On the structure of positive maps II: low dimensional matrix algebras

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Abstract

We use a new idea that emerged in the examination of exposed positive maps between matrix algebras to investigate in more detail the difference between positive maps on $M_2(\mathbb{C})$ and $M_3(\mathbb{C})$. Our main tool stems from classical Grothendieck theorem on tensor product of Banach spaces and is an older and more general version of Choi-Jamiołkowski isomorphism between positive maps and block positive Choi matrices. It takes into account the correct topology on the latter set that is induced by the uniform topology on positive maps. In this setting we show that in $M_2(\mathbb{C})$ case a large class of nice positive maps can be generated from the small set of maps represented by self-adjoint unitaries, $2P_x$ with $x$ maximally entangled vector and $p \otimes \mathbb{1}$ with $p$ rank 1 projector. We show why this construction fails in $M_3(\mathbb{C})$ case. There are also similarities.

In both $M_2(\mathbb{C})$ and $M_3(\mathbb{C})$ cases any unital positive map represented by self-adjoint unitary is unitarily equivalent to the transposition map. Consequently we obtain a large family of exposed maps. We also investigate a convex structure of the Choi map, the first example of non-decomposable map. As a result the nature of the Choi map will be explained. This gives an information on the origin of appearance of non-decomposable maps on $M_3(\mathbb{C})$.

1 Introduction

Positive maps between $n \times n$ matrix algebras play an important role in the entanglement theory as they can be used do classify entangled states on two $n$-level quantum systems. Furthermore, it seems that positive (not only completely positive) maps play an important role in description of some special dynamical systems (see e.g. [1] and [2]). The problem of characterizing all positive maps was unsolved for over 50 years even for matrix of dimension $n = 3$ or higher. Very recently, a general characterization of unital positive maps, for finite dimensional case, was given in [3]. To complete an analysis of the structure of positive maps, it is natural to ask a question what is an essential difference between simple case of maps between $n = 2$ matrix algebras and maps between $n = 3$ matrix algebras. In that way one hopes to fully understand the origin of appearance of non-decomposable maps for the $n = 3$ case.

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In this paper we will shed some light on this problem using new idea. It originated from the attempt to characterize exposed points of the set of positive maps between matrix algebras [3]. In that work the following set of Choi matrices naturally emerges

\[ \mathcal{D} = \{ \text{symmetries, } nP_x, p \otimes 1 \} \]

where symmetries are selfadjoint unitaries, \( x \) is fully entangled vector on \( \mathbb{C}^n \otimes \mathbb{C}^n \) and \( p \) is some rank one projector. We will show that this set is rich enough to describe all regular extreme positive maps in the \( n = 2 \) case (i.e. maps with the property that their restriction to diagonal subalgebra is still extreme, cf. Def. 5). We will also show at which point it fails in the \( n = 3 \) case. To further examine \( n = 3 \) case we explore relation of Choi matrices given by symmetries to Choi matrix of transposition map. Finally analysis of the convex structure of Choi map will be presented. This gives now information on the nature of the first example of non-decomposable map.

The article is organized as follows. It the Section 2 we recall some basic notions and introduce useful tools. In the Section 3 we consider the case of extremal decomposable map. Finally analysis of the convex structure of Choi map will be presented. This gives now information on the nature of the first example of non-decomposable map.

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2 Preliminaries

2.1 Basic definitions and notation

By the \( a^\dagger \) we will denote as usual the transpose of the matrix \( a \). Occasionally when the function-of-argument notation will be more convenient we will use \( \tau(a) \) to denote transposition map. By \( \text{id} \) we will denote identity map. The \( \circ \) will represent ordinary composition of maps. We implicitly assume that all discussed maps between matrix algebras are linear.

Recall that the linear map \( \phi: M_n(\mathbb{C}) \to M_m(\mathbb{C}) \) between the algebra of \( n \times n \) matrices and \( m \times m \) matrices is called positive when it maps positive semidefinite matrices\(^1\) (denoted by \( M_n(\mathbb{C})^+ \)) into positive semidefinite matrices. We will denote the set of all positive maps from \( M_n(\mathbb{C}) \) to \( M_m(\mathbb{C}) \) by \( \mathcal{L}^+(M_n(\mathbb{C}), M_m(\mathbb{C})) \).

We will write \( \mathcal{L}^+(M_n(\mathbb{C})) \) instead of \( \mathcal{L}^+(M_n(\mathbb{C}), M_n(\mathbb{C})) \). A map is called completely positive when maps \( \phi \circ \text{id}: M_n(\mathbb{C}) \otimes M_k(\mathbb{C}) \to M_m(\mathbb{C}) \otimes M_k(\mathbb{C}) \) are positive for any \( k \). We will denote by \( \mathcal{L}^{\text{cop}}(M_n(\mathbb{C}), M_m(\mathbb{C})) \) the set of all completely positive maps from \( M_n(\mathbb{C}) \) to \( M_m(\mathbb{C}) \). A map is called completely copositive, if \( \tau \circ \phi \) is a completely positive map. A positive map is called decomposable if it can be written as a sum of completely positive and completely copositive map. It is well known that in the case \( \mathcal{L}^+(M_2(\mathbb{C})), \mathcal{L}^+(M_2(\mathbb{C}), M_2(\mathbb{C})), \mathcal{L}^{\text{cop}}(M_2(\mathbb{C}), M_2(\mathbb{C})) \) all maps are decomposable [4, 5].

More generally, we can consider a positive and completely positive maps from a C*-algebra \( \mathfrak{A} \) into algebra of bounded operators \( \mathcal{B}(\mathcal{H}) \) acting on some Hilbert space \( \mathcal{H} \). In that case we will denote by \( \mathcal{L}^+(\mathfrak{A}, \mathcal{B}(\mathcal{H})) \) and \( \mathcal{L}^{\text{cop}}(\mathfrak{A}, \mathcal{B}(\mathcal{H})) \) sets of positive and completely positive maps respectively. The case of \( M_n(\mathbb{C}) \) is a special case of

\(^1\)We consider a matrix to be positive semi-definite when its spectrum lies on positive half-line.
this general approach as matrix algebra is a finite dimensional $C^*$-algebra. Another example, important in this article, is the set of positive maps from the algebra of continuous complex-valued functions on a locally compact Hausdorff space (this is canonical example of a commutative $C^*$-algebra) to some matrix algebra. It is well known that for a commutative $\mathfrak{A}$ the sets $\mathcal{L}^+(\mathfrak{A},B(\mathfrak{H}))$ and $\mathcal{L}^{c*}(\mathfrak{A},B(\mathfrak{H}))$ are equal.

A linear map $\phi : M_n(C) \to M_m(C)$ is called unital if $\phi(\mathbb{1}_n) = \mathbb{1}_m$ ($\mathbb{1}_n$ denotes identity matrix in $M_n(C)$; if the dimension will be clear from the context we will drop index $n$). Norm of a map $\phi : M_n(C) \to M_m(C)$ is defined as usual, i.e. $\|\phi\| = \sup\{\|\phi(a)\| \mid a \in M_n(C), \|a\| = 1\}$, where $\|a\|$ for $a \in M_n(C)$ denotes operator norm.

The set of all positive maps is a convex cone in the set of all linear and continuous maps. The subset of normalized, unital positive maps is a convex subset of the set of all positive maps. The subset of normalized and unital completely positive maps is a convex subset of the set of normalized unital positive maps.

### 2.2 Isomorphism between functionals and states

The relation between mapping spaces and continuous bilinear forms on a tensor products follows from the works of Grothendieck [5]. In the general setting it was already known in 1960s (cf. [7]), and later was reformulated in the linear algebra terms for finite dimensional case by Choi and Jamiołkowski ([5] and [8]) and now is widely known as Choi-Jamiołkowski isomorphism. However, as the underlying geometry will play the crucial role in the sequel we will use following consequence of the Grothendieck construction.

**Lemma 1** (cf. [8]). There is an isometric isomorphism between $\mathcal{L}(M_n(C),M_n(C))$ and bilinear forms in $(M_n(C) \otimes \pi M_n(C))^*$ given by 

$$\tilde{\phi} (\sum_{i} a_i \otimes b_i) = \sum_{i} \mathrm{Tr}(\phi(a_i)b_i^*) .$$

Moreover, the map $\phi \in \mathcal{L}^+(M_n(C),M_n(C))$ if and only if $\tilde{\phi}$ is positive on $M_n(C)^* \otimes \pi M_n(C)^+$.

The $M_n(C) \otimes \pi M_n(C)$ that appeared in the Lemma is by definition a Banach space completion of an algebraic tensor product in the projective norm given by 

$$\pi(x) = \inf \left\{ \sum_{i} \|a_i\| \|b_i\| \mid x = \sum_{i} a_i \otimes b_i, a_i \in M_n(C), b_i \in M_n(C) \right\}$$

The norm $\| \cdot \|_1$ denotes the trace norm, i.e. $\|a\|_1 = \mathrm{Tr}|a| = \mathrm{Tr}(a^*a)^{1/2}$.

As we work on finite dimensional spaces, we can represent the bilinear form $\tilde{\phi}$ corresponding to a positive map $\phi$ by a density matrix $\rho_{\phi}$ given by a well-known formula 

$$\rho_{\phi} = \sum_{i,j} E_{i,j} \otimes \phi(E_{i,j}),$$

where $E_{i,j}$ are matrix units. The positivity condition from the Lemma can now be restated: a map $\phi$ is positive if and only if corresponding $\rho_{\phi}$ is block-positive, what we denote by 

$$\rho_{\phi} \geq_{bp} 0 \iff (x \otimes y, \rho_{\phi} x \otimes y) \geq 0, \quad \forall x, y \in C^n.$$
Very important feature of the cited Lemma [1] is the fact that it establishes isometric isomorphism, thus normed maps are mapped into normed functionals. But as these functionals are defined on projective tensor product, the corresponding functional norm must be dual to the projective norm. We will denote this norm by $\alpha$ and the duality tells us that

$$
\alpha(\rho_a) = \sup \left\{ \frac{\text{Tr} \rho_a a}{\pi(a)} \mid a \in \mathcal{M}_n(\mathbb{C}) \otimes_n \mathcal{M}_n(\mathbb{C}), a \neq 0 \right\}.
$$

(2)

Using this we can specify the set of Choi matrices corresponding to normalized positive maps

$$
\mathcal{D}_0 := \{ \rho \in \mathcal{M}_n(\mathbb{C}) \otimes_n \mathcal{M}_n(\mathbb{C}) \mid \rho = \rho^*, \alpha(\rho) = 1, \rho \geq_\text{vp} 0 \},
$$

and the set Choi matrices corresponding to normalized, unital maps (for a detailed justification see [3])

$$
\mathcal{D} := \{ \rho \in \mathcal{M}_n(\mathbb{C}) \otimes \mathcal{M}_n(\mathbb{C}) \mid \rho = \rho^*, \alpha(\rho) = 1, \rho \geq_\text{vp} 0, \text{Tr} \rho = n \}.
$$

As was mentioned in the Introduction, in the study of exposed points of the set $\mathcal{D}$ a distinguished role is played by selfadjoint unitaries (see [3]), thus we recall a definition.

**Definition 2.** An operator $s$ is called a symmetry if it is a selfadjoint unitary, i.e. $s = s^*$ and $s^2 = 1$. The set of all symmetries in the set $\mathcal{B}(\mathcal{H})$ of all bounded operators acting on Hilbert space $\mathcal{H}$ will be denoted by $\mathcal{S}(\mathcal{H})$.

An operator $s$ is called a partial symmetry or e-symmetry if $s$ is selfadjoint and $s^2 = e$, where $e$ is some orthogonal projector on $\mathcal{H}$.

Note that any symmetry admits a canonical decomposition $s = p - q$, where $p, q$ are orthogonal projectors such that $p + q = 1$. Namely $p = 1/2(1 + s)$ and $q = 1/2(1 - s)$. In particular we can write $s = 1 - 2q$. Symmetries are also useful in computing the $\alpha$-norm, as we see in following lemma.

**Lemma 3** ([3], Lemma 16). Let $\sigma \in \mathcal{M}_n(\mathbb{C}) \otimes_n \mathcal{M}_n(\mathbb{C})$, then

$$
\alpha(\rho) = \max \{ \text{Tr} \rho s \otimes p \mid s \in \mathcal{S}(\mathbb{C}^n), p \in \text{Proj}^1(\mathbb{C}^n) \},
$$

where $\text{Proj}^1(\mathbb{C}^n)$ stands for the set of rank one orthogonal projectors on Hilbert space $\mathbb{C}^n$.

