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AN ALGORITHM FOR CHECKING EXTREMALITY OF ENTANGLED STATES WITH POSITIVE PARTIAL TRANSPOSES

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Abstract. We characterize extreme rays of the cone $\mathbb{T}$ of all positive semi-definite block matrices whose partial transposes are also positive semi-definite. We also construct an algorithm checking whether a given PPTES generates an extreme ray in the cone $\mathbb{T}$ or not. Using this algorithm, we give an example of $4 \otimes 4$ PPT entangle state of the type $(5, 5)$, which generates extreme ray of the cone $\mathbb{T}$

1. Introduction

Quantum entanglement has been investigated during the last few decades in connection with the quantum information theory and quantum communication theory. The characterization and classification of the entanglement are a central problem in the field of quantum information. In particular it is of primary importance to test whether a given quantum state is separable or entangled.

A density matrix A in $(M_n \otimes M_m)^+$ is said to be *entangled* if it does not belong to $M_n^+ \otimes M_m^+$, where M_n^+ denotes the cone of all positive semi-definite $n \times n$ matrices over the complex fields. A density matrix is said to be *separable* if it belongs to $M_n^+ \otimes M_m^+$. Note that a density matrix defines a state on the matrix algebra by the Schur or Hadamard product.

One of the criteria for separability was given by Choi [1] and Peres [14], which says that the partial transpose of every separable state is positive semi-definite. The *partial transpose* or *block transpose* A^τ of

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$A \in M_n \otimes M_m$ is define by

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

This necessary condition for separability is called the positive partial transpose (PPT) criterion for separability. It was shown by Horodecki et al. [9] that PPT criterion is also sufficient condition for separability in the cases of $M_2 \otimes M_2$ and $M_2 \otimes M_3$. Existence of PPT entangled $3 \otimes 3$ state was known already in terms of cones by Choi [1]. On physical ground, first examples of entangled states that are PPT were found by Horodecki [10], following Woronowicz construction [17]. See the review paper [11] and references therein for other separability criteria.

Still more efforts have been done to find various type of PPT entangled states (PPTES). PPTES may be classified by their range dimensions as was studied in [16]. A PPTES A is said to be of the type (s, t) if the range dimension of A is s, and the range dimension of A^τ is t. There are some examples of $(4, 4)$, $(5, 5)$, $(6, 5)$, $(7, 5)$, $(8, 5)$, $(6, 6)$ and $(6, 7)$ PPTES in the literature. See the references [2, 6, 7] for example.

In this note, we denote by $\mathbb{T}$ the convex cone of all positive semidefinite block matrices whose partial transposes are also positive semidefinite, that is to say

$$\mathbb{T} = \{A \in (M_n \otimes M_m)^+ \,:\, A^\tau \in (M_n \otimes M_m)^+\}.$$

Note that the convex set of all $n \otimes m$ entangled states with positive partial transpose is of the form

$$\{A \in \mathbb{T} \,:\, \mathrm{Tr}(A) = 1\}$$

where Tr denotes the usual trace of a matrix in $M_n \otimes M_m = M_{n\times m}$. To understand this convex cone $\mathbb{T}$, the author with Kye [5] characterized the face of $\mathbb{T}$ in terms of pairs of subspaces of the space $M_{m\times n}$ of all $m \times n$ matrices. Recall that 1-dimensional face of a given convex cone is extreme ray. We say that a PPTES is *extremal* if it generates an extreme ray in the convex cone $\mathbb{T}$. It was shown that some PPTES of type $(4, 4), (5, 5)$ and $(6, 6)$ in [2, 6, 7] are extremal by a direct argument [4, 8, 12]. Moreover, Leinaas et al. [13] formulated a criterion for finding extreme points of the convex set of density matrices with positive partial transpose. They reduced the question of extremality to the problem of solving a system of linear equations.

The purpose of this note is to construct a practical algorithm for checking whether a given PPTES is extremal in the convex cone $\mathbb{T}$ or not. We explain very briefly in the next section the facial structures of the cone $\mathbb{T}$, and investigate what kinds of faces of $\mathbb{T}$ are extreme rays using our previous results [5] on the facial structure of $\mathbb{T}$. In the final section, we construct an algorithm for checking the extremality of PPTES and discuss an implementation of this algorithