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FACIAL STRUCTURES FOR SEPARABLE STATES

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ABSTRACT. The convex cone \mathbb{V}_1 generated by separable states is contained in the cone \mathbb{T} of all positive semi-definite block matrices whose block transposes are also positive semi-definite. We characterize faces of the cone \mathbb{V}_1 induced by faces of the cone \mathbb{T} which are determined by pairs of subspaces of matrices.

1. Introduction

Let M_n denote the C^* -algebra of all $n \times n$ matrices of complex entries, and M_n^+ the cone of all positive semi-definite matrices in M_n . Then the positive cone $(M_n \otimes M_m)^+$ of the tensor product $M_n \otimes M_m$ of two C^* -algebras M_n and M_m is strictly larger than the tensor product $M_n^+ \otimes M_m^+$ of two positive cones M_n^+ and M_m^+ , that is, we have

$$M_n^+ \otimes M_m^+ \subsetneq (M_n \otimes M_m)^+,$$

even in the simplest case of $m = n = 2$.

This is the starting point of the notion of entanglement, which is one of the key research area of quantum physics during the last two decades in connection with quantum information theory and quantum communication theory. Note that the tensor product of two positive cones coincides with the positive cone of the tensor product of the two commutative C^* -algebras, that is, we have

$$\mathcal{A}^+ \otimes \mathcal{B}^+ = (\mathcal{A} \otimes \mathcal{B})^+$$

for commutative C^* -algebras \mathcal{A} and \mathcal{B} . This is why entanglement arising in quantum mechanics has no counterpart in classical mechanics.

A positive semi-definite block matrix in $(M_n \otimes M_m)^+$ is said to be *separable* if it belongs to $M_n^+ \otimes M_m^+$, and it is said to be *entangled* if it belongs to

$$(M_n \otimes M_m)^+ \setminus M_n^+ \otimes M_m^+.$$

Following the notations in [13], we denote by \mathbb{V}_1 the cone of all separable positive semi-definite block matrices, which is nothing but $M_n^+ \otimes M_m^+$. Recall

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that a matrix itself represents a linear functional on the matrix algebra via the Hadamard product, and so an element in $M_n^+ \otimes M_m^+$ represents a *separable state* on the matrix algebra if it is normalized.

It is very difficult to determine if a given positive semi-definite block matrix is separable or entangled, and it had been one of the main research topics in quantum physics to find useful criteria to distinguish separable ones from entanglement. One of the early criterion for separability was given by Choi [11] in mathematics side and Peres [26] in physics side, which says that a positive semi-definite block matrix A is separable then the block transpose, or the partial transpose A^τ of A is also positive semi-definite. There are many other criteria even though it is now known [14] that it is *NP* hard in general to determine if a given one is separable or entangled. See Chapter 15 in [5] for various separability criteria.

We denote by \mathbb{T} the convex cone of all positive semi-definite block matrices in $(M_n \otimes M_m)^+$ whose partial transposes are also positive semi-definite. The above mentioned criterion, called PPT criterion by quantum physicists, tells us the relation

$$\mathbb{V}_1 \subset \mathbb{T}$$

holds in general. Woronowicz [31] showed that $\mathbb{V}_1 = \mathbb{T}$ if and only if $(m, n) = (2, 2), (2, 3)$ or $(3, 2)$, and gave an explicit example in $\mathbb{T} \setminus \mathbb{V}_1$ in the case of $(m, n) = (2, 4)$. This kind of example is called a *positive partial transpose entangled state* (PPTES) when it is normalized. An example of a PPTES in $(m, n) = (3, 3)$ was firstly given by Choi [11]. Much efforts have been given since nineties to find various types of PPTES's. See [6], [7], [12], [15], [16] and [17], for example.

Finding an example of a PPTES is equivalent to find a non-decomposable positive linear map between matrix algebras, by the duality theory between entanglement and positive linear maps, as was seen in [31], [29] and [13]. In mathematics side, operator algebraists have been interested in the theory of positive linear maps since the fifties [27], [28]. Actually, the above mentioned examples of PPTES's in [31] and [29] are byproducts of the efforts to show that there exist non-decomposable positive linear maps. In these days, many mathematicians are interested in the entanglement theory itself. See [1], [2], [21] and [30], for example.

One of the standard method to understand a given convex set is to characterize the facial structures. In this vein, the second author with Ha [15] characterized the faces of the cone \mathbb{T} in terms of pairs of subspaces of the inner product space $M_{m \times n}$ of all $m \times n$ matrices. On the other hands, the facial structures for the cone \mathbb{V}_1 is not clear, even though its extremal rays are easy to find by the definition. Recently, faces of \mathbb{V}_1 whose interior points have the range spaces with low dimensions have been studied [1] in mathematics side.

Two convex cones \mathbb{T} and \mathbb{V}_1 share faces in various ways. For examples, if subspaces characterizing a face of \mathbb{T} is low dimensional, then this face of \mathbb{T}

itself becomes a face of \mathbb{V}_1 by [20]. On the other hands, some faces of \mathbb{T} are independent of the cone \mathbb{V}_1 . For example, if a face of \mathbb{T} has a so called edge PPTES as an interior point, then this face has no intersection with \mathbb{V}_1 except the zero. Therefore, it is natural to ask what kinds of faces of \mathbb{T} also give rise to faces of \mathbb{V}_1 , and that is the purpose of this paper to answer.

Let C_0 be a convex subset of a convex set C_1 . A face F_1 of the convex set C_1 gives rise to a face $C_0 \cap F_1$ of C_0 whenever it is nonempty. Note that two different faces of C_1 may give rise to the same face of C_0 , in general. We say that a face F_0 of C_0 is *induced* by a face F_1 of C_1 , or F_1 *induces* F_0 , if the following conditions

$$(1) \quad F_0 = C_0 \cap F_1, \quad \text{int } F_0 \subset \text{int } F_1$$

hold, where $\text{int } C$ denotes the relative interior of the convex set C with respect to the hyperplane spanned by C . Then every induced face of C_0 is induced by a unique face of C_1 , and every inducing face of C_1 induces a unique face of C_0 . It is easy to see that a face F_1 of C_1 induces a face of C_0 if and only if the condition

$$(2) \quad C_0 \cap \text{int } F_1 \neq \emptyset$$

holds. If this is the case, then the face F_1 of C_1 induces the face $C_0 \cap F_1$ of the smaller convex set C_0 .