### 2.3 Notions of extremality

In the setting of positive maps different notions of extremality arise. The most obvious is a notion of extreme point of a convex set. The map $\phi \in \mathcal{L}^+(\mathcal{A}, \mathcal{B}(\mathcal{H}))$ is called extreme when it cannot be written as a convex combination of other positive maps.

Now consider a completely positive map $\phi \in \mathcal{L}^+(\mathcal{A}, \mathcal{B}(\mathcal{H}))$. One can write it in following way: $\phi = \sum \phi_i t_i$, where $t_i \in \mathcal{B}(\mathcal{H})$ such that $\sum t_i^* t_i = 1$, all $t_i$ are invertible and all $\phi_i$ are completely positive (there is always a trivial decomposition). Such map is called $C^*$-extreme in the set of completely positive maps whenever for all such decompositions all $\phi_i$ are unitarily equivalent to $\phi$ (for details see [10]).
Finally, we can define an order structure in $\mathcal{L}^{\text{cp}}(\mathcal{A}, \mathcal{B}(\mathcal{H}))$ in the following way: $\psi \preceq \phi$ if $\phi = \psi$ is completely positive. Then we call a completely positive map $\phi$ pure if $\psi \preceq \phi$ implies $\psi = \lambda \phi$ (thus it is a natural generalization of the notion of a pure state).

In general, for completely positive maps following inclusions are valid

$$\text{pure maps} \subseteq C^*-\text{extreme maps} \subseteq \text{extreme maps}$$

In many cases it is known that some of these inclusions are proper. For our case it will be important to note that in general for maps $\mathcal{L}^+(C(X), M_n(\mathbb{C}))$ there are extreme maps that are not $C^*$-extreme. In the section 3 we will reexamine this problem in the special case of $\mathcal{L}^+(C(X), M_2(\mathbb{C}))$ using the Arveson characterization [11] of extreme maps in $\mathcal{L}^{\text{cp}}(C(X), M_n(\mathbb{C}))$.

**Definition** ([11]). A family of subspaces $\{\mathcal{M}_1, \ldots, \mathcal{M}_n\}$ of Hilbert space $\mathcal{H}$ is weakly independent if whenever there are given $\{T_i \in \mathcal{B}(\mathcal{H})\}^n_{i=1}$ such that the range of $T_i$ and $T_i^*$ lies in $\mathcal{M}_i$, equality $T_1 + \cdots + T_n = 0$ implies that $T_1 = \cdots = T_n = 0$.

**Remark** (see [11]). This condition is equivalent to a linear independence of the family of subspaces $\{\mathcal{M}_1, \ldots, \mathcal{M}_n\}$ of $\mathcal{H} \otimes \mathcal{H}$, where $\mathcal{M}_i := [\xi \otimes \eta] \mid \xi, \eta \in \mathcal{M}_i]$.

**Theorem 4** ([11], Thm 1.4.10 and also cf. [12]). Let $X$ be a compact Hausdorff space and let $\mathcal{H}$ be a finite dimensional Hilbert space. Then extreme points of the set of unital completely positive maps $C(X) \to M_n(\mathbb{C})$ are maps of the form

$$\phi(f) = f(x_1)K_1 + \cdots + f(x_k)K_k, \quad f \in C(X),$$

where $k \geq 1$, $x_1, \ldots, x_k$ are distinct points of $X$ and $K_1, \ldots, K_k$ are positive operators satisfying

(i) $K_1 + \cdots + K_k = I$,

(ii) $\{[K_1 \mathbb{C}^n], \ldots, [K_k \mathbb{C}^n]\}$ is weakly independent family of subspaces, where $[h]$ denotes smallest subspace containing subset $h$.

Note that any $C^*$-extreme map $\phi$ in $\mathcal{L}^{\text{cp}}(C(X), \mathbb{C}^n)$ is also extreme, thus can be represented in the way showed in the previous theorem. Farenick and Morenz [13] showed that the extreme $\phi \in \mathcal{L}^{\text{cp}}(C(X), \mathbb{C}^n)$ is $C^*$-extreme if and only if $K_i$ are orthogonal projectors. This equivalently means that $\phi$ is multiplicative.

We will relate the commutative case to the noncommutative case of $\mathcal{L}(M_n(\mathbb{C}))$ by considering the restriction of a positive map $\phi \in \mathcal{L}^+(M_n(\mathbb{C}))$ to the abelian subalgebra $\text{diag}_n(\mathbb{C}) := \{a \in M_n(\mathbb{C}) \mid a \text{ is diagonal matrix}\}$ of diagonal matrices. It is well known fact that $a \in \text{diag}_n(\mathbb{C})$ can be identified with $a_f \in C(X)$, $X = \{1, \ldots, n\}$, i.e. the complex valued (trivially) continuous function on the set $X$. Thus $\mathcal{L}^{\text{cp}}(\text{diag}_n(\mathbb{C}), M_n(\mathbb{C}))$ can be identified with $\mathcal{L}^{\text{cp}}(C(X), M_n(\mathbb{C}))$. We introduce following notion.

**Definition 5.** Let $\phi$ be a linear, extreme map in the set $\mathcal{L}^+(M_n(\mathbb{C}))$ or $\mathcal{L}^{\text{cp}}(M_n(\mathbb{C}))$. If the map $\phi_0 := \phi|_{\text{diag}_n(\mathbb{C})}$ is extreme in the set of $\mathcal{L}^{\text{cp}}(\text{diag}_n(\mathbb{C}), M_n(\mathbb{C}))$ then we call $\phi$ a regular extreme positive map.
3 Extremality vs. $C^*$-extremality in abelian case

Firstly, let us consider a special case of $\mathcal{L}^\sigma(C(X), M_2(\mathbb{C}))$, where $X = \{1, 2\}$. For $\phi$ extreme in unital $\mathcal{L}^\sigma(C(X), M_2(\mathbb{C}))$ we conclude from Theorem 4 that

$$\phi(f) = f(x_0)K_0 \text{ or } \phi(f) = f(1)K_1 + f(2)K_2.$$  

The first case implies that $K_0 = I$, so corresponding $\mathcal{M}_0 := [K_0 I] = \mathcal{H} = \mathbb{C}^2$. Thus any map of this form is also $C^*$-extreme.

Now take a closer look into the second case. Let $e_1$ and $e_2$ are unit vectors corresponding to projections onto $\mathcal{M}_1 = [K_1 I]$ and $\mathcal{M}_2 = [K_2 I]$ respectively. As $\mathcal{M}_i$ are weakly independent subspaces $\mathcal{M}_i = \{e_i \otimes e_i\}, i = 1, 2$ are linearly independent. Moreover we know that $K_i$ are positive and rank one operators. But any rank one operator can be written in the form $|x\rangle \langle y|$, and such operator is hermitian if and only if $x = y$. So $K_i = |x_i\rangle \langle x_i|$. But

$$I = K_1 + K_2 = |x_1\rangle \langle x_1| + |x_2\rangle \langle x_2|.$$  

Now acting on $x_1$ on the right and taking scalar multiplication from the left by $x_1$ we get that $(x_1, x_2) = 0$ so $K_i$ are orthogonal projectors. Thus by the Farenick and Morenz result any such map is also $C^*$-extreme and therefore multiplicativ (for details see [13] and [10]). As a result we proved the following.

Lemma 6. Any extreme map in $\mathcal{L}^\sigma(C(\{1, 2\}), \mathbb{C}^2)$ is $C^*$-extreme.

We will now discuss a more complicated case of $\mathcal{L}^\sigma(\text{diag}_3(\mathbb{C}), M_3(\mathbb{C}))$. Here, using the Arveson Theorem [11] we conclude that the dimensions of $\mathcal{M}_i$ can be equal to 1, 2, 3. The case of dimension 3 is trivial, as before. Let us then consider the case when one of $\mathcal{M}_i$’s have the dimension equal to 2.

Example 7. Take

$$K_1 = |e_1\rangle \langle e_1|,$$

$$K_2 = |e_2\rangle \langle e_2|,$$

$$K_3 = \frac{1}{2} |e_1 + e_3\rangle \langle e_1 + e_3| + |e_3\rangle \langle e_3|.$$  

Then $K_1 + K_2 + K_3 = I + P \equiv S$, where $P = \frac{1}{2} |e_1 + e_3\rangle \langle e_1 + e_3|$. Note that $S$ is invertible thus we can define

$$\tilde{K}_1 = S^{-\frac{1}{2}} K_1 S^{-\frac{1}{2}}.$$  

This does not change the rank of $K_1$ as $S^{-\frac{1}{2}}$ is a non-singular matrix. It is also self-adjoint, thus this operation preserves positivity. Moreover $\tilde{K}_1 + \tilde{K}_2 + \tilde{K}_3 = I$. Thus we can define an extreme map $\mathcal{L}^\sigma(C(X), M_3(\mathbb{C}))$ by

$$\tilde{\phi}(f) = f(x_1)\tilde{K}_1 + f(x_2)\tilde{K}_2 + f(x_3)\tilde{K}_3.$$  

But using the matrix representation we compute that

$$\tilde{K}_1 \tilde{K}_3 = \begin{pmatrix} \frac{1}{\sqrt{2}} \left(5 + 2\sqrt{6}\right) & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \left(5 - 2\sqrt{6}\right) \end{pmatrix}$$  

thus $K_1$ and $K_3$ are not orthogonal and by remark following the Theorem 4 we conclude that the map $\phi$ is not multiplicative, so it is not $C^*$-extreme.
This example indeed shows that the set of $C^*$-extreme maps in $\mathscr{L}^+(\text{diag}_3(\mathbb{C}), M_3(\mathbb{C}))$ is indeed a proper subset of the set of all extreme maps. It is not surprising as even in $\mathscr{L}^+(C([1,2,3]), M_2(\mathbb{C}))$ there are examples of extreme maps that are not $C^*$-multiplicative \cite{10}.

4 Extreme positive maps on $2 \times 2$ vs. $3 \times 3$ matrices

The results from the previous section allows us to get deeper insight into the structure of the well known case of $\mathscr{L}^+(M_2(\mathbb{C}))$, as well as understand a bit more the nature of qualitative change when we increase the dimension by 1.

Fix a normalized unital $\phi \in \mathscr{L}^+(M_2(\mathbb{C}))$. Using the formula (1) we introduce following notation:

$$\rho_\phi = \sum_{ij} E_{ij} \otimes \phi(E_{ij}) = \sum_{ij} E_{ij} \otimes \rho_{ij}, \quad \text{where } E_{ij} = |e_i\rangle \langle e_j|$$

From the definition of $\rho_{ij}$ we immediately get that $\rho_{11} \geq 0, \rho_{22} \geq 0, \rho_{11} + \rho_{22} = \mathbb{1}$ and $\rho_{ij} = \rho_{ji}^*$. In two dimensional case the structure of $\rho$ can be explicitly given, namely:

**Proposition 8.** The Choi matrix $\rho_\phi$ corresponding to the regular extreme normalized unital map $\phi \in \mathscr{L}^+(M_2(\mathbb{C}))$ can be written in one of following block forms in some matrix representation

$$\rho_\phi = \begin{pmatrix} |y_1\rangle \langle y_1| & c_0 |y_1\rangle \langle y_2| + c |y_2\rangle \langle y_1| \\ c_0 |y_1\rangle \langle y_2| & |y_2\rangle \langle y_2| \end{pmatrix} \quad \text{or } \rho_\phi = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix},$$

where $c_0 \geq 0, c \in \mathbb{C}$ and $\{y_1, y_2\}$ is some basis in $\mathbb{C}^2$.

