned} \tag{10}$$

and the characteristic polynomial of $D \otimes D - A \otimes A$

$$\begin{aligned} q(x) = &- x^9 + 36x^8 + 5420x^7 + 104400x^6 - 427924x^5 - 14134608x^4 + 10924160x^3 \\ &+ 415328832x^2 - 1106058240x + 671846400. \end{aligned} \tag{11}$$

Observe that $p(x) - q(x) = kx^3$ for some $k > 0$. As $D \otimes D + A \otimes A$ and $D \otimes D - A \otimes A$ are real symmetric matrices, p and q have only real roots. Notice that neither p nor q has 0 as a root. As $p(x) - q(x) = kx^3$, p and q do not have a common root.
We can factorize the polynomials, writing

$$\begin{aligned} p(x) &= (-1)(x - r_1) \cdots (x - r_9) \\ q(x) &= (-1)(x - s_1) \cdots (x - s_9) \end{aligned}$$

with $r_1, ...r_9, s_1, ..., s_9 \in \mathbb{R}$.
Assume that all roots of p and q are positive. Then all coefficients of

$$\begin{aligned} p(-x) =&(-1)(-x-r_1)\cdots(-x-r_9) \\ =&(x+r_1)\cdots(x+r_9) \end{aligned}$$

and analogous $q(-x)$, would be positive.
Looking at the polynomials (10), (11), we see that the coefficient at x^7 is negative in both $p(-x)$ and $q(-x)$. Therefore, p and q have negative roots.
Let m_q be the smallest root of q and m_p the smallest root of p.
Suppose, for the sake of contradiction, that $m_q < m_p$.
Then $m_q < m_p \leq r_i$ for all i. Therefore, $p(m_q) = (-1)(m_q - r_1)\cdots(m_q - r_9)$ is positive as a product of 10 negative numbers.
On the other hand $p(m_q) = p(m_q) - q(m_q) = k(m_q)^3 < 0$, which contradicts $p(m_q) > 0$.
As p and q have no common roots, we have shown that $m_p < m_q$.
$|m_q| + m_p$ is an eigenvalue of $C^{t_2} = |m_q| Id \otimes Id + D \otimes D + A \otimes A$. From above, we know that $0 > m_p - m_q = m_p + |m_q|$, as m_q is negative. Thus, C^{t_2} is not positive semidefinite and therefore C is not PPT.

Therefore, we found one counterexample. This leads to the question whether this is the only one, or if there are more non-separable quantum states.
First we test variations of the asymmetric matrix A.

$$\tilde{C} = |m_c| Id \otimes Id + D \otimes D - (cA) \otimes (cA)$$

with m_c being the smallest eigenvalue of $D \otimes D - (cA) \otimes (cA)$. Calculating the eigenvalues of the partial transpose for $c \in \{1/2, 2, 5, 50, -5\}$ shows that $\tilde{C}$ is entangled in this cases. The testing indicates that many more values for c might be possible, even $c \in \mathbb{R} \backslash \{0\}$.
The analytic proof for the explicit counterexample from above uses three properties of the characteristic polynomials p and q:

1. $p(x) - q(x) = kx^3$ with $k > 0$
2. $p(0) \neq 0$ and $q(0) \neq 0$
3. $p(-x), q(-x)$ have a negative coefficient.

Using Mathematica, we get the characteristic polynomial p of $D \otimes D + (cA) \otimes (cA)$

$$\begin{aligned} p(x) = &\, 729000000 - 58320000c^4 + 1166400c^8 - 1108890000x \\ &+ 1101600c^4x + 1730160c^8x + 385236000x^2 + 29342160c^4x^2 \\ &+ 750672c^8x^2 + 8425800x^3 + 2556724c^4x^3 + 163592c^6x^3 \\ &+ 105228c^8x^3 - 13505580x^4 - 630648c^4x^4 + 1620c^8x^4 \\ &- 376561x^5 - 51282c^4x^5 - 81c^8x^5 + 104904x^6 - 504c^4x^6 \\ &+ 5402x^7 + 18c^4x^7 + 36x^8 - x^9 \end{aligned}$$

and the characteristic polynomial q of $D \otimes D - (cA) \otimes (cA)$

$$\begin{aligned} q(x) = {} & 729000000 - 58320000c^4 + 1166400c^8 - 1108890000x \\ & + 1101600c^4x + 1730160c^8x + 385236000x^2 + 29342160c^4x^2 \\ & + 750672c^8x^2 + 8425800x^3 + 2556724c^4x^3 - 163592c^6x^3 \\ & + 105228c^8x^3 - 13505580x^4 - 630648c^4x^4 + 1620c^8x^4 \\ & - 376561x^5 - 51282c^4x^5 - 81c^8x^5 + 104904x^6 - 504c^4x^6 \\ & + 5402x^7 + 18c^4x^7 + 36x^8 - x^9 \end{aligned}$$