Recall again that every face of \mathbb{T} corresponds to a pair of subspaces of $M_{m \times n}$, as mentioned above. In the next section, we characterize faces of \mathbb{T} which induce faces of \mathbb{V}_1 in terms of the corresponding pairs of subspaces. In Section 3, we concentrate on the $2 \otimes n$ case, and investigate the possible range of dimensions of pairs of subspaces of $M_{2 \times n}$ for which the corresponding faces of \mathbb{T} induce faces of \mathbb{V}_1 . In the Section 4, We characterize faces of \mathbb{V}_1 which are induced by faces of \mathbb{T} , and give an example of a face of \mathbb{V}_1 which is not induced by a face of \mathbb{T} in the $3 \otimes 3$ case in the final section.

Throughout this paper, every vector will be considered as a column vector. If $x \in \mathbb{C}^m$ and $y \in \mathbb{C}^n$, then x will be considered as an $m \times 1$ matrix, and y^* will be considered as a $1 \times n$ matrix, and so xy^* is an $m \times n$ rank one matrix whose range is generated by x and whose kernel is orthogonal to y . For natural numbers m and n , we denote by $m \vee n$ and $m \wedge n$ the maximum and minimum of m and n , respectively. Finally, $\{e_{i,j} : i = 1, \dots, m, j = 1, \dots, n\}$ denotes the usual matrix units in $M_{m \times n}$.

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2. Faces of PPT's inducing faces for separable states

To begin with, we review briefly the facial structures for the convex cone \mathbb{T} of all positive semi-definite block matrices whose block transposes are also positive semi-definite [15]. We identify a matrix $z \in M_{m \times n}$ and a vector $\tilde{z} \in \mathbb{C}^n \otimes \mathbb{C}^m$

as follows: For $z \in [z_{ik}] \in M_{m \times n}$, we define

$$z_i = \sum_{k=1}^n z_{ik} e_k \in \mathbb{C}^n, \quad i = 1, 2, \dots, m,$$

$$\tilde{z} = \sum_{i=1}^m z_i \otimes e_i \in \mathbb{C}^n \otimes \mathbb{C}^m.$$

Then $z \mapsto \tilde{z}$ defines an inner product isomorphism from $M_{m \times n}$ onto $\mathbb{C}^n \otimes \mathbb{C}^m$. We also define

$$\mathbb{V}_s = \text{conv} \{ \tilde{z} \tilde{z}^* \in M_n \otimes M_m : \text{rank } z \leq s \},$$

$$\mathbb{V}^s = \text{conv} \{ (\tilde{z} \tilde{z}^*)^\tau \in M_n \otimes M_m : \text{rank } z \leq s \}$$

for $s = 1, 2, \dots, m \wedge n$, where $\text{conv } X$ means the convex cone generated by X , and A^τ denotes the *block-transpose* of A , that is,

$$\left(\sum_{i,j=1}^m a_{ij} \otimes e_{ij} \right)^\tau = \sum_{i,j=1}^m a_{ji} \otimes e_{ij}.$$

It is clear that $\mathbb{V}_{m \wedge n}$ coincides with the cone of all positive semi-definite $mn \times mn$ matrices. We have the following chains

$$\mathbb{V}_1 \subset \mathbb{V}_2 \subset \dots \subset \mathbb{V}_{m \wedge n}, \quad \mathbb{V}^1 \subset \mathbb{V}^2 \subset \dots \subset \mathbb{V}^{m \wedge n}$$

of inclusions. The cone

$$\mathbb{T} = \mathbb{V}_{m \wedge n} \cap \mathbb{V}^{m \wedge n}$$

consists of all positive semi-definite matrices whose block transposes are also positive semi-definite, or positive semi-definite matrices with positive partial transposes in the language of quantum physics. If $z = xy^* \in M_{m \times n}$ is a rank one matrix, then $\tilde{z} = \bar{y} \otimes x$, and we have

$$\tilde{z} \tilde{z}^* = \bar{y} \bar{y}^* \otimes x x^*,$$

and so it follows that

$$\mathbb{V}_1 = M_n^+ \otimes M_m^+.$$

We also have

$$(3) \quad (\tilde{z} \tilde{z}^*)^\tau = (\bar{y} \bar{y}^*) \otimes (x x^*)^\dagger = \bar{y} \bar{y}^* \otimes \bar{x} \bar{x}^* = \tilde{w} \tilde{w}^*$$

with $w = \bar{x} \bar{y}^*$, and so we have $\mathbb{V}_1 = \mathbb{V}^1$.

For subspaces D and E of $M_{m \times n}$, we define

$$\Psi_D = \{ A \in \mathbb{V}_{m \wedge n} : \mathcal{R}A \subset \tilde{D} \},$$

$$\Psi^E = \{ A \in M_n \otimes M_m : A^\tau \in \Psi^E \},$$

where $\mathcal{R}A$ denotes the range space of A , and $\tilde{E} = \{ \tilde{z} : z \in E \} \subset \mathbb{C}^n \otimes \mathbb{C}^m$. Note that we have

$$(4) \quad \text{int } \Psi_D = \{ A \in \Psi_D : \mathcal{R}A = \tilde{D} \},$$

$$\text{int } \Psi^E = \{ A \in \Psi^E : \mathcal{R}A^\tau = \tilde{E} \}.$$

Every pair (D, E) of subspaces of $M_{m \times n}$ gives rise to a nontrivial face

$$(5) \quad \tau(D, E) := \Psi_D \cap \Psi^E$$

of the convex cone \mathbb{T} , whenever the intersection is not trivial. Conversely, every face of \mathbb{T} is of the form (5) for a unique pair (D, E) of subspaces under the condition

$$\text{int } \tau(D, E) \subset \text{int } \Psi_D \cap \text{int } \Psi^E.$$

This condition actually implies the following

$$(6) \quad \text{int } \tau(D, E) = \text{int } \Psi_D \cap \text{int } \Psi^E$$

by [16], Proposition 2.1. In this way, a face of \mathbb{T} corresponds to a pair of subspaces of $M_{m \times n}$.