**Proof.** If we consider a restriction of the map $\phi$ to diagonal matrices, then based on results of the previous section and the Def.\ref{def} we conclude that either

$$\rho_{ii} = |y_i\rangle \langle y_i|$$

or

$$\rho_{11} = \mathbb{1}, \quad \rho_{22} = 0.$$  

Firstly we will consider non-trivial case. Assume $\rho_{ii} = |y_i\rangle \langle y_i|$. The block-positivity property of the $\rho$ gives us

$$(x \otimes y, \sum_{ij}(E_{ij} \otimes \rho_{ij})x \otimes y) = \sum_{ij}(x, e_i)(e_j, x)(y, \rho_{ij}y) \geq 0.$$  

Now let us take $x = \varepsilon e_1 + \lambda e_2$ and $y = y_1$, with $\varepsilon > 0$ and $\lambda$ real. Note that $x$ does not have to be normalized vector. Then the inequality above gives us

$$\varepsilon^2 + \varepsilon \lambda(y_1, \rho_{12}y_1) + \varepsilon \lambda(y_1, \rho_{21}y_1) + 0 \geq 0$$

So we get

$$\lambda(y_1, (\rho_{12} + \rho_{12}^*)y_1) \geq -\varepsilon.$$  

As vector $x$ can be chosen arbitrary, we can also take the vector $\varepsilon e_1 - \lambda e_2$ and then we get

$$\varepsilon \geq \lambda(y_1, (\rho_{12} + \rho_{12}^*)y_1)$$
Fixing $\epsilon$ and taking arbitrary $\lambda$ we conclude that
\[
(y_1, (\rho_{12} + \rho_{12}^*) y_1) = 0
\]
(3)

If we proceed by the same way using vectors $\epsilon \epsilon_1 + i \lambda \epsilon_2$ and $\epsilon \epsilon_1 - i \lambda \epsilon_2$ we conclude that
\[
(y_1, (\rho_{12} - \rho_{12}^*) y_1) = 0
\]
(4)

Combining these two we get that $(y_1, \rho_{12} y_1) = 0$. If we choose $y = y_2$ and repeat all the above reasoning we arrive to conclusion that $(y_2, \rho_{12} y_2) = 0$, so finally we get that
\[
\rho_{12} = c_1 |y_1\rangle \langle y_2| + c_2 |y_2\rangle \langle y_1|.
\]
(5)

Now we do a unitary transformation $y_1 \mapsto e^{-i \arcc \epsilon} y_1$, $y_2 \mapsto y_2$, which gives us the desired result.

In the case when $\rho_{11} = \mathbb{1}$ and $\rho_{22} = 0$ we repeat all above calculations with the only difference that we get $(y, \rho_{12} y) = 0$ for any $y$. Thus $\rho_{12} = 0$ and this corresponds to the second form. \qed

Let us now discuss admissible values of coefficients $c_0$ and $c$. In this part we will extensively use the fact, than $\rho$ is normalized in $\alpha$-norm, i.e. $\alpha(\rho_\phi) = 1$. In particular, the definition of $\alpha$-norm tells us that
\[
1 = \alpha(\rho_\phi) \geq |\text{Tr} \rho_\phi a \otimes b|,
\]
for any $a$ and $b$ such that $\tau(a \otimes b) = 1$. Note that if $\|a\| = 1$ and $\|b\| = 1$ then $\tau(a \otimes b) = 1$. Take for $a = E_{12} + \lambda E_{21}$ and $b = |y_2\rangle \langle y_1|$, with $|\lambda| = 1$. From the definition of the operator norm one instantly gets that $\|a\| = 1$. On the other hand $\|b\| = \text{Tr} |y_2\rangle \langle y_1| = \text{Tr} (|y_1\rangle \langle y_2| |y_2\rangle \langle y_1|)^{1/2} = \text{Tr} |y_1\rangle \langle y_1| = 1$. Consequently
\[
1 \geq |\text{Tr} (\rho_\phi (E_{12} + \lambda E_{21}) \otimes |y_2\rangle \langle y_1|)| = |\text{Tr} (\phi (E_{12} + \lambda E_{21}) \tau(|y_2\rangle \langle y_1|))|,
\]
due to definition of $\rho_\phi$ (cf. Lemma [1]). Now applying the Proposition [3] we get
\[
1 \geq |\text{Tr} (c_0 |y_1\rangle \langle y_2| + c |y_2\rangle \langle y_1| + \lambda c_0 |y_2\rangle \langle y_1| + \lambda^* |y_1\rangle \langle y_2|) | = |\text{Tr} (c |y_2\rangle \langle y_1| + \lambda c_0 |y_2\rangle \langle y_1|)|
\]
Calculating the trace one arrives to $1 \geq |c + \lambda c_0|$. Because $\lambda$ here is arbitrary complex number of modulus 1, we can take in particular $\lambda = e^{i \arcc \epsilon}$. Thus
\[
1 \geq |c_0| + |c| = c_0 + |c|.
\]
(6)

Now it is easy to show that

**Theorem 9.** Any regular extreme normalized unital map in $\mathcal{L}^+ (M_2(\mathbb{C}))$ corresponds to an element of the following subset of $\mathcal{D}$

$$\{\mathcal{S}(\mathbb{C}^2), 2P_x, p \otimes \mathbb{1}, \rho_\phi \} = \mathcal{D} \cup \{\rho_\phi \}, \text{where } \rho_\phi = \begin{pmatrix} |y_1\rangle \langle y_1| & 0 \\ 0 & |y_2\rangle \langle y_2| \end{pmatrix},$$

and $x$ is a maximally entangled vector in some basis $\{y_1, y_2\}$ of $\mathbb{C}^2$ and $p$ is a rank one projector in $\mathbb{C}^2$. 

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Proof. If $\phi \in \mathcal{L}^+(M_2(\mathbb{C}))$ is regular extreme, then from Proposition 8 we know that $\rho_\phi$ is of the form

$$
\rho_\phi = \begin{pmatrix}
|y_1\rangle \langle y_1| & c_0 |y_1\rangle \langle y_2| + c |y_2\rangle \langle y_1| \\
(c_0 |y_2\rangle \langle y_1| + \overline{c}|y_1\rangle \langle y_2| & |y_2\rangle \langle y_2|
\end{pmatrix} \quad \text{or} \quad \rho_\phi = \begin{pmatrix}
I & 0 \\
0 & 0
\end{pmatrix},
$$

Let us consider the first case. Then $\{y_1, y_2\}$ fix basis in one Hilbert space. Let us use the same symbol to denote basis in the second Hilbert space (that is fixed by the matrix representation). Define $\tilde{y}_1 = y_1, \tilde{y}_2 = e^{i\arg c} y_2$ and

$$
w = \sum_{i,j=1}^{2} |\tilde{y}_i\rangle \langle \tilde{y}_j| \otimes |y_j\rangle \langle y_i| = \begin{pmatrix}
|y_1\rangle \langle y_1| & e^{i\arg c} |y_1\rangle \langle y_2| \\
e^{-i\arg c} |y_1\rangle \langle y_2| & |y_2\rangle \langle y_2|
\end{pmatrix}.
$$

By straightforward calculation we check that $w$ is a symmetry. Now take $x = 1/\sqrt{2} (y_1 \otimes y_1 + y_2 \otimes y_2)$ and define

$$
\rho_0 = 2P_x = \begin{pmatrix}
|y_1\rangle \langle y_1| & |y_1\rangle \langle y_2| \\
|y_2\rangle \langle y_1| & |y_2\rangle \langle y_2|
\end{pmatrix}.
$$

Then one gets that

$$
\rho_\phi = c_0 \rho_0 + |c| w + (1 - c_0 - |c|) \rho_\phi.
$$

Due to (5) we see that $\rho_\phi$ must be a convex combination of maps form $\bar{D}$ and $\rho_\phi$. As we assumed that $\phi$ is extreme, the claim follows.

In the case when

$$
\rho_\phi = \begin{pmatrix}
I & 0 \\
0 & 0
\end{pmatrix},
$$

we immediately see that it is equal to $|y_1\rangle \langle y_1| \otimes I$ in the basis fixed by matrix representation.

\[\Box\]

Remark. The element $\rho_\phi$ corresponds to the map projecting element $a$ onto the subalgebra of diagonal matrices in some basis fixed by matrix representation. Namely

$$
\tilde{\phi}(a) = \begin{pmatrix}
a_{11} & 0 \\
0 & a_{22}
\end{pmatrix}.
$$

Remark. It is also noteworthy to mention that maps corresponding to elements $2P_x$ are isomorphisms and those corresponding to symmetries are anti-isomorphisms. The last claim follows from the fact that in the $n = 2$ case all symmetries in $\mathcal{D}$ are locally unitary equivalent to the Choi matrix of transposition map (for a simple proof see [3]).

The situation in the case of $\phi \in \mathcal{L}^+(M_3(\mathbb{C}))$ is much more complicated. Our results concerns only regular maps. Nevertheless example 7 shows that even in this case we cannot infer that the block-diagonal part of Choi matrix, i.e. elements $\phi(e_{ij})$, are formed by the orthogonal projectors. Moreover for $n = 3$ there appear non-decomposable maps. Illustration of this fact is given by generalized Choi maps.

Example 10. Consider a generalized Choi map of the form [14, 5, 15]

$$
\phi(a) = \frac{1}{2} \begin{pmatrix}
a_{11} + a_{33} & -a_{1,2} & -a_{1,3} \\
-a_{2,1} & a_{22} + a_{11} & -a_{2,3} \\
-a_{3,1} & -a_{3,2} & a_{33} + a_{22}
\end{pmatrix}.
$$
It is known that this is an extreme positive map. Arverson’s decomposition of its restriction to commutative algebra diag₃(ℂ) is given by

\[ \phi(f) = f(x_1)K_1 + f(x_2)K_2 + f(x_3)K_3, \]

where

\[
K_1 = \frac{1}{2}(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2|)
\]

\[
K_2 = \frac{1}{2}(|e_2\rangle\langle e_2| + |e_3\rangle\langle e_3|)
\]

\[
K_3 = \frac{1}{2}(|e_1\rangle\langle e_1| + |e_3\rangle\langle e_3|).
\]

It is apparent that in this example \(K_1K_2 \neq 0\).

5 Convex analysis of Choi map

In this section we will study the structure of Choi map \(\phi\) that was recalled in the Example 10. It is worth remembering that this was the first and very important example of a non-decomposable positive map. Denote by \(\rho_C\) Choi matrix corresponding to \(\phi\) and by \(\tilde{\rho}_C\) partial transpose of \(\rho_C\). From [3] we know that partial transposition preserves the set \(\mathcal{D}\). In fact \(\tilde{\rho}_C\) corresponds to the map \(\tau \circ \phi\) and is also extreme and indecomposable. The analysis of \(\tilde{\rho}_C\) is nicer than \(\rho_C\). Thus to understand the nature of the Choi map we will carry out an examination of \(\tilde{\rho}_C\).

Lemma 11. Let

\[ w^- = \sum_{i,j=1}^{3} \epsilon_{ij}E_{ij} \otimes E_{ji}, \text{ where } \epsilon_{ij} = \begin{cases} 1 & \text{for } i = j, \\ -1 & \text{for } i \neq j. \end{cases} \]

Then \(w^-\) is a symmetry (but not block positive) and \(\alpha(w^-) = 5/3\).

Proof. The fact that \(w^-\) is a symmetry follows from the direct calculation. To see that it is not block positive it is enough to consider \(x = 1/2(e_1 + e_2) + 1/\sqrt{2}e_2\) and calculate that

\[ (x \otimes w^- x \otimes x) = -\frac{1}{4}. \]

In order to calculate \(\alpha(w^-)\) we will use Lemma 3 i.e.

\[ \alpha(w^-) = \sup_{s,p} |\text{Tr} w^- s \otimes p|, \]

where \(s\) is a symmetry and \(p\) is a rank 1 projector. Because \(s \in M_3(ℂ)\), we can write it as \(s = \mathbb{1} - 2q\), where \(q\) is projector. Without loss of generality we can assume that this is rank 1 projector, as case rank 0 is trivial and rank 2 can be reduced to rank 1 by \(\mathbb{1} - 2q = 2q' - \mathbb{1} = -(\mathbb{1} - 2q')\) where \(q' = \mathbb{1} - q\), and \(q'\) is rank 1. Thus

\[ \alpha(w^-) = \sup_{q,p} |\text{Tr} w^- \mathbb{1} \otimes p - 2 \text{Tr} w^- q \otimes p|. \]

Let \(p = |x\rangle\langle x|\) and \(q = |y\rangle\langle y|\). By explicit calculation we see that \(\text{Tr} w^- \mathbb{1} \otimes p = ||x||^2 = 1\), so to obtain supremum we need to find extreme values of \(\text{Tr} w^- q \otimes \)}
Denote by \( \{x_i\} \) and \( \{y_i\} \) coefficients of \( x \) and \( y \) in canonical basis. Then we calculate

\[
\text{Tr} w^{-1} \otimes p = |x_1|^2|y_1|^2 - x_1\overline{x_2}y_2\overline{y_1} - x_1\overline{x_3}y_3\overline{y_1} - x_2\overline{x_1}y_1\overline{y_2} - x_2\overline{x_3}y_3\overline{y_2} - x_3\overline{x_1}y_1\overline{y_3} - x_3\overline{x_2}y_2\overline{y_3} + |x_3|^2|y_3|^2
= |x_1|^2|y_1|^2 + |x_2|^2|y_2|^2 + |x_3|^2|y_3|^2
- 2\Re x_1\overline{x_2}y_2\overline{y_1} - 2\Re x_1\overline{x_3}y_3\overline{y_1} - 2\Re x_2\overline{x_3}y_3\overline{y_2}.
\]

We can rewrite this using a polar decomposition of complex coefficients \( x_j = \xi_j e^{i\phi_j}, y_j = \eta_j e^{i\psi_j} \).