We now check, whether points 1. - 3. are satisfied:

1. $p(x) - q(x) = 327184c^6x^3$, $k = 327184c^6 > 0$ for all $c \in \mathbb{R}\backslash\{0\}$
2. $p(0) = q(0) = 729000000 - 58320000c^4 + 1166400c^8 \neq 0$ for all $c \in \mathbb{R}\backslash\{-\sqrt{5}, \sqrt{5}\}$
3. The coefficient of x^7 of $p(-x)$ and $q(-x)$ is $-(5402 + 18c^4) < 0$ for all $c \in \mathbb{R}$.

We see that all three point are satisfied for $c \in \mathbb{R}\backslash\{-\sqrt{5}, 0, \sqrt{5}\}$, therefore, following the proof from above, $\tilde{C}$ is entangled for all $c \in \mathbb{R}\backslash\{-\sqrt{5}, 0, \sqrt{5}\}$.
Using the same method, we can also show that

$$C_2 = |m| Id \otimes Id + (eD) \otimes (eD) - (cA) \otimes (cA)$$

is entangled for all $e \in \mathbb{R}\backslash\{0\}$ and $c \in \mathbb{R}\backslash\{-\sqrt{5}e, 0, \sqrt{5}e\}$. Here m is again the smallest eigenvalue of $(eD) \otimes (eD) - (cA) \otimes (cA)$.
We now adapt this counterexample to the case of A and D being 4×4 matrices. Set

$$D = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & -10 \end{pmatrix}; \quad A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ -1 & 0 & 1 & 1 \\ -1 & -1 & 0 & 1 \\ -1 & -1 & -1 & 0 \end{pmatrix}$$

and m as the smallest eigenvalue of $D \otimes D - A \otimes A$. Then

$$C := |m| Id \otimes Id + D \otimes D - A \otimes A$$

is not separable, which can be proven by calculating the eigenvalues of C^{t_2} with a CAS. This indicates that there likely are entangled bipartite quantum states in higher dimensions as well. So the general rule for operator Schmidt rank 2 quantum states cannot be transferred to states with operator Schmidt rank 3.

5 Conclusion

This thesis on Operator Systems and Separability of Quantum States outlines the proof of Theorem 3.1, which states that every bipartite quantum state with operator Schmidt rank 2 is separable. It also highlights an example of an entangled state with operator Schmidt rank 3. First, we have introduced the underlining concepts of separability, the tensor product and positive semidefinite matrices, then we have given the definition of convex cones, (free) spectrahedra and operator systems. We have further exhibited that a free spectrahedron is an operator system and that there is a minimal and a maximal operator system containing a given convex cone. After introducing the simplex cone, we have shown that the maximal and the minimal operator system containing a given simplex cone are equal and hence any operator system containing this cone is equal to the minimal operator system. This presented all the tools required to start the proof of the main theorem.

Given a quantum state $\rho = P_1 \otimes Q_1 + P_2 \otimes Q_2$, the spectrahedron $C = S(P_1, P_2) \in \mathbb{R}^2$, can have three different shapes: $C = \{0\}$, C is single ray or C is a simplex cone. While we have used a direct way to proof the theorem for cases one and two, case three needed the poof that the free spectrahedron $FS(P_1, P_2)$ equals the minimal operator system containing C.

In Section 4 we defined the PPT-criterion, proved that it is well defined and a necessary condition for separability. Afterwards we used it to see that an explicit quantum state with operator Schmidt rank 3 is not separable. Therefore, Theorem 3.1 is not true for quantum states with operator Schmidt rank 3.

We further revealed that the counterexample provided is not the only one, but that there is a whole set of entangled matrices of this kind.

Overall, we have demonstrated that every bipartite quantum state with operator Schmidt rank 2 is separable, but not every state with operator Schmidt rank 3 is separable. We also clarified the connection between the theory of quantum states and the theory of operator systems and free spectrahedra.

In literature, only a few additional criterions for separability can be found, with no general solution to this problem. However, not many approaches were made using operator systems and free spectrahedra, thus looking at the problem from this angle might lead to even more insights in the field of quantum states.

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