Theorem 2.1. *Let (D, E) be a pair of subspaces of $M_{m \times n}$. Then the following are equivalent:*

- (i) *The pair (D, E) gives rise to a nontrivial face $\tau(D, E)$ of \mathbb{T} which induces a face of \mathbb{V}_1 .*
- (ii) *There exist $x_1, \dots, x_\alpha \in \mathbb{C}^m$ and $y_1, \dots, y_\alpha \in \mathbb{C}^n$ such that*

$$D = \text{span} \{x_1 y_1^*, \dots, x_\alpha y_\alpha^*\}, \quad E = \text{span} \{\overline{x_1} y_1^*, \dots, \overline{x_\alpha} y_\alpha^*\}.$$

Proof. Assume (i), and let F be the induced face of \mathbb{V}_1 by $\tau(D, E)$. Choose an interior point

$$(7) \quad A = \sum_{i=1}^{\alpha} \tilde{z}_i \tilde{z}_i^*$$

of F with rank one matrices $z_i = x_i y_i^*$ for $i = 1, 2, \dots, \alpha$. Then A is also an interior point of $\tau(D, E)$ by (1). It follows that A is also an interior point of Ψ_D by (6), and so we see that

$$D = \text{span} \{x_1 y_1^*, \dots, x_\alpha y_\alpha^*\}$$

by (4). Similarly, we also see that A^τ is an interior point of Ψ^E , from which we have

$$E = \text{span} \{\overline{x_1} y_1^*, \dots, \overline{x_\alpha} y_\alpha^*\}$$

by (3) and (4).

Conversely, we assume (ii), and define $A \in \tau(D, E)$ as in (7). Then we see that $A \in \mathbb{V}_1$ is an interior point of $\tau(D, E)$ as above. Therefore, $\tau(D, E)$ induces a face of \mathbb{V}_1 by (2). \square

Note that if the rank of a block matrix $A \in M_n \otimes M_m$ is less than or equal to $m \vee n$, then $A \in \mathbb{T}$ if and only if $A \in \mathbb{V}_1$ [20]. Therefore, if a pair (D, E) of subspaces gives rise to a nontrivial face of \mathbb{T} and $\dim D \leq m \vee n$ or $\dim E \leq m \vee n$, then we see that the pair (D, E) already satisfies the conditions of Theorem 2.1. See also [1] for the structures of faces of \mathbb{V}_1 whose interior points have ranks less than or equal to $m \vee n$.

The range criterion for separability [19] tells us that $A \in (M_n \otimes M)^+$ is separable then the pair $(\mathcal{R}A, \mathcal{R}A^\tau)$ satisfies the condition (ii) of the theorem, where we confuse subspaces of $M_{m \times n}$ and $\mathbb{C}^n \otimes \mathbb{C}^m$ by the correspondence $z \mapsto \tilde{z}$. We note that the proof of this criterion is already contained in the proof of Theorem 2.1. It is known [4] that the range criterion is not sufficient for separability. In this line, Theorem 2.1 tells us that if a block matrix $A \in (M_n \otimes M_m)^+$ satisfies the range criterion, in other words, if the pair $(\mathcal{R}A, \mathcal{R}A^\tau)$ satisfies the condition (ii) of the theorem, then there is a separable state B with

$$(\mathcal{R}A, \mathcal{R}A^\tau) = (\mathcal{R}B, \mathcal{R}B^\tau)$$

such that A and B lie in the same face of \mathbb{T} as interior points. We also note that the condition (ii) of the theorem appeared in [24] to classify faces of the cone of all decomposable positive linear maps.

In the simplest $2 \otimes 2$ case, every possible pairs of subspaces satisfying the condition (ii) of Theorem 2.1 are listed in [15]. The possible pairs of dimensions of subspaces are

$$(1, 1), (2, 2), (3, 3), (3, 4), (4, 3), (4, 4).$$

This is a byproduct of the characterization [8] of faces of the cone of all positive linear maps between M_2 . See also [23]. It is worthwhile to note that if V is a rank two matrix in $M_{2 \times 2}$, then the pair $(V^\perp, M_{2 \times 2})$ satisfies the condition (ii) of the theorem by the following explicit construction: If we write $V = xy^* + \mu zw^*$ for nonzero $\mu \in \mathbb{C}$ and unit vectors x, y, z and w with for $x \perp z, y \perp w$ by the polar decomposition, then we have

$$V^\perp = \text{span} \{xw^*, zy^*, (\bar{\mu}x - z)(y + w)^*, (\bar{\mu}x - (1 - i)z)((1 + i)y + w)^*\},$$

$$M_{2 \times 2} = \text{span} \{\bar{x}w^*, \bar{z}y^*, \overline{(\bar{\mu}x - z)(y + w)^*}, \overline{(\bar{\mu}x - (1 - i)z)((1 + i)y + w)^*}\},$$

as was desired. See [8], Proposition 3.7.