\[
\text{Tr} w^{-1} \otimes p = \xi_1^2\eta_1^2 + \xi_2^2\eta_2^2 + \xi_3^2\eta_3^2
- 2\xi_1\xi_2\eta_1\eta_2 \cos(\phi_1 - \phi_2 + \psi_2 - \psi_1)
- 2\xi_1\xi_3\eta_1\eta_3 \cos(\phi_1 - \phi_3 + \psi_3 - \psi_1)
- 2\xi_2\xi_3\eta_2\eta_3 \cos(\phi_2 - \phi_3 + \psi_3 - \psi_2)
\geq \xi_1^2\eta_1^2 + \xi_2^2\eta_2^2 + \xi_3^2\eta_3^2 - 2\xi_1\xi_2\eta_1\eta_2 - 2\xi_1\xi_3\eta_1\eta_3 - 2\xi_2\xi_3\eta_2\eta_3 = m,
\]

with equality e.g. for \( \phi_1 = 0 = \psi_j \), and \( M = \xi_1^2\eta_1^2 + \xi_2^2\eta_2^2 + \xi_3^2\eta_3^2 + 2\xi_1\xi_2\eta_1\eta_2 + 2\xi_1\xi_3\eta_1\eta_3 + 2\xi_2\xi_3\eta_2\eta_3 \geq \text{Tr} w^{-1} \otimes p \).

with equality e.g. for \( \phi_1 = \phi_2 = \pi \) and other \( \phi_i = 0, \psi_i = 0 \). We use the normalization of \( x \) and \( y \) to introduce parametrization

\[
\xi_1 = \sin \alpha \sin \beta, \quad \xi_2 = \cos \alpha \sin \beta, \quad \xi_3 = \cos \beta,
\eta_1 = \sin \mu \sin \nu, \quad \eta_2 = \cos \mu \sin \nu, \quad \eta_3 = \cos \nu,
\]

Substitution and simplification yields

\[
m = \cos^2 \beta \cos^2 \nu + \cos^2(\alpha + \mu) \sin^2 \beta \sin^2 \nu - \cos \beta \sin \beta \cos(\alpha - \mu) \sin 2\nu
= (\cos \beta \cos \nu - \cos(\alpha + \mu) \sin \beta \sin \nu)^2 - 4 \cos \beta \sin \beta \sin \alpha \mu \sin \nu \cos \nu,
\]

and

\[
M = (\cos \beta \cos \nu + \cos(\alpha - \mu) \sin \beta \sin \nu)^2.
\]

Now we substitute

\[
\alpha^- = \alpha - \mu, \quad \alpha^+ = \alpha + \mu,
\beta^- = \beta - \nu, \quad \beta^+ = \beta + \nu
\]

and get

\[
m = \frac{1}{4} (\cos \beta^- + \cos \beta^+ - \cos \alpha^+ \cos \beta^- + \cos \alpha^- \cos \beta^+)^2
- \frac{1}{4} (\cos \beta^- + \cos \beta^+)(\cos \beta^- - \cos \beta^+)(\cos \alpha^- - \cos \alpha^+)
M = \frac{1}{4} (\cos \beta^- + \cos \beta^+ + \cos \alpha^- \cos \beta^- - \cos \alpha^- \cos \beta^+)^2.
\]

(7)
Finally we denote
\[ a = \cos \beta, \quad b = \cos \beta^+ \quad c = \cos \alpha^+, \quad d = \cos \alpha^- \]
to get
\[
m = \frac{1}{4}(a + b - c + a b - c b) - \frac{1}{2}(a + b)(a - b)(d - c)
\]
\[
M = \frac{1}{4}(a + b + d - c a - d b)
\]
By direct calculation the minimum value of \( m \) is equal to \(-1/3 \) (e.g. for \( a = -1, b = 1/3, c = 0, d = 1 \)) and maximum value of \( M \) equals 1, so the \( \alpha \)-norm of \( w^- \) equals \( 5/3 \).

**Remark.** For \( n = 2 \) analogously defined \( w^- \) belongs to \( \mathcal{D} \).

Simple calculation leads to following conclusion.

**Proposition 12.** Choi matrix \( \tilde{\rho}_C \) is a convex combination of \( w^- \) and matrix
\[
r = E_{11} \otimes E_{22} + E_{22} \otimes E_{33} + E_{33} \otimes E_{11},
\]
amely
\[
\tilde{\rho}_C = \frac{1}{2}r + \frac{1}{2}w^-.
\]

**Remark.** Matrix \( r \) is positive and it is straightforward to check that \( r \in \mathcal{D} \).

Let us recall the definition of generalized Choi map (see e.g. \[15\]):
\[
\phi_{a,b,c}(x) = \psi_{a,b,c}(x) - x,
\]
where
\[
\psi_{a,b,c}(x) = \begin{pmatrix} ax_{11} + bx_{22} + cx_{33} & 0 & 0 \\ 0 & ax_{22} + bx_{33} + cx_{11} & 0 \\ 0 & 0 & ax_{33} + bx_{11} + cx_{22} \end{pmatrix}.
\]
Such map is positive if and only if following conditions are satisfied
(i) \( a \geq 1 \),
(ii) \( a + b + c \geq 3 \),
(iii) \( bc \geq (2 - a)^2 \) if \( 1 \leq a \leq 2 \).

Now one can see that partial transpose of \( w^- \) is a Choi matrix corresponding to generalized Choi map \( \phi_{2,0,0} \). Then for any \( 0 \leq \lambda \leq 1 \)
\[
\rho_\lambda = \lambda r + (1 - \lambda)w^-
\]
corresponds to generalized Choi map \( (1 - \lambda)\phi_{2,0,0}/(1 - \lambda) \). The factor \( (1 - \lambda) \) in front ensures that the map is always unital. Conditions under which the generalized Choi map is positive imply that for \( \lambda \geq 1/2 \) the Choi matrix \( \rho_\lambda \) belongs to \( \mathcal{D} \).
6 Properties of symmetries in $\mathcal{D}$

To further examine the $n = 3$ case we will focus on a local unitary equivalence of those Choi matrices that are represented by symmetries. We know that in $n = 2$ case all symmetries in $\mathcal{D}$ are locally unitarily equivalent to Choi matrix representing transposition map. The natural question arise whether it is still true in $n = 3$ case or can symmetries also represent some non-decomposable maps.

Through this section we adopt convention that coefficients of Schmidt decomposition are non-negative (any possible phase is included in vectors of Schmidt decomposition). To simplify notation we used the same symbol $e_i$ to denote basis vectors in the first and the second Hilbert space, but clearly this is only a matter of convenience.

6.1 Technical lemmas

**Lemma 13.** Let $s$ be a block positive symmetry, with decomposition $s = p - q$. Then

(i) any eigenvector of $q$ must have Schmidt rank greater than one;

(ii) any eigenvector of $q$ that have Schmidt rank equal to 2 must have both Schmidt coefficients equal to $\frac{1}{\sqrt{2}}$.

**Proof.** Block positivity condition implies that for normalized vectors $(x \otimes y, qx \otimes y) \leq \frac{1}{2}$.

The (i) part is then obvious, as one could take for $x \otimes y$ eigenvector of $q$ that have Schmidt rank equal to one and violate above inequality.

For (ii) let us consider the Schmidt rank 2 normalized eigenvector $v$ of $q$. Its Schmidt decomposition can be written as $v = \cos \alpha \ e_1 \otimes f_1 + \sin \alpha \ e_2 \otimes f_2$ with $\alpha \in (0, \pi/2)$. Then:

$$(e_1 \otimes f_1, P_v e_1 \otimes f_1) = \cos^2 \alpha,$$

$$(e_2 \otimes f_2, P_v e_2 \otimes f_2) = \sin^2 \alpha,$$

where $P_v$ denotes orthogonal projector on vector $v$. But when $\cos^2 \alpha \leq 1/2$ then $\sin^2 \alpha \geq 1/2$ with equality only when both equal 1/2. So Schmidt coefficients of $v$ must be equal to $1/\sqrt{2}$.

Following lemma about $\alpha$-norm will be used very often and we will use it without an explicit mention.

**Lemma 14.** Let $\rho \in \mathcal{D}$. Then for any one-dimensional projector $p$

$$a(\rho) = \text{Tr}(\mathbb{1} \otimes p)\rho = 1$$

**Proof.** From the Lemma we have

$$a(\rho) = \max\{|\text{Tr} \rho s \otimes p| \mid s \in \mathcal{S}(\mathcal{H}), p \in \text{Proj}^1(\mathcal{H})\}$$

Because $\rho \in \mathcal{D}$, then there exists positive and unital map $\phi_\rho : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$. For any symmetry $s$ and projector $p$ we thus have

$$\text{Tr} \rho s \otimes p = \text{Tr} \phi_\rho(s)p^\dagger.$$
Next, we notice that from the Kadison inequality we have that
\[ \mathbb{1} = \phi_p(s^2) \geq \phi_p(s)^2, \]
thus \( \mathbb{1} \geq |\phi_p(s)| \) and by the Proposition 2.2.13c in [17],
\[ p^* \geq p|\phi_p(s)|p^*. \]
Let \( p^* = |x\rangle \langle x| \). By \( P_\lambda \) we denote spectral projections of \( \phi_p(s) \). Taking trace we have
\[ \text{Tr} p^* \geq \text{Tr} p^*|\phi_p(s)|p^* = (x, |\phi_p(s)|x) = \sum_{\lambda \in \sigma(\phi_p(s))} |\lambda|(x, P_\lambda x) \geq |\lambda(x, P_\lambda x) = |\text{Tr} \phi_p(s)p^*| = |\text{Tr} ps \otimes (p^*)^*| \]
On the other hand we have \( \mathbb{1} = \text{Tr} p^* = \text{Tr} \phi_p(\mathbb{1})p^* = \text{Tr} \mathbb{1} \otimes p \), for any \( p \). \( \square \)

The following Lemma is in fact valid for any finite dimensional Hilbert space \( \mathcal{H} \). Although it seems to be well known for sake of completeness we give here the proof because this lemma is the crucial element of many proofs in the sequel.

**Lemma 15.** Let \( x = \sum_{i=1}^N \lambda_i e_i \otimes f_i \) be the Schmidt decomposition of vector \( x \). Then for any one-dimensional projector \( P \)
\[ \text{Tr}(\mathbb{1} \otimes p)P \leq \max \lambda_i^2. \]
Moreover \( \text{Tr}(\mathbb{1} \otimes P_\lambda)P \leq \max \lambda_i^2 \) if and only if
\[ z \in \text{span}\{f_i \} \text{ where } i \text{ is such that } \lambda_i = \max \lambda_k. \]

**Proof.** Let \( z = \sum_{i=1}^k z_if_i \) (if \( k < N \), where \( N \) is a dimension of a corresponding Hilbert space then we define \( f_i \) for \( i = k+1, \ldots, N \) as mutually orthonormal vectors to \( f_i, i = 1, \ldots, k \), such that \( \{f_i\}_{i=1,\ldots,N} \) is a basis). Then
\[ \text{Tr}(\mathbb{1} \otimes P_\lambda)P \leq \sum_{i,j} \lambda_i \lambda_j \text{Tr}(\mathbb{1} \otimes f_i) |e_i \rangle \langle e_j|f_j\rangle = \sum_{i,j} \lambda_i \lambda_j \text{Tr}(\mathbb{1} \otimes f_i) |e_i \rangle \langle e_j|f_j\rangle \]
\[ = \sum_{i,j=1}^n \lambda_i \lambda_j \sum_{m=1} x_m \sum_{n=1} \text{Tr}(\mathbb{1} \otimes f_m) |e_i \rangle \langle e_j|f_j\rangle \]
\[ = \sum_{i,j=1}^n \lambda_i \lambda_j \sum_{m=1} x_m \sum_{n=1} \delta_{ij} \delta_{mj} \]
\[ = \sum_{i,j} \lambda_i \lambda_j \sum_{m=1} x_m \delta_{ij} \]
\[ = \sum_{i} \lambda_i \sum_{m=1} x_m \delta_{ij} \]
\[ = \sum_{i} \lambda_i \sum_{m=1} x_m \delta_{ij} = \sum_i \lambda_i \sum_{m=1} x_m \delta_{ij} \]
Denote \( \lambda_{\max} = \max \lambda_i \). Then
\[ \lambda_i^2 |z_i|^2 \leq \sum_i \lambda_{\max}^2 |z_i|^2 = \lambda_{\max}^2. \]
For a second claim, let us assume that \( \lambda_i \) are sorted and the first \( n \) of \( \lambda_i \) are equal \( \lambda_{\max} \) (\( n \) can be smaller than \( N \), in particular \( n \) can be equal \( 1 \)). The “if” part is obvious: substitution of \( \lambda_{\max} \) for \( \lambda_i \) does not change anything. The “only if” part follows from the fact, that if \( z = \sum_{i=1}^n z_if_i + z_jf_j \), \( j > n \) (with possible \( z_i = 0 \) for \( i \in 1 \ldots n \)), then \( \lambda_j^2 |z_j|^2 \leq \lambda_{\max}^2 |z_j|^2 \). \( \square \)
We adopt following notation for partial transpose: $\mathbb{1} \otimes \tau \equiv \tau_s$.