In general, it is very difficult to determine if a given pair of subspaces satisfies the condition (ii) of the theorem or not. It was recently shown in [25] that if the rank of $A \in M_{m \times n}$ is greater than or equal to 2 and $B \in M_{m \times n}$ satisfies the following condition

$$(x | Ay) = 0 \implies (x | B\bar{y}) = 0 \text{ for each } x \in \mathbb{C}^m \text{ and } y \in \mathbb{C}^n,$$

then $B = 0$, where $(|)$ denotes the inner product in \mathbb{C}^m . This shows that if the rank of $A \in M_{m \times n}$ is greater than or equal to 2, then the pair $(A^\perp, M_{m \times n})$ satisfies the condition (ii) of the theorem. Indeed, if we collect all rank one matrices $\{xy^*\}$ orthogonal to A in $M_{m \times n}$, then the above result shows that matrices $\{\bar{x}\bar{y}^*\}$ for those collection generate the whole space $M_{m \times n}$, and so does the set $\{\bar{x}\bar{y}^*\}$, by the relation

$$(x | Ay) = (xy^* | A),$$

where $(|)$ of the right side denotes the inner product in $M_{m \times n}$.

If the pair (D, E) satisfies the condition (ii) of the theorem and xy^* is orthogonal to D , then it is clear that $\bar{x}\bar{y}^*$ is orthogonal to E . Therefore, if the

pair $(D, M_{m \times n})$ satisfies the condition (ii) of the theorem, then D^\perp has no rank one matrices. Therefore, we have the following:

Proposition 2.2. *Let D be a subspace of $M_{m \times n}$ of codimension one with $A \in D^\perp$. Then the pair $(D, M_{m \times n})$ satisfies the condition (ii) of the theorem if and only if $\text{rank } A \geq 2$.*

It would be very nice to know sufficient and necessary conditions on subspaces D of $M_{m \times n}$ for which the pairs $(D, M_{m \times n})$ satisfy the condition (ii). The absence of rank one matrices in the orthogonal complement D^\perp is an obvious necessary condition. But, this is not sufficient. There is a 4-dimensional subspace D of $M_{3 \times 3}$ without rank one matrices for which D^\perp has only six rank one matrices up to scalar multiplications [17]. In fact, every generic 4-dimensional subspace of M_3 , in the sense of algebraic geometry, has no rank one matrices and its orthogonal complement has only six rank one matrices up to constant multiples. In this case, the pair $(D^\perp, M_{3 \times 3})$ never satisfies the condition (ii) of the theorem.

3. Examples in $2 \otimes n$ cases

Now, we consider an example of a pair of subspaces satisfying the condition of Theorem 2.1 for which the difference of dimensions of two spaces is big. In [22], a 5-dimensional subspace of $M_{2 \times 4}$ spanned by rank one matrices has been considered. See also [3]. Following this example, we put

$$x_\alpha = \begin{pmatrix} 1 \\ \alpha \end{pmatrix} \in \mathbb{C}^2, \quad y_\alpha = \begin{pmatrix} 1 \\ \bar{\alpha} \\ \vdots \\ \bar{\alpha}^{n-1} \end{pmatrix} \in \mathbb{C}^n$$

for $\alpha \in \mathbb{C}$, and consider the set

$$(8) \quad \left\{ x_\alpha y_\alpha^* = \begin{pmatrix} 1 & \alpha & \cdots & \alpha^{n-1} \\ \alpha & \alpha^2 & \cdots & \alpha^n \end{pmatrix} : \alpha \in \mathbb{C} \right\}$$

of rank one matrices in $M_{2 \times n}$.

We first show that the set

$$(9) \quad \{x_\alpha y_\alpha^* : \alpha = \alpha_0, \alpha_1, \dots, \alpha_n\}$$

is linearly independent, whenever $\alpha_0, \alpha_1, \dots, \alpha_n$ are mutually distinct complex numbers. To to this, let

$$c_0 x_{\alpha_0} y_{\alpha_0}^* + c_1 x_{\alpha_1} y_{\alpha_1}^* + \cdots + c_n x_{\alpha_n} y_{\alpha_n}^* = 0.$$

Note that the $(1, k)$ -entry of the above matrix is $\sum_{j=0}^n \alpha_j^{k-1} c_j$ for $k = 1, 2, \dots, n$ and the $(2, n)$ -entry is $\sum_{j=0}^n \alpha_j^n c_j$. So, we have

$$\alpha_0^k c_0 + \alpha_1^k c_1 + \cdots + \alpha_n^k c_n = 0$$

for each $k = 0, 1, \dots, n$. Whenever $\alpha_0, \alpha_1, \dots, \alpha_n$ are mutually distinct complex numbers the matrix

$$\begin{pmatrix} 1 & 1 & \dots & 1 \\ \alpha_0 & \alpha_1 & \dots & \alpha_n \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_0^n & \alpha_1^n & \dots & \alpha_n^n \end{pmatrix}$$

is non-singular, and so the set (9) is linearly independent. Therefore, we see that the span D_n of (8) is an $(n+1)$ -dimensional subspace of $M_{2 \times n}$ whose orthogonal complement is spanned by

$$\{e_{1,j+1} - e_{2,j} : j = 1, 2, \dots, n-1\}.$$

We note that D_n^\perp has no rank one matrices.

Now, we proceed to show that the set

$$\left\{ \overline{x_\alpha} y_\alpha^* = \begin{pmatrix} 1 & \alpha & \dots & \alpha^{n-1} \\ \overline{\alpha} & \overline{\alpha}\alpha & \dots & \overline{\alpha}\alpha^{n-1} \end{pmatrix} : \alpha \in \mathbb{C} \right\}$$

generates the whole space $M_{2 \times n}$. To do this, we show that the set

$$(10) \quad \{ \overline{x_\alpha} y_\alpha^* : \alpha = 0, r_1, r_2, \dots, r_{n-1}, ir_1, ir_2, \dots, ir_n \},$$

consisting of $2n$ rank one matrices, is linearly independent, whenever r_1, r_2, \dots, r_n are mutually distinct nonzero real numbers. Suppose that

$$a_0 x_0 y_0^* + \sum_{j=1}^{n-1} a_j \overline{x_{r_j}} y_{r_j}^* + \sum_{j=1}^n b_j \overline{x_{ir_j}} y_{ir_j}^* = 0.$$

We look at the $(1, k+1)$ and $(2, k)$ entries of the above matrix, to see

$$(11) \quad \begin{aligned} \sum_{j=1}^{n-1} r_j^k a_j + i^k \sum_{j=1}^n r_j^k b_j &= 0, & k = 1, 2, \dots, n-1 \\ \sum_{j=1}^{n-1} r_j^k a_j - i^k \sum_{j=1}^n r_j^k b_j &= 0, & k = 1, 2, \dots, n \end{aligned}$$

respectively. Therefore, we have

$$(12) \quad \sum_{j=1}^{n-1} r_j^k a_j = \sum_{j=1}^n r_j^k b_j = 0, \quad k = 1, 2, \dots, n-1.$$

From the relation $\sum_{j=1}^{n-1} r_j^k a_j = 0$, we have $a_j = 0$ for $j = 1, 2, \dots, n-1$. If we put this results in the second relation of (11) with $k = n$, then we see that the relation $\sum_{j=1}^n r_j^k b_j = 0$ in (12) also holds for $k = n$. Therefore, we see that $b_j = 0$ for $j = 1, 2, \dots, n$. Finally, we have $a_0 = 0$, and so we conclude that the set (10) is linearly independent and the pair $(D_n, M_{2 \times n})$ satisfies the condition of Theorem 2.1.

We denote by $S_{m,n}$ the set of all pairs (p, q) of natural numbers for which there exist pairs (D, E) of subspaces of $M_{m \times n}$ satisfying the condition of Theorem 2.1 with

$$\dim D = p, \quad \dim E = q.$$

The above example shows that $(n + 1, 2n) \in S_{2,n}$ for each $n = 2, 3, \dots$, or equivalently

$$(k, 2k - 2) \in S_{2,k-1}$$

for $k = 3, 4, \dots$. Note that $(p, q) \in S_{m,n}$ implies that $(p, q) \in S_{m',n'}$ whenever $m' \geq m$ and $n' \geq n$. Since $(2, 2) \in S_{2,2}$, we have the following:

Proposition 3.1. *Let $n = 2, 3, \dots$. Then $(k, 2k - 2) \in S_{2,n}$ for each $k = 2, 3, \dots, n + 1$.*

The following proposition shows that this gives us a maximal gap between the two dimensions of the pair satisfying the condition of Theorem 2.1.

Proposition 3.2. *Let $n = 2, 3, \dots$. Then $(k, 2k - 1) \notin S_{2,n}$ for each $k = 2, 3, \dots, n$. We also have $(1, 2) \notin S_{2,n}$.*

Proof. Assume that $(k, 2k - 1) \in S_{2,n}$ for some $k = 2, 3, \dots, n$, then there exists a pair (D, E) of subspaces of $M_{2 \times n}$ with $\dim D = k$, $\dim E = 2k - 1$ such that

$$D = \text{span} \{x_i y_i^* : i = 1, 2, \dots, \alpha\}, \quad E = \text{span} \{\bar{x}_i y_i^* : i = 1, 2, \dots, \alpha\}$$

for some $\alpha \in \mathbb{N}$ and $x_i \in \mathbb{C}^2$, $y_i \in \mathbb{C}^n$. If $\dim \text{span} \{y_i\} \leq k - 1$, then

$$\dim E \leq 2(k - 1) < 2k - 1.$$

Therefore, the span of $\{y_i : 1 \leq i \leq \alpha\}$ must be of dimension k . Without loss of generality, we may assume that $\{y_1, y_2, \dots, y_k\}$ is linearly independent.

Choose an orthonormal basis $\{\eta_{k+1}, \dots, \eta_n\}$ of the space $\{y_1, \dots, y_k\}^\perp$ in \mathbb{C}^n , and $w_1, \dots, w_k \in \text{span} \{y_1, y_2, \dots, y_k\}$ so that $y_i \perp w_j$ for $i \neq j$. Finally, choose $z_i \in \mathbb{C}^2$ ($i = 1, 2, \dots, k$) so that $z_i \perp x_i$ for $i = 1, 2, \dots, k$. Then, it is easy to see that the two sets

$$\{z_i w_i^* : 1 \leq i \leq k\} \cup \{e_j \eta_j^* : i = 1, 2, j = k + 1, \dots, n\}$$

and

$$\{\bar{z}_i w_i^* : 1 \leq i \leq k\} \cup \{\bar{e}_j \eta_j^* : i = 1, 2, j = k + 1, \dots, n\}$$

are linearly independent, and contained in the spaces D^\perp and E^\perp , respectively. Therefore, we see that

$$\dim E^\perp \geq k + 2(n - k) = 2n - k,$$

and $2k - 1 = \dim E \leq k$, which cannot happen when $k \geq 2$. Therefore we conclude that $(k, 2k - 1) \notin S_{2,n}$ for any $k = 2, 3, \dots, n$.

Finally, if $\text{span} \{x_i y_i^*\}$ is one dimensional, then so is $\text{span} \{\bar{x}_i y_i^*\}$. Therefore, $(1, 2) \notin S_{m,n}$. □

Proposition 3.3. *For $p < q$, if $(p, q) \in S_{m,n}$ and $p \leq s \leq q$, then $(p, s) \in S_{m,n}$.*

Proof. Suppose that $(p, q) \in S_{m,n}$, then there exists a pair of subspaces (D, E) with $\dim D = p$ and $\dim E = q$ so that

$$D = \text{span} \{x_i y_i^* : 1 \leq i \leq \alpha\}, \quad E = \text{span} \{\bar{x}_i y_i^* : 1 \leq i \leq \alpha\}$$

for some $\alpha \in \mathbb{N}$ and $x_i \in \mathbb{C}^m, y_i \in \mathbb{C}^n$. We may assume that $\{x_i y_i^* : 1 \leq i \leq p\}$ is linearly independent by rearrangement. Then, we have

$$\dim \text{span} \{\bar{x}_i y_i^* : 1 \leq i \leq p\} \leq p < q = \dim \text{span} \{\bar{x}_i y_i^* : 1 \leq i \leq \alpha\}.$$