**Lemma 16.** Let $a \in B(\mathcal{H}) \otimes B(\mathcal{H})$ and $U, V$ are unitaries acting on $\mathcal{H}$. Then
\[
(\tau_s \circ \text{Ad}_{U \otimes V}) a = (\text{Ad}_{U \otimes (V^*)} \circ \tau_s) a
\]

**Proof.** Let $a = \sum a_i \otimes b_i$ then
\[
\tau_s(U \otimes V a U^* \otimes V^*) = \sum \lambda_i a_i \otimes (\tau(V b_i V^*))
\]
\[
= \sum \lambda_i a_i \otimes (\tau(V^*) \tau(b_i) \tau(V))
\]
\[
= U \otimes \tau(V^*) \left( \sum \lambda_i (a_i \otimes \tau(b_i)) \right) U^* \otimes \tau(V)
\]
\[
= (U \otimes \tau(V^*)) \tau_s(a) (U^* \otimes \tau(V)).
\]

\[\square\]

### 6.2 Building blocks of symmetries in $\mathcal{D}$

**Proposition 17.** Let $\xi_1, \xi_2, \xi_3$ be three orthonormal vectors in $\mathcal{H} \otimes \mathcal{H}$ with Schmidt decompositions of the form:

\[
\xi_1 = \sum_{i=1}^3 \lambda_i e_i \otimes f_i, \quad \lambda_i > 0, \quad \sum_{i=1}^3 \lambda_i^2 = 1,
\]
\[
\xi_2 = \frac{1}{\sqrt{2}} (h_1 \otimes g_1 + h_2 \otimes g_2),
\]
\[
\xi_3 = \frac{1}{\sqrt{2}} (k_1 \otimes l_1 + k_2 \otimes l_2).
\]

Then the symmetry $s = \mathbb{1} - 2q$, where $q = \sum P_{\xi_i}$, is not in $\mathcal{D}$.

**Proof.** Assume that Schmidt coefficients of $\xi_1$ are sorted and the greatest is $\lambda_1$. We will consider separately three cases exhausting all possible values for $\lambda_1$, namely $\lambda_1 > 1/\sqrt{2}$, $\lambda_1 \in [1/\sqrt{3}, 1/\sqrt{2})$, and $\lambda_1 = 1/\sqrt{2}$ ($\lambda_1$ is the greatest Schmidt coefficient, so must be greater or equal to $1/\sqrt{3}$). Last two parts will be proved by contradiction: we assume that $s$ is in $\mathcal{D}$ and show that then $a(s) \neq 1$.

If $\lambda_1 > 1/\sqrt{3}$ then $(e_j \otimes f_1, g_j \otimes f_1) > 1/2$ so $s$ is not block positive.

If $\lambda_1 \in [1/\sqrt{3}, 1/\sqrt{2})$, take the $l_i$ such that $\{l_i\}$ is a basis in $\mathcal{H}$. Then $\text{Tr}(\mathbb{1} \otimes P_{\xi_1}) P_{\xi_1} = 0$. But from the Lemma\textsuperscript{15} $\text{Tr}(\mathbb{1} \otimes P_{\xi_1}) P_{\xi_1} < 1/2$ and $\text{Tr}(\mathbb{1} \otimes P_{\xi_2}) P_{\xi_2} \leq 1/2$. Consequently
\[
\text{Tr}(\mathbb{1} \otimes P_{\xi_1}) s = \text{Tr}(\mathbb{1} \otimes P_{\xi_2}) \mathbb{1} - 2 \text{Tr}(\mathbb{1} \otimes P_{\xi_2}) q = 3 - 2 \text{Tr}(\mathbb{1} \otimes P_{\xi_2}) q > 3 - 2(1/2 + 1/1 + 2/0) = 1,
\]
and $s$ can not be in $\mathcal{D}$.

It remains to consider the case when $\lambda_1 = 1/\sqrt{2}$. Notice that then $\lambda_2, \lambda_3 < 1/\sqrt{3}$. Let $g_3, h_3, k_3$ and $l_3$ be orthonormal vectors to, respectively, $\{g_1, g_2\}, \{h_1, h_2\}, \{k_1, k_2\}$ and $\{l_1, l_2\}$. Then either (a) $f_1 \neq g_3$ or (b) $f_1 = g_3$. In the case (a), from the Lemma\textsuperscript{15} we infer that
\[
\text{Tr}(\mathbb{1} \otimes P_{\xi_3}) P_{\xi_1} < \frac{1}{2},
\]

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as the maximal Schmidt coefficient equals to $1/\sqrt{2}$, and $g_3$ does not belong to one dimensional subspace spanned by $f_1$. But as $\text{Tr}(\mathbb{1} \otimes P_{g_3})P_{\xi_3} = 0$ ($g_3$ is orthogonal to $g_1$ and $g_2$), and $\text{Tr}(\mathbb{1} \otimes P_{g_3})P_{\xi_3} \leq 1/2$ (Lemma 15 again), we conclude that

$$\text{Tr}(\mathbb{1} \otimes P_{g_3})s > 3 - 2(1/2 + 1/2) = 1,$$

and $s$ is not in $\mathcal{D}$ this case.

If $f_1 = g_3$, then we repeat previous reasoning, i.e. either (b1) $f_1 \neq l_3$ or (b2) $f_1 = l_3$. The case (b1) can be treated exactly in the same manner as it was done previously in the case (a): $\text{Tr}(\mathbb{1} \otimes P_{l_3})P_{\xi_1} < 1/2$ and the rest follows as before, so $s \notin \mathcal{D}$.

For (b2) we conclude that $g_3 = l_3$ and notice that $\text{Tr}(\mathbb{1} \otimes P_{g_3})P_{\xi_3} = 1/2$ (obvious) and $\text{Tr}(\mathbb{1} \otimes P_{g_3})P_{\xi_3} = 1/2$ (again Lemma 15 as $g_1$ being orthogonal to $l_3 = g_3$ belongs to the subspace spanned by $l_1, l_2$) and $\text{Tr}(\mathbb{1} \otimes P_{g_3})P_{\xi_3}$ must be strictly greater than zero as $\{f_1, f_2, f_3\}$ spans whole $\mathcal{H}$, so

$$\text{Tr}(\mathbb{1} \otimes P_{g_3})s = \text{Tr}(\mathbb{1} \otimes P_{g_3})P_{\xi_1} + \text{Tr}(\mathbb{1} \otimes P_{g_3})P_{\xi_2} + \text{Tr}(\mathbb{1} \otimes P_{g_3})P_{\xi_3} > 1,$$

and also it that case $\text{Tr}(\mathbb{1} \otimes P_{g_3})s \neq 1$. We excluded all possibilities, so such $s$ cannot be in $\mathcal{D}$. \qed

In the tensor product $\mathcal{H} \otimes \mathcal{H}$ the subspace of Schmidt rank 3 vectors is one dimensional [18,19], thus it is impossible to have two or more such orthonormal vectors. Thus we arrive at the following conclusion.

**Corollary 18.** Let $s$ be a block positive symmetry in $\mathcal{D}$, and $s = p - q$. Then all eigenvectors of $q$ are Schmidt rank 2 vectors with both Schmidt coefficients equal to $1/\sqrt{2}$.

### 6.3 Local unitary equivalence of a certain class of symmetries

It will be less complicated if we show locally unitary equivalence to the following symmetry in $\mathcal{D}$ (which is locally unitary equivalent to symmetry corresponding to transposition map).

**Lemma 19.** Let

$$x_1 = \frac{1}{\sqrt{2}}(e_1 \otimes e_1 + e_2 \otimes e_2),$$

$$x_2 = \frac{1}{\sqrt{2}}(e_1 \otimes e_3 + e_3 \otimes e_2),$$

$$x_3 = \frac{1}{\sqrt{2}}(e_2 \otimes e_3 - e_3 \otimes e_1).$$

Then $s_0 = 1 - 2 \sum_i P_{x_i}$ is a block positive symmetry in $\mathcal{D}$ locally unitary equivalent to the symmetry corresponding to the transposition map.

**Proof.** By direct calculation one sees that partial transpose of $s_0$, is equal to $3P_x$, where $x$ is maximally entangled vector:

$$x = \frac{1}{\sqrt{3}}(e_3 \otimes e_3 - e_1 \otimes e_2 + e_2 \otimes e_1).$$
Now let $w$ be the Choi matrix corresponding to the transposition map (in the basis introduced above). Let $y$ be the vector defined by $3P_y = \tau_y(w)$, i.e.

$$y = \frac{1}{\sqrt{3}}(e_1 \otimes e_1 + e_2 \otimes e_2 + e_3 \otimes e_3)$$

We remind that if two vectors have exactly the same Schmidt coefficients then they are locally unitarily equivalent, so $x = U \otimes V y$ for some unitaries $U, V$. Consequently $P_x = U \otimes V P_y U^* \otimes V^*$. Finally, by the Lemma 16

$$s_0 = \tau_y(3P_y) = \tau_y(U \otimes V 3P_y U^* \otimes V^*) = U \otimes \tau(V^*) \tau_y(3P_y) U^* \otimes \tau(V) = \text{Ad}_{U \otimes \tau(V^*)} w.$$

Now we can prove our first equivalence result.

**Proposition 20.** Let $s$ be a symmetry in $\mathcal{D}$ and let $s = \mathbb{1} - 2q$. Assume that eigenvectors of $q$ are of the form

$$x_1 = \frac{1}{\sqrt{2}}(e_1 \otimes e_1 + e_2 \otimes e_2),$$

$$x_2 = \frac{1}{\sqrt{2}}(e_1 \otimes e_1 \pm e_2 \otimes e_1),$$

$$x_3 \text{ arbitrary consistent with assumptions},$$

then $s$ is locally unitary equivalent to the symmetry $s_0$.

**Proof.** Recall that the block positivity condition is equivalent to $(x \otimes y, qx \otimes y) \leq 1/2$. Take $x = 1/\sqrt{2}(e_1 + e_2) = y$, then $(x \otimes y, P_s x \otimes y) = 1/2$. Thus $(x \otimes y, P_s x \otimes y) = 0$. By the analogous argument we infer that $(e_1 \otimes e_1, P_s e_1 \otimes e_1) = 0$ and $(e_2 \otimes e_2, P_s e_2 \otimes e_2) = 0$. Consequently $x_2$ must belong to the subspace spanned by six basis vectors $e_1 \otimes e_2, e_2 \otimes e_3, e_2 \otimes e_1, e_2 \otimes e_2, e_3 \otimes e_3$ and $1/\sqrt{2}(e_1 \otimes e_2 - e_2 \otimes e_1)$. Due to assumed form of $x_2$ we have following possibilities (without normalization constant)

(i) $e_1 \otimes e_3 \pm e_2 \otimes e_3$ 
(ii) $e_1 \otimes e_3 \pm e_3 \otimes e_1$ 
(iii) $e_1 \otimes e_3 \pm e_3 \otimes e_1$

(iv) $e_1 \otimes e_3 \pm e_3 \otimes e_3$ 
(v) $e_2 \otimes e_3 \pm e_3 \otimes e_1$ 
(vi) $e_2 \otimes e_3 \pm e_3 \otimes e_2$

(vii) $e_2 \otimes e_3 \pm e_3 \otimes e_3$ 
(viii) $e_2 \otimes e_3 \pm e_3 \otimes e_2$ 
(ix) $e_2 \otimes e_3 \pm e_3 \otimes e_3$

(x) $e_3 \otimes e_2 \pm e_2 \otimes e_3$ 
(xi) $e_1 \otimes e_2 - e_2 \otimes e_1$

Note that (i), (iv), (vii), (viii), (ix), (x) are Schmidt rank 1 vectors, thus it remains to consider

1. $e_1 \otimes e_3 \pm e_3 \otimes e_1$,
2. $e_1 \otimes e_3 \pm e_3 \otimes e_2$,
3. $e_2 \otimes e_3 \pm e_3 \otimes e_1$,
4. $e_2 \otimes e_3 \pm e_3 \otimes e_2$,
5. $e_1 \otimes e_2 - e_2 \otimes e_1$. 

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Note that it suffices to consider only ‘+’ case, as we can get minus by performing local unitary transformation $e_3 \rightarrow -e_3$ on the first Hilbert space component and leave everything else unchanged.

Let us examine the first case. We will use once more the block positivity condition. Take $x = 1/\sqrt{2}(e_1 + e_3) = y$. Then one calculates $(x \otimes y, P_{x^*} x \otimes y) = \frac{1}{2}$ but $(x \otimes y, P_{x^*} x \otimes y) = 1/8$, thus this violates block positivity and the first case is excluded. By the analogous argument we also exclude the fourth case.

In the second case $x_3$ can be a linear combination of the remaining $e_2 \otimes e_3, e_1 \otimes e_3, e_3 \otimes e_2, e_1 \otimes e_2$ and $1/\sqrt{2}(e_1 \otimes e_2 - e_2 \otimes e_1)$ (as it must be orthogonal to $x_1$ and $x_2$). When we consider $x = 1/\sqrt{2}(e_1 + e_3), y = 1/\sqrt{2}(e_2 + e_3)$ we get $(x \otimes y, P_{x^*} x \otimes y) = \frac{1}{2}$, what excludes $e_3 \otimes e_2$ from the list (as in that case $(x \otimes y, P_{x^*} x \otimes y) > 0$). Now consider $\text{Tr}(\mathbb{1} \otimes P_{x_2})(P_{x_1} + P_{x_2}) = 1$. From Lemma 21 it follows that $\alpha$-normalization demands that $\text{Tr}(\mathbb{1} \otimes P_{x_2})P_{x_3} = 0$ which excludes $1/\sqrt{2}(e_1 \otimes e_2 - e_2 \otimes e_1)$ from $x_3$. Thus, $x_3 = 1/\sqrt{3}(e_2 \otimes e_3 \pm e_3 \otimes e_1)$. In fact there must be a ‘−’ sign, as for $x = 1/\sqrt{3}(e_1 + e_2 + e_3)$ plus sign gives $(x \otimes x, x \otimes x) = 2/3$. In the third case $x_2$ and $x_3$ are swapped.

Finally in the last case we have that $\text{Tr}(\mathbb{1} \otimes P_{x_3})(P_{x_1} + P_{x_3}) = 1$ and $\text{Tr}(\mathbb{1} \otimes P_{x_3})(P_{x_1} + P_{x_3}) = 1$, thus $\text{Tr}(\mathbb{1} \otimes P_{x_2})P_{x_3}$ and $\text{Tr}(\mathbb{1} \otimes P_{x_3})P_{x_2}$ must equal zero (again we use $\alpha$-normalization and Lemma 21). This cannot be true if $x_3$ has Schmidt rank 2, so we arrive to contradiction.

Remark. Notice that in the Proposition above we indeed put restriction only on one vector, namely $x_2$. Form of $x_1$ only specifies the basis.

Lemma 21. Let $x = 1/\sqrt{2}(e_1 \otimes e_2 - e_2 \otimes e_1)$ and $y = 1/\sqrt{2}(g_1 \otimes e_3 + e_3 \otimes g_2)$, where $g_1, g_2 \in \text{span}\{e_1, e_2\}$ (all vectors are normalized). Then $z = c_1 x + c_2 y$ for any nonzero $c_1, c_2 \in \mathbb{C}$ have Schmidt rank equal to 3 unless $g_1 = \pm g_2$.

Proof. Firstly let us rewrite

$$
g_1 = \sin \alpha e_1 + e^{i \phi} \cos \alpha e_2,$$
$$
g_2 = \sin \beta e_1 + e^{i \psi} \cos \beta e_2,$$
$$
y = \frac{1}{\sqrt{2}}(g_1 \otimes e_3 + e^{i \eta} e_2 \otimes g_2),$$
$$
z = c(\cos \gamma x + e^{ix} \sin \gamma y).$$

This is exactly equivalent to the statement of the theorem, but now parameters $\alpha, \beta, \gamma, \phi, \psi, \chi, \eta$ are real, and only $c$ is complex. Now recall that the Schmidt rank of the vector $z$ is equal to the rank of the matrix formed by coefficients $z_{ij} = (e_i \otimes e_j, z)$. Thus if $z$ have Schmidt rank less than 3, then $\det(z_{ij}) = 0$. By the explicit calculation we have

$$
\det(z_{ij}) = -\frac{1}{2\sqrt{2}} e^2 \sin^2 \gamma \cos \gamma e^{i(\eta + 2\chi)} (e^{i \phi} \sin \alpha \cos \beta - e^{i \phi} \cos \alpha \sin \beta)
$$

This is equal to zero only when $(e^{i \phi} \sin \alpha \cos \beta - e^{i \phi} \cos \alpha \sin \beta) = 0$, i.e. either $\sin(\alpha - \beta) = 0$ and $\phi - \psi = 0$ or $\sin(\alpha + \beta) = 0$ and $\phi - \psi = \pi$. In the first case $g_1 = g_2$ and in the second $g_1 = -g_2$. 

\[\square\]
Lemma 22. Let $\xi_1, \xi_2, \xi_3$ are three orthonormal vectors in $\mathcal{H} \otimes \mathcal{H}$ with Schmidt rank equal 2. Let us put $\xi_1 = 1/\sqrt{2}(e_1 \otimes e_1 + e_2 \otimes e_2)$. If one of remaining vectors is of the form

$$c_1(e_1 \otimes e_2 + e_2 \otimes e_1) + c_2 e_1 \otimes e_3 + c_3 e_2 \otimes e_3 + c_4 e_3 \otimes e_2 + c_5 e_3 \otimes e_1,$$

where $c_i \in \mathbb{C}$, then the symmetry $s = 1 - 2g$, where $g = \sum_i P_{\xi_i}$ is not in $\mathcal{D}$ unless $c_5 = 0$.

Proof. Without loss of generality assume that $\xi_2$ is of the form above. Then it can be written in the same form as $z$ in the proof of the Lemma 21 precisely

$$x = 1/\sqrt{2}(e_1 \otimes e_2 - e_2 \otimes e_1),$$

$$g_1 = \sin \alpha e_1 + e^{i\phi} \cos \alpha e_2,$$

$$g_2 = \sin \beta e_1 + e^{i\psi} \cos \beta e_2,$$

$$\gamma = 1/\sqrt{2}(g_1 \otimes e_3 + e^{i\eta} e_3 \otimes g_2),$$

$$\xi_2 = \cos \gamma x + e^{i\chi} \sin \gamma y.$$

But then we easily see that $\text{Tr}(\mathbb{I} \otimes P_{\xi_2})P_{\xi_2} = 1/2 \sin^2 \gamma$. As $\text{Tr}(\mathbb{I} \otimes P_{\xi_2})P_{\xi_2} = 0$, by the $\alpha$-normalization and Lemma 14 we need $\text{Tr}(\mathbb{I} \otimes P_{\xi_2})P_{\xi_2} = 1 - 1/2 \sin^2 \gamma$. But $1 - 1/2 \sin^2 \gamma > 1/2$ for $\gamma \neq \pi/2$ or $3/2\pi$. Then, by the Lemma 15 one of the Schmidt coefficients of $\xi_3$ would have to be greater than $1/\sqrt{3}$, so the thesis is proved (see Corollary 15). On the other hand if $\gamma = \pi/2$ or $\gamma = 3/2\pi$ then, turning back to notation from the statement of the lemma, we get $c_1 = 0$.

Lemma 23. Let $\xi_1, \xi_2, \xi_3$ are three orthonormal vectors in $\mathcal{H} \otimes \mathcal{H}$ with Schmidt rank equal 2. Let us put $\xi_1 = 1/\sqrt{2}(e_1 \otimes e_1 + e_2 \otimes e_2)$. If one of remaining vectors is of the form

$$c_1 e_1 \otimes e_3 + c_2 e_2 \otimes e_3 + c_3 e_3 \otimes e_2 + c_4 e_3 \otimes e_1 + c_5 e_3 \otimes e_3,$$

where $c_i \in \mathbb{C}$, then the symmetry $s = 1 - 2g$, where $g = \sum_i P_{\xi_i}$ is not in $\mathcal{D}$ unless $c_5 = 0$.

Proof. Without loss of generality let us assume that the $\xi_2$ is of the form above. The $\alpha$-normalization demands that $\text{Tr}(\mathbb{I} \otimes P_{\xi_2})q = 1$ but $\text{Tr}(\mathbb{I} \otimes P_{\xi_2})P_{\xi_2} = 0$, thus we infer that $\text{Tr}(\mathbb{I} \otimes P_{\xi_2})P_{\xi_2} = 1/2 = \text{Tr}(\mathbb{I} \otimes P_{\xi_2})P_{\xi_2}$ (note that the trace cannot be greater than 1/2 as the maximal Schmidt coefficient is equal to $1/\sqrt{3}$, cf. Lemma 15). Then

$$\text{Tr}(\mathbb{I} \otimes P_{\xi_2})P_{\xi_2} = |c_1|^2 + |c_2|^2 + |c_3|^2 = 1/2.$$

So $|c_3|^2 + |c_4|^2 = 1/2$ due to normalization. Now we are going to show that $c_5$ must equal to zero. Consider the family of vectors of the form:

$$u_\phi = c_4 e_1 + c_4 e_2 + e^{i\phi}/\sqrt{2} e_3.$$

Now we directly calculate

$$\text{Tr}(\mathbb{I} \otimes P_{u_\phi})P_{\xi_2} = \frac{1}{2} + \frac{1}{\sqrt{2}}(c_4^2 e^{i\phi} + c_5 e^{-i\phi}).$$

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As Tr(\(I \otimes P_{\xi_2}\))\(\xi_2\) must be less or equal to 1/2, then

\[ c_2^2 e^{i\phi} + c_5 e^{-i\phi} \leq 0. \]

If we take \(\phi = 0\), we get that \(\Re c_5 \leq 0\). For \(\phi = \pi\) we get \(\Re c_5 \geq 0\). \(\phi = \pi/2\) implies \(3c_5 \geq 0\) and \(\phi = 3/2\pi\) gives \(3c_5 \leq 0\). Thus \(c_5 = 0\).

**Lemma 24.** Let \(\xi_1, \xi_2, \xi_3\) are three orthonormal vectors in \(\mathcal{H} \otimes \mathcal{H}\) with Schmidt rank equal 2. Let us put \(\xi_1 = 1/\sqrt{2}(e_1 \otimes e_1 + e_2 \otimes e_2)\). If one of remaining vectors is of the form

\[ c_1 \frac{1}{\sqrt{2}}(e_1 \otimes e_2 - e_2 \otimes e_1) + c_2 e_1 \otimes e_3 + c_3 e_2 \otimes e_3 + c_4 e_3 \otimes e_2 + c_5 e_3 \otimes e_1 + c_6 e_3 \otimes e_3, \]

then the symmetry \(s = I - 2q\), where \(q = \sum P_{\xi}\), is not in \(\mathcal{D}\) if both \(c_1\) and \(c_6\) are not equal to 0.