Since $p \leq s \leq q$, we see that there exists $k \in \mathbb{N}$ with $p \leq k \leq \alpha$ so that

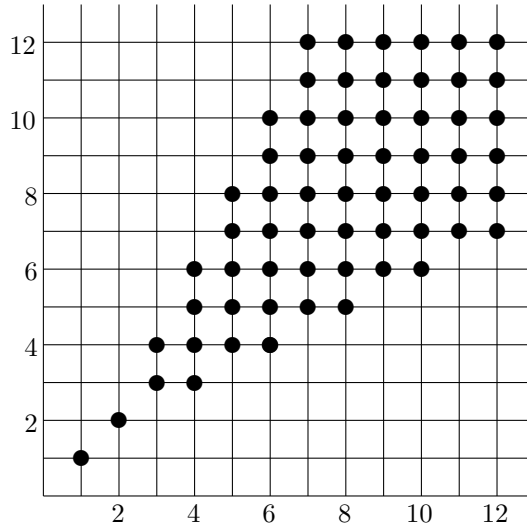
$$\dim \text{span} \{\bar{x}_i y_i^* : 1 \leq i \leq k\} = s.$$

Put

$$D' = \text{span} \{x_i y_i^* : 1 \leq i \leq k\}, \quad E' = \text{span} \{\bar{x}_i y_i^* : 1 \leq i \leq k\}.$$

Then we see the $\dim D' = p$ and $\dim E' = s$, and so $(p, s) \in S_{m,n}$. □

With the above propositions, we can now figure out the set $S_{2,n}$ as is shown in the following diagram:



4. Faces for separable states induced by PPT

For a subset S of $M_n \otimes M_m$, we define

$$S^\tau = \{A^\tau : A \in S\}.$$

Note that the map $A \mapsto A^\tau$ is an affine isomorphism of $M_n \otimes M_m$ which preserves both convex cones \mathbb{T} and \mathbb{V}_1 . Therefore, if F is a face of \mathbb{T} (respectively \mathbb{V}_1), then F^τ is also a face of \mathbb{T} (respectively \mathbb{V}_1). If $F = \sigma(D, E)$ is a face of \mathbb{T} , then we have

$$F^\tau = \sigma(E, D).$$

Recall that extremal rays of a face F of a convex cone C are determined by the extremal rays of C which belong to F . For a face F of \mathbb{V}_1 , we denote by R_F the set of all $m \times n$ rank one matrices z such that $\widetilde{z}\widetilde{z}^* \in F$, which generate extremal rays of F . It is clear that

$$(13) \quad xy^* \in R_F \iff \overline{xy}^* \in R_{F^\tau}$$

for $x \in \mathbb{C}^m$ and $y \in \mathbb{C}^n$, by the relation (3). Nevertheless, it should be noted that two subspaces $\text{span } R_F$ and $\text{span } R_{F^\tau}$ of $M_{m \times n}$ has no direct relations. It may happen that nonzero $xy^* \notin \text{span } R_F$ but $\overline{xy}^* \in \text{span } R_{F^\tau}$, as we will see in the next section.

Lemma 4.1. *If F is induced by $\tau(D, E)$, then we have*

$$(14) \quad D = \text{span } R_F, \quad E = \text{span } R_{F^\tau}.$$

Proof. If z is a rank one matrix, then it is clear that $z \in R_F$ implies $z \in D$ by the relation $F = \tau(D, E) \cap \mathbb{V}_1$. Therefore, we have $\text{span } R_F \subset D$. Take an interior point A of $\tau(D, E)$ in \mathbb{V}_1 . Then $A = \sum \widetilde{z}_i \widetilde{z}_i^*$ for rank one matrices z_i , and D is the span of $\{z_i\}$. Since F is a face and $\sum \widetilde{z}_i \widetilde{z}_i^* \in F$, we see that $\widetilde{z}_i \widetilde{z}_i^* \in F$. Therefore $z_i \in R_F$, and we see that $\text{span } R_F = D$.

For the second relation, we note that F^τ is a face of \mathbb{V}_1 which is induced by $\tau(D, E)^\tau = \tau(E, D)$. Therefore, we have $E = \text{span } R_{F^\tau}$. \square

Now, we characterize faces of \mathbb{V}_1 which are induced by faces of \mathbb{T} .

Theorem 4.2. *For a face F of \mathbb{V}_1 , the following are equivalent:*

- (i) *The face F of \mathbb{V}_1 is induced by a face of \mathbb{T} .*
- (ii) *If xy^* is a rank one matrix in $(\text{span } R_F) \setminus R_F$, then $\overline{xy}^* \notin \text{span } R_{F^\tau}$.*

Proof. If the face F of \mathbb{V}_1 is induced by a face of \mathbb{T} , then $F = \tau(D, E) \cap \mathbb{V}_1$ with D and E as in (14) by Lemma 4.1. We assume that (ii) does not hold, and take a rank one matrix $z = xy^*$ so that $xy^* \in \text{span } R_F \setminus R_F$ and $\overline{xy}^* \in \text{span } R_{F^\tau}$. Then we have $\widetilde{z}\widetilde{z}^* \in \tau(D, E) \cap \mathbb{V}_1$ but $\widetilde{z}\widetilde{z}^* \notin F$. This leads to a contradiction, and so we see that (i) implies (ii).