**Proof.** We will prove the statement by the contradiction, thus assume that \(c_1 \neq 0\), \(c_6 \neq 0\) and \(s\) is in \(\mathcal{D}\). Firstly, let us assume that \(\xi_2\) is of the claimed form, and we get rid off irrelevant overall phase factor assuming that \(c_6\) real. We know from Lemma [x] that \(\xi_2\) must be Schmidt rank 2 with equal Schmidt coefficients. Then, it is well known that the coefficient matrix \((a_{ij})\), where \(a_{ij} := (e_i \otimes e_j, \xi_2)\) must have zero determinant (otherwise it would be full rank and this would mean that \(\xi_2\) must by Schmidt rank 3). By the explicit calculation one finds that

\[ \det(a_{ij}) = \frac{1}{2} c_1 \left(c_6 c_1 + \sqrt{2}(c_3 c_5 - c_2 c_4)\right). \]

Let us denote by \(\delta = (c_3 c_5 - c_2 c_4)\). As we assumed that \(c_1 \neq 0\), this means that

\[ c_1 c_6 + \sqrt{2} \delta = 0. \]

We can multiply it by \(\bar{c}_1\) to get \(|c_1|^2 c_6 + \sqrt{2} \delta \bar{c}_1 = 0\). Now adding this equation and its conjugate together we can express the necessary condition for \(\xi_2\) to be Schmidt rank 2 as (we remind that \(c_6\) is chosen to be real)

\[ \sqrt{2}(\delta \bar{c}_1 + \bar{c}_1) = -2|c_1|^2 c_6. \] (10)

Now note that as we demand that \(\xi_2\) is Schmidt rank 2 with equal Schmidt coefficients we can assume that \(\xi_2 = 1/\sqrt{2}(f_1 \otimes g_1 + f_2 \otimes g_2)\) for appropriate vectors \(f_i\) and \(g_i\). Now take the projector \(P_{\xi_2}\) onto the vector \(\xi_2\) and calculate partial trace \(\omega = \text{Tr}_2 P_{\xi_2}\) with respect to the second Hilbert space. Partial trace does not depend on basis and we see that eigenvalues of \(\omega\) are equal to squares of Schmidt coefficients of \(\xi_2\), thus must be equal to 1/2. On the other hand we know that the eigenvalues of \(\omega\) are roots of characteristic polynomial, which in case of \(3 \times 3\) matrix can be written in the form

\[ \det(\lambda I - \omega) = \lambda^3 + a\lambda^2 + b\lambda + d = 0. \]

The \(d\) is simply equal to \(\det(\omega)\) and must equal to zero, otherwise \(\xi_2\) would be Schmidt rank 3 vector. Thus

\[ \lambda(\lambda^2 + a\lambda + b) = 0. \]

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Let us for while forget about the assumptions that two non-zero roots must be equal. As always here the non-zero solutions $\lambda_1$ and $\lambda_2$ are the squares of Schmidt coefficients, which are positive and their squares sum up to 1 (due to normalization), we can assume that

$$\lambda_1 = \sin^2 \theta, \quad \lambda_2 = \cos^2 \theta, \quad 0 < \theta < \frac{\pi}{2}.$$ 

Then we immediately see that $\lambda_1 \lambda_2 \leq 1/4$ and is equal 1/4 if and only if $\sin \theta = 1/\sqrt{2} = \cos \theta$, thus in case of equal Schmidt coefficients. We then use Vieta's formula to express necessary condition for a $\lambda_1$ and $\lambda_2$ to be equal

$$\lambda_1 \lambda_2 = b = \frac{1}{4}$$

By the explicit calculation one find that $b$ can be expressed as

$$b = \frac{1}{4} \left( 2\sqrt{2}c_5 \left( (c_3 c_5 - c_2 c_4)\bar{c}_1 + c_1 (\bar{c}_3 c_5 - \bar{c}_2 c_4) \right) + 4 \left( |c_2|^2 + |c_3|^2 \right) \left( |c_4|^2 + |c_5|^2 \right) + 2|c_1|^2 \left( 2|c_2|^2 + 2|c_3|^2 + 2|c_4|^2 + 2|c_5|^2 + |c_1|^4 \right) \right).$$

To simplify this expression we will use the fact that $\alpha$-normalization of $s$ demands that $\text{Tr}(I \otimes P_\xi) P_\xi = 1/2$ (cf. proof of Lemma 23). By explicit calculation this means that

$$|c_2|^2 + |c_3|^2 + c_5^2 = \frac{1}{2},$$

and this combined with normalization of vector $\xi_2$ yields

$$|c_1|^2 + |c_4|^2 + |c_5|^2 = \frac{1}{2}.$$ 

We will use these equalities to eliminate $|c_2|^2, |c_3|^2, |c_4|^2$ and $|c_5|^2$ from the $b$. We will also substitute $\delta$ where it applies. We get

$$b = \frac{1}{4} \left( 2\sqrt{2}c_5 (\delta \bar{c}_1 + \bar{c}_1) + 4 \left( \frac{1}{2} - c_2^2 \right) \left( \frac{1}{2} - |c_1|^2 \right) + 2|c_1|^2 (c_6^2 - |c_1|^2 + 1) + |c_1|^4 \right).$$

Now we substitute eq. (10) and simplify expression to get

$$b = 1/4 \left( 2|c_1|^2 c_6^2 - 2c_6^2 - |c_1|^4 + 1 \right) = 1/4.$$ 

This is satisfied when

$$2|c_1|^2 c_6^2 - 2c_6^2 - |c_1|^4 = 0$$

To simplify notation denote $|c_1|^2 = \alpha$ and $c_6^2 = \beta$. Now one can immediately see that the equation

$$2\alpha \beta - 2\beta - 2\alpha^2 = 0$$

does not have solutions for $0 < \alpha, \beta < 1$. Thus we arrived to the contradiction. □

**Corollary 25.** If a symmetry $s = 1 - 2q$, where $q = \sum_i P_{x_i}$ is in $\mathcal{D}$ then

- $x_1 = \frac{1}{\sqrt{2}} (e_1 \otimes e_1 + e_2 \otimes e_2),$
- $x_2 = \frac{1}{\sqrt{2}} (g_1 \otimes e_3 + e_3 \otimes h_2),$
- $x_3 = \frac{1}{\sqrt{2}} (k_1 \otimes e_3 + e_3 \otimes l_2),$
Proof. We know that \( x_2 \) and \( x_3 \) must be a linear combination of the form
\[
c_1 \frac{1}{\sqrt{2}} (e_1 \otimes e_2 - e_2 \otimes e_1) + c_2 e_1 \otimes e_3 + e_3 \otimes e_2 + c_3 e_3 \otimes e_2 + c_4 e_3 \otimes e_1 + c_5 e_1 \otimes e_3 + e_3 \otimes e_3 \otimes e_3,
\]

but Lemma 23 and 22 imply together that \( c_1 = 0 \) and \( c_6 = 0 \). Then we get the desired form.

Lemma 26. Let \( s = \mathbb{I} - 2q \in \mathcal{D} \) be the symmetry where \( q = \sum_i P_{x_i} \),
\[
x_1 = \frac{1}{\sqrt{2}} (e_1 \otimes e_1 + e_2 \otimes e_2),
\]
\[
x_2 = \frac{1}{\sqrt{2}} (g_1 \otimes e_3 + e_3 \otimes h_2),
\]
\[
x_3 = \frac{1}{\sqrt{2}} (k_1 \otimes e_3 + e_3 \otimes l_2),
\]
then \( h_2 \perp l_2 \) and \( g_1 \perp k_1 \).

Proof. Let us calculate \( \text{Tr}(\mathbb{I} \otimes P_{x_2})P_{x_3} \). For \( P_{x_i} \), we get \( 1/2 \), as \( h_2 \) belongs to the span of \( e_1 \) and \( e_2 \) (it is shown in the previous proof). Obviously for \( P_{x_2} \) this also equals \( 1/2 \), so for \( P_{x_1} \) it must equal 0. We thus calculate \( \text{Tr}(\mathbb{I} \otimes P_{x_3})P_{x_3} \) (once more we use the fact, that non-diagonal terms in the first tensor product factor will vanish)
\[
\text{Tr}(\mathbb{I} \otimes P_{x_3})P_{x_3} = \frac{1}{2} \left((h_2|e_3) (e_3|h_2) + (h_2|l_2) (l_2|h_2)\right) = \frac{1}{2} (h_2, l_2)^2
\]
so the first claim follows. Then using the fact that \( (x_2, x_3) = 0 \), we get
\[
(x_2, x_3) = \frac{1}{2} (g_1 \otimes e_3 + e_3 \otimes h_2, k_1 \otimes e_3 + e_3 \otimes l_2) = \frac{1}{2} ((g_1, k_1) + (h_2, l_2)) = \frac{1}{2} (g_1, k_1),
\]
and the second claim follows.

Theorem 27. For \( n = 2, 3 \) any symmetry in \( \mathcal{D} \) is locally unitarily equivalent to Choi matrix corresponding to the transposition map.

Proof. For \( n = 2 \) the result is already known (see [3]). For \( n = 3 \), take a symmetry \( s \in \mathcal{D} \). Denote \( s = \mathbb{I} - 2q \) where \( q = \sum_i P_{x_i} \). Then from the Corollary 25 we know that
\[
y_1 = \frac{1}{\sqrt{2}} (e_1 \otimes e_1 + e_2 \otimes e_2),
\]
\[
y_2 = \frac{1}{\sqrt{2}} (g_1 \otimes e_3 + e_3 \otimes h_2),
\]
\[
y_3 = \frac{1}{\sqrt{2}} (k_1 \otimes e_3 + e_3 \otimes l_2).
\]
According to the Lemma 23 \( h_2 \perp l_2 \) and \( g_1 \perp k_1 \). Moreover we know that \( g_1 \perp e_3 \), \( k_1 \perp e_3 \), \( h_2 \perp e_3 \) and \( l_2 \perp e_3 \). Thus \( \{g_1, k_1, e_3\} \) and \( \{h_2, l_2, e_3\} \) are two sets of mutually orthogonal vectors that we can consider as a bases in corresponding Hilbert spaces. This allows us to define two unitary operators:
\[
U g_1 = e_1, \quad \quad U k_1 = -e_3, \quad \quad U e_3 = e_2,
\]
\[
V h_2 = e_2, \quad \quad V l_2 = e_3, \quad \quad V e_3 = e_1.
\]
Then

\[ U \otimes V y_1 = \frac{1}{\sqrt{2}} (U e_1 \otimes V e_1 + U e_2 \otimes V e_2), \]
\[ U \otimes V y_2 = \frac{1}{\sqrt{2}} (e_1 \otimes e_1 + e_2 \otimes e_2), \]
\[ U \otimes V y_3 = \frac{1}{\sqrt{2}} (-e_3 \otimes e_1 + e_2 \otimes e_3). \]

These three vectors satisfy assumptions of the Proposition [20] so \( s \) is locally unitarily equivalent to \( s_0 \). But \( s_0 \) is locally unitarily equivalent to the Choi matrix of transposition map and the claim follows.

Remark. Consider case \( n = 3 \). It is clear that any antisomorphism is represented by a symmetry. Above theorem establishes the converse: any symmetry corresponds to a Choi matrix of the form \( 3P_x \), for some maximally entangled vector \( x \).

6.4 Symmetries as exposed points of \( \mathcal{D} \)

Our goal is to show that the Choi matrix corresponding to transposition map in \( M_3(\mathbb{C}) \) is an exposed (so also an extreme) point of \( \mathcal{D} \). We start with a lemma.

**Lemma 28.** Let \( w = \sum_{i,j=1}^{n} E_{ij} \otimes E_{ji} \) and \( \sigma \in \mathcal{D} \) such that \( \text{Tr} w \sigma = n^2 \). Then

(i) \( (e_j, \sigma_{ij} e_i) = 1 \),

(ii) \( \sum_i \sigma_{ii} = 1 \),

(iii) \( \sigma_{ii} \geq 0 \), and \( (e_i, \sigma_{jj} e_j) = 0 \) for \( i \neq j \),

(iv) \( (e_i, \sigma_{ij} e_j) = 0 \) for \( i \neq j \),

where we adopted notation \( \sigma = \sum_{ij} E_{ij} \otimes \sigma_{ij} \).

**Proof.** For (i) we firstly note that

\[ \text{Tr} w \sigma = \sum_{i,j=1}^{n} (e_i \otimes e_j, \sigma e_j \otimes e_i), \]

but on the other hand due to \( a(\sigma) = 1 \), i.e.

\[ \sup \{ |\text{Tr} \sigma a| \mid a \in M_3(\mathbb{C}), \pi(a) = 1 \} = 1, \]

one has

\[ |\text{Tr} \sigma E_{ji} \otimes E_{ij}| = |(e_i \otimes e_j, \sigma e_j \otimes e_i)| \leq 1. \]

These and the assumption that \( \text{Tr} w \sigma = n^2 \) implies (i).

Property (ii) follows immediately:

\[ \sum_i \sigma_{ii} = \sum_i \phi(E_{ii}) = \phi(1) = 1, \]

where \( \phi \) is a positive unital normalized map corresponding to \( \sigma \).
To show (iii) we need to apply block-positivity condition $\sigma \succeq_{bp} 0$. In particular

$$0 \leq (e_m \otimes y, \sigma e_m \otimes y) = \sum_{ij}(e_m \otimes y, E_{ij} \otimes \sigma_{ij} e_m \otimes y) = (y, \sigma_{mm} y).$$

Now, due to (ii) $(e_k, \sum_m \sigma_{mm} e_k) = 1$, due to (i) $(e_k, \sigma_{kk} e_k) = 1$ and due to last inequality $(e_k, \sigma_{mm} e_k) \geq 0$. Thus we obtained desired result.

Finally to show (iv) we proceed as in the proof of Prop. 8. We take $x = e_i \pm \lambda e_j$, and $y = e_j$, with $i \neq j$ and $\epsilon > 0, \lambda \in \mathbb{R}$ (so the vectors are not necessarily normalized). Then block positivity gives us

$$0 \leq (x \otimes e_i, \sum_{kl} E_{kl} \otimes \sigma_{kl} x \otimes e_i)$$

$$= e^2_i (e_i, e_i) + \epsilon \lambda (e_i, e_j e_i) + e \lambda (e_i, e_j e_i) + \lambda^2 (e_i, e_j e_i)$$

Due to our assumptions and results already obtained this means that

$$\lambda (e_i, (\sigma_{ij} + \sigma_{ji} e_i)) \geq -\epsilon.$$

Repeating this for $x = e e_i - \lambda e_j, x = e e_i + i \lambda e_j, x = e e_i - i \lambda e_j$, we conclude that $(e_i, \sigma_{ij} e_i) = 0$ for $i \neq j$.