For the converse, we assume (ii) and define subspaces D and E as in (14). We proceed to show the relation

$$(15) \quad F = \tau(D, E) \cap \mathbb{V}_1.$$

If $z = xy^*$ is a rank one matrix and $\widetilde{z}\widetilde{z}^* \in F$, then it is clear that $\widetilde{z}\widetilde{z}^*$ belongs to $\tau(D, E) \cap \mathbb{V}_1$. If $\widetilde{z}\widetilde{z}^* \in \tau(D, E) \cap \mathbb{V}_1$, then $z = xy^* \in D = \text{span } R_F$ and $\overline{xy}^* \in E = \text{span } R_{F^\tau}$. By the assumption (ii), we have $z = xy^* \in R_F$ and $\widetilde{z}\widetilde{z}^* \in F$. Therefore, we have the relation (15). From the relation (14), we can choose finite set $\{z_i = x_i y_i^*\}$ in R_F such that $D = \text{span } \{x_i y_i^*\}$ and $E = \text{span } \{\overline{x_i y_i^*}\}$. Then it is clear that $\sum_i \widetilde{z}_i \widetilde{z}_i^* \in \mathbb{V}_1$ is an interior point of $\tau(D, E)$, which induces the face $\tau(D, E) \cap \mathbb{V}_1 = F$ of \mathbb{V}_1 . \square

If the face F of \mathbb{V}_1 is induced by a face $\tau(D, E)$ of \mathbb{T} , then we have

$$(16) \quad xy^* \in R_F \iff xy^* \in D \text{ and } \bar{xy}^* \in E.$$

Using this relation, we examine how the second condition of Theorem 4.2 works in several cases of $m = n = 2$.

First, consider the case of $F = \tau(V^\perp, M_{2 \times 2})$, where V is of rank 2. In this case, R_F consists of rank one matrices which is orthogonal to V . We have $\text{span } R_F = V^\perp$, and there is no rank one matrix in $(\text{span } R_F) \setminus R_F$.

Next, we consider the case of $F = \tau(M_{2 \times 2}, V^\perp)$, where V is of rank 2. In this case, R_F consists of rank one matrices xy^* such that $\bar{xy}^* \perp V$, and we have $\text{span } R_F = M_{2 \times 2}$. Note that xy^* belongs to $(\text{span } R_F) \setminus R_F$ if and only if \bar{xy}^* is not orthogonal to V if and only if $xy^* \notin R_{F^\tau}$.

Finally, we consider the case of $F = \tau(V^\perp, W^\perp)$, where V and W are of ranks 2 and there are rank one matrices $x_i y_i^*$ such that

$$V^\perp = \text{span} \{x_i y_i^* : i = 1, 2, 3\}, \quad W^\perp = \text{span} \{\bar{x}_i y_i^* : i = 1, 2, 3\}.$$

See [8], Proposition 3.6. In this case, we see that

$$\begin{aligned} R_F &= \{xy^* : xy^* \perp V, \bar{xy}^* \perp W\}, & \text{span } R_F &= V^\perp, \\ R_{F^\tau} &= \{xy^* : xy^* \perp W, \bar{xy}^* \perp V\}, & \text{span } R_{F^\tau} &= W^\perp. \end{aligned}$$

Therefore, we see that the second condition of Theorem 4.2 is immediate.

It would be nice if we find an intrinsic characterization for subsets R of rank one matrices for which there exist faces F of \mathbb{V}_1 such that $R = R_F$. We say that a subset R of rank one matrices in $M_{m \times n}$ is *locally full* if there is no rank one matrices in $(\text{span } R) \setminus R$. This is equivalent to say that there exists a subspace D of $M_{m \times n}$ spanned by rank one matrices such that R coincides with the set of all rank one matrices in D .

For a set R of rank one matrices, we write

$$\bar{R} = \{\bar{xy}^* : xy^* \in R\}.$$

Note that xy^* is parallel to zw^* if and only if \bar{xy}^* is also parallel to \bar{zw}^* . If R is a subset of $M_{m \times n}$ which consists of rank one matrices, then it is clear that the pair $(\text{span } R, \text{span } \bar{R})$ satisfies the second condition of Theorem 2.1, and so we see that

$$F_R = \tau(\text{span } R, \text{span } \bar{R}) \cap \mathbb{V}_1$$

is a face of \mathbb{V}_1 . In this case,

$$xy^* \in R_{F_R} \iff xy^* \in \text{span } R \text{ and } \bar{xy}^* \in \text{span } \bar{R}$$

by (16). Therefore, we see that the relation

$$R \subset R_{F_R}$$

holds in general. Suppose that R is locally full. If $xy^* \in R_{F_R}$, then $xy^* \in \text{span } R$, which implies $xy^* \in R$. Therefore, we see that $R = R_{F_R}$. This is also the case when \bar{R} is locally full. Indeed, if $xy^* \in R_{F_R}$, then $\bar{xy}^* \in \text{span } \bar{R}$. If \bar{R}

is locally full, then this implies $\overline{xy^*} \in \overline{R}$ and $xy^* \in R$. Therefore, we have the following:

Proposition 4.3. *Let R be a subset of $M_{m \times n}$ consisting of rank one matrices. If either R or \overline{R} is locally full, then there exists a face F of \mathbb{V}_1 such that $R = R_F$. Furthermore, this face F is induced by a face of \mathbb{T} .*

Recall the three cases discussed just after Theorem 4.2. In the case of $F = \tau(V^\perp, M_{2 \times 2})$, we see that R_F is locally full. On the other hands, if $F = \tau(M_{2 \times 2}, V^\perp)$, then $\overline{R_F}$ is locally full. In the case of $F = \tau(V^\perp, W^\perp)$, neither R_F nor $\overline{R_F}$ is locally full, and so we see that the converse of Proposition 4.3 does not hold.

5. Examples in $3 \otimes 3$ case

In this section, we give an example of a face of \mathbb{V}_1 which is not induced by a face of \mathbb{T} . To begin with, we review the duality theory between block matrices and positive linear maps in matrix algebras.