**Theorem 29.** The Choi matrix $w$

$$w = \sum_{ij} E_{ij} \otimes E_{ji} \quad (11)$$

corresponding to transposition map in $M_n(\mathbb{C})$ is an exposed point of $\mathcal{D}$.

**Proof.** We will show that the value of functional $\omega(\sigma) = \text{Tr} w \sigma$ is strictly less than $n^2$ for $\sigma \in \mathcal{D}$ unless $\sigma = w$.

Because $\text{Tr} w \sigma = \sum_{i,j=1}^n (e_i \otimes e_j, \sigma e_i \otimes e_j)$ and due to $\alpha$-normalization of $\sigma$ we have that $\text{Tr} w \sigma \leq n^2$. It is clear that $\text{Tr} w w = n^2$. Let us take arbitrary $\sigma \in \mathcal{D}$ such that $\text{Tr} w \sigma = n^2$. From the previous lemma we know that $\sigma_{ii} \geq 0$ and

$$(e_1, \sigma_{11} e_1) = 1, \quad (e_2, \sigma_{11} e_2) = 0, \quad (e_3, \sigma_{11} e_3) = 0,$$

from which we infer that $e_2, e_3 \in \ker \sigma_{11}$, so $\sigma_{11} = |e_1 \rangle \langle e_1|$. Analogously we show that $\sigma_{22} = |e_2 \rangle \langle e_2|$ and $\sigma_{33} = |e_3 \rangle \langle e_3|$.

Now let us consider $\sigma_{12}$. From the Lemma 28 we immediately get that

$$(e_2, \sigma_{12} e_1) = 1 \quad (12)$$

and

$$(e_1, \sigma_{12} e_1) = 0. \quad (13)$$

Due to the fact that $\sigma$ is hermitian, $(e_2, \sigma_{12} e_2) = (\sigma_{21} e_2, e_2) = (e_2, \sigma_{21} e_2) = 0$, so

$$(e_2, \sigma_{12} e_2) = 0.$$

Now we proceed as in the proof of Prop. 8. Precisely, take $x_\pm = e_1 \pm \lambda, e_2$, with $e > 0, \lambda \in \mathbb{R}$ and $y_\pm = e_i \pm e_3$. Then

$$0 \leq (x_+ \otimes y_+, \sigma x_+ \otimes y_+) + (x_- \otimes y_-, \sigma x_- \otimes y_-) = 2e^2 + 4e \lambda \Re (e_3, \sigma_{12} e_3)$$
and 
\[ 0 \leq (x_- \otimes y_+, \sigma x_- \otimes y_+) + (x_- \otimes y_-, \sigma x_- \otimes y_-) = 2e^2 - 4e \Re(e_3, \sigma_{12} e_3), \]

so \(-e \leq 2\Re(e_3, \sigma_{12} e_3) \leq e\). Due to arbitrariness of \(\lambda\), \(\Re(e_3, \sigma_{12} e_3) = 0\). Analogous calculations for \(u_\pm = e_1 \pm i e_3\) instead of \(x_\pm\) yield that \(\Im(e_3, \sigma_{12} e_3) = 0\), so

\[ (e_3, \sigma_{12} e_3) = 0. \]

Using these results we see that

\[
0 \leq (x_+ \otimes y_+, \sigma x_+ \otimes y_+) = e^2 + 2e \Re((e_1, \sigma_{12} e_3) + (e_3, \sigma_{12} e_1))
\]
\[
0 \leq (x_+ \otimes y_-, \sigma x_+ \otimes y_-) = e^2 - 2e \Re((e_1, \sigma_{12} e_3) + (e_3, \sigma_{12} e_1))
\]
\[
0 \leq (u_+ \otimes y_+, \sigma u_+ \otimes y_+) = e^2 - 2e \Im((e_1, \sigma_{12} e_3) + (e_3, \sigma_{12} e_1))
\]
\[
0 \leq (u_+ \otimes y_-, \sigma u_+ \otimes y_-) = e^2 + 2e \Im((e_1, \sigma_{12} e_3) + (e_3, \sigma_{12} e_1))
\]

so \((e_1, \sigma_{12} e_3) + (e_3, \sigma_{12} e_1) = 0\). Analogous results for \(v_\pm = e_1 \pm i e_3\) yield that \((e_1, \sigma_{12} e_3) - (e_3, \sigma_{12} e_1) = 0\), so

\[ (e_1, \sigma_{12} e_3) = 0, \quad (e_3, \sigma_{12} e_1) = 0. \]

Repeating the same arguments for \(y_\pm = e_2 \pm e_3\), \(v_\pm = e_2 \pm i e_3\) we get that

\[ (e_2, \sigma_{12} e_3) = 0, \quad (e_3, \sigma_{12} e_2) = 0. \]

It remains to show that \((e_1, \sigma_{12} e_2) = 0\). Firstly we take \(e = 1, \lambda = 1, y_\pm = e_1 \pm e_2\) and \(v_\pm = e_1 \pm i e_2\) and see that

\[
0 \leq (u_+ \otimes v_+, \sigma u_+ \otimes v_+) = 2\Re(e_1, \sigma_{12} e_2),
\]
\[
0 \leq (x_+ \otimes v_-, \sigma x_+ \otimes v_-) = -2\Re(e_1, \sigma_{12} e_2),
\]

so \(\Re(e_1, \sigma_{12} e_2) = 0\). Now for \(z_\pm = ee_1 \pm (1 \pm i)e_2\) we calculate (using previous results) that

\[
0 \leq (z_+ \otimes v_+, \sigma z_+ \otimes v_+) = 1 - 2ie(e_1, \sigma_{12} e_2),
\]
\[
0 \leq (z_- \otimes v_-, \sigma z_- \otimes v_-) = 1 + 2ie(e_1, \sigma_{12} e_2),
\]

so that for every \(e > 0\)

\[
\frac{1}{2e} \leq \Im(e_1, \sigma_{12} e_2) \leq \frac{1}{2e}
\]

We conclude that \(\Im(e_1, \sigma_{12} e_2) = 0\). Gathering all those results together we see that

\[ \sigma_{12} = |e_2\rangle \langle e_1| . \]

Using the same methods we show that

\[ \sigma_{13} = |e_3\rangle \langle e_1|, \quad \sigma_{23} = |e_3\rangle \langle e_2|. \]

Thus if for any \(\sigma \in \mathcal{D}\), \(\text{Tr}\sigma = n^2\), then \(\sigma = w\), otherwise \(\text{Tr}\sigma < n^2\), so \(w\) is an exposed point of \(\mathcal{D}\).
Combining this result with previous section we see that.

**Corollary 30.** Any symmetry \( s \in \mathcal{D} \) is an exposed point of \( \mathcal{D} \). Also any Choi matrix of the form \( 3P_v \), where \( x \) maximally entangled vector, is an exposed point of \( \mathcal{D} \).

**Remark.** This corollary immediately follows from results in [20] and repeats the result already given in [21] (which was obtained via convex analysis). Also the criterion given in [22] shows that transposition map is an exposed map. Moreover the proof of mentioned criterion allows us to construct other functionals 'supporting' exposedness of \( w \), so such functionals are far from being unique. Despite those two overlaps we decided to presented the longer proof to make it more consistent with Section [4] and emphasizes some similarities between \( n = 2 \) and \( n = 3 \) cases.

### 6.5 Partial symmetries

It is easy to see that for \( n = 2 \) there can be no partial symmetries belonging to \( \mathcal{D} \). For \( n = 3 \) the situation is different. The unitality condition \( \text{Tr} \rho = 3 \) and decomposition \( \rho = p - q \) imply that \( v = p + q \) must be of rank 5 or 7. Moreover, it is known that for \( n = 4 \) maps corresponding to partial symmetries can be exposed and indecomposable, see [22] and [23]. This advocates the importance of examination of partial symmetries in \( n = 3 \) case.

The easiest example of block positive symmetry can be obtained by perturbation of swapping operator in \( n = 2 \) embedded in \( n = 3 \).

**Example 31.** Let

\[
w = \sum_{i,j=1}^{2} E_{ij} \otimes E_{ji}, \quad \text{and} \quad x = \frac{1}{\sqrt{2}} (e_1 + e_2) \otimes e_3
\]

then

\[
s_0 = w + P_x
\]

is an e-symmetry. The rank of \( s_0 \) is equal to 5. This map is coCP as partial transpose of \( s_0 \) is a positive matrix.

One observe that that the image of map corresponding to \( s_0 \) is 4 dimensional subspace of \( M_3(\mathbb{C}) \). Thus in fact it is a map of the form \( M_3(\mathbb{C}) \to M_2(\mathbb{C}) \to M_3(\mathbb{C}) \).

It is known that any map \( M_3(\mathbb{C}) \to M_2(\mathbb{C}) \) is decomposable. It is natural to ask if there are other e-symmetries such that corresponding maps are not of this form. Affirmative answer is given by the following examples.

**Example 32.** Let \( w \) be as in previous example and \( x = e_3 \otimes e_3 \). Let us put

\[
s = w + P_x
\]

Then \( s^2 \) is a partial symmetry with \( s^2 \) of rank 5. It is block positive because partial transpose of \( s \) is positive. Thus the above map is coCP. The image of this map is a 5 dimensional subspace of \( M_3(\mathbb{C}) \).

Despite extensive study we did not find any example of partial symmetry \( s \) in \( \mathcal{D} \) for \( n = 3 \) with rank of \( s^2 \) equal to 7 nor we didn't found any partial symmetry corresponding to a non-decomposable map. This led us to following conjecture.

**Conjecture.** For \( n = 3 \), if \( s \in \mathcal{D} \) is a partial symmetry then (i) rank of \( s^2 \) is equal to 5, (ii) \( s \) corresponds to decomposable positive map.
7 Final remarks

Up to now we have studied block positive symmetries as well as Choi matrices of the form $nP_x$, where $x$ is maximally entangled vector. To complete the picture let us focus for a while on Choi matrices of the form $p \otimes \mathbb{1}$.

**Proposition 33.** Choi matrices of the form $p \otimes \mathbb{1}$, where $p$ is rank 1 projector, are extreme points of $\mathcal{D}$ for any $n$.

**Proof.** Suppose that $p \otimes \mathbb{1} = \lambda \sigma_1 + (1 - \lambda) \sigma_2$ and $p = |f \rangle \langle f |$. Then for any vector $g$ we have

$$ (f \otimes g, p \otimes \mathbb{1} f \otimes g) = 1 = \lambda (f \otimes g, \sigma_1 f \otimes g) + (1 - \lambda) (f \otimes g, \sigma_2 f \otimes g). \quad (14) $$

Due to $\alpha$-normalization of $\sigma_i$ we have $\text{Tr}(\mathbb{1} \otimes P_g) \sigma_i = 1$. So

$$ \text{Tr} P_f \otimes P_g \sigma_i + \text{Tr}(\mathbb{1} - P_f) \otimes P_g \sigma_i = 1 $$

Due to block positivity of $\sigma_i$ both terms must be greater than 0, so

$$ (f \otimes g, \sigma_i f \otimes g) \leq 1, $$

but due to (14) we need to have equality. Consequently for any $f'$ orthogonal to $f$ and any $g$ we have that $(f' \otimes g, \sigma_i f' \otimes g) = 0$, so both $\sigma_i$ must equal $p \otimes \mathbb{1}$, so $p \otimes \mathbb{1}$ is extremal.

Consequently we conclude that the set

$$ \tilde{\mathcal{D}} = \{\text{symmetries}, nP_x, p \otimes \mathbb{1}\} $$

naturally arise as a subset of extremal Choi matrices. In fact we have shown that symmetries, thus also Choi matrices of the form $nP_x$ are exposed points of $\mathcal{D}$ for $n = 2, 3$. We saw that the simple set $\tilde{\mathcal{D}}$ is enough to describe all regular extreme points of $\mathcal{D}$ for $n = 2$. We also indicated how much deficient $\tilde{\mathcal{D}}$ is for $n = 3$ due to appearance of

1. partial symmetries (although their independence of $\tilde{\mathcal{D}}$ for $n = 3$ does not seem to be trivial and need further investigation),

2. non-decomposable maps, with Choi map as a standard example,

3. various concepts of extremality even when restricted to diagonal subalgebra.

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