In [13], we have considered the bi-linear pairing between $M_n \otimes M_m$ and the space $\mathcal{L}(M_m, M_n)$ of all linear maps from M_m into M_n , given by

$$\langle A, \phi \rangle = \text{Tr} \left[\left(\sum_{i,j=1}^m \phi(e_{ij}) \otimes e_{ij} \right) A^t \right] = \sum_{i,j=1}^m \langle \phi(e_{ij}), a_{ij} \rangle$$

for $A = \sum_{i,j=1}^m a_{ij} \otimes e_{ij} \in M_n \otimes M_m$ and a linear map ϕ from M_m into M_n , where the bi-linear form in the right side is given by $\langle X, Y \rangle = \text{Tr}(YX^t)$ for $X, Y \in M_n$. This is equivalent to define

$$\langle y \otimes x, \phi \rangle = \text{Tr}(\phi(x)y^t)$$

for $x \in M_m$ and $y \in M_n$. If $z = xy^*$ is a rank one matrix in $M_{m \times n}$, then we have

$$\langle \widetilde{zz^*}, \phi \rangle = (\phi(xx^*)|yy^*),$$

where $(|)$ denotes the usual inner product in the matrix algebra M_n , which is linear in the first variable and conjugate-linear in the second variable.

We denote by \mathbb{P}_1 (respectively \mathbb{D}) the convex cone of all positive linear maps (respectively decomposable positive linear maps) from M_m into M_n . In this duality, the pairs

$$(\mathbb{V}_1, \mathbb{P}_1), \quad (\mathbb{T}, \mathbb{D})$$

are dual each other, in the sense

$$\begin{aligned} A \in \mathbb{V}_1 &\iff \langle A, \phi \rangle \geq 0 \text{ for each } \phi \in \mathbb{P}_1, \\ \phi \in \mathbb{P}_1 &\iff \langle A, \phi \rangle \geq 0 \text{ for each } A \in \mathbb{V}_1, \end{aligned}$$

and similarly for the other pair. This gives us a criterion of separability using positive linear maps in matrix algebras. See also [18].

We begin with an example [10] of an indecomposable positive linear map in M_3 which generates an extremal ray. See also [9]. This map is given by

$$\phi : [a_{ij}] \mapsto \begin{bmatrix} a_{11} + a_{33} & -a_{12} & -a_{13} \\ -a_{21} & a_{22} + a_{11} & -a_{23} \\ -a_{31} & -a_{32} & a_{33} + a_{22} \end{bmatrix}.$$

Let F be the dual face of \mathbb{V}_1 given by this map, that is,

$$(17) \quad F = \{A \in \mathbb{V}_1 : \langle A, \phi \rangle = 0\}.$$

By a direct calculation, we see that R_F consists of the following rank one matrices

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & \alpha & \bar{\gamma} \\ \bar{\alpha} & 1 & \beta \\ \gamma & \bar{\beta} & 1 \end{pmatrix},$$

where $\alpha\beta\gamma = 1$ with $|\alpha| = |\beta| = |\gamma| = 1$. We show that

$$(18) \quad \text{span } R_F = \{[a_{ij}] \in M_3 : a_{11} = a_{22} = a_{33}\}.$$

It is clear that every matrix $[a_{ij}]$ in $\text{span } R_F$ has the relation $a_{11} = a_{22} = a_{33}$, and so the dimension of $\text{span } R_F$ is at most 7. We see that the following four matrices

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix}$$

together $e_{1,3}, e_{2,1}, e_{3,2}$ are linearly independent rank one matrices belonging to R_F . This proves the relation (18), and so $\text{span } R_F$ is a 7-dimensional subspace of $M_{3 \times 3}$.

Next, we show that the set R_{F^τ} spans M_3 . To do this, put

$$x_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, x_2 = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, x_3 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, x_4 = \begin{pmatrix} 1 \\ -i \\ 1 \end{pmatrix}, x_5 = \begin{pmatrix} 1 \\ 1 \\ -i \end{pmatrix}, x_6 = \begin{pmatrix} 1 \\ -i \\ -i \end{pmatrix}$$

and $y_i = x_i$ for $i = 1, 2, 3, 4, 5, 6$. We also define

$$x_7 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, x_8 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, x_9 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, y_7 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, y_8 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, y_9 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

Then it is easy to see that $x_i y_i^* \in R_{F^\tau}$. It remains to show that the set

$$\{\bar{x}_i y_i^* : i = 1, 2, \dots, 9\}$$

is linearly independent. Suppose that $B = \sum_{i=1}^9 a_i \bar{x}_i y_i^* = 0$, and look at the entries of the matrix B . Then we have

$$\begin{aligned} B_{11} &= a_1 + a_2 + a_3 + a_4 + a_5 + a_6 = 0, \\ B_{12} &= a_1 - a_2 + a_3 + ia_4 + a_5 + ia_6 = 0, \\ B_{22} &= a_1 + a_2 + a_3 - a_4 + a_5 - a_6 = 0, \\ B_{23} &= a_1 - a_2 - a_3 + ia_4 + ia_5 - a_6 = 0, \\ B_{31} &= a_1 + a_2 - a_3 + a_4 + ia_5 + ia_6 = 0, \\ B_{33} &= a_1 + a_2 + a_3 + a_4 - a_5 - a_6 = 0. \end{aligned}$$

With this relation, we have $a_i = 0$ for $i = 1, 2, \dots, 6$, from which we also have $a_7 = a_8 = a_9 = 0$.

Although every self-adjoint rank one matrix in $\text{span } R_F$ belongs to R_F , there are many rank one matrices in $\text{span } R_F$ which do not belong to R_F . Actually, a rank one matrix with zero diagonals is in the space $\text{span } R_F$ if and only if it has only one nonzero column or row. A rank one matrix with nonzero diagonals is in the space $\text{span } R_F$ if and only if it is a scalar multiple of the matrix of the form

$$\begin{pmatrix} 1 & a & b \\ \frac{1}{a} & 1 & \frac{b}{a} \\ \frac{1}{b} & \frac{a}{b} & 1 \end{pmatrix}$$

with nonzero complex numbers a and b . When $|a| \neq 1$, above matrix belongs to $\text{span } R_F \setminus R_F$. Since $\text{span } R_{F^c}$ is the full matrix algebra, we conclude that the face F is not induced by a face of \mathbb{T} by Theorem 4.2.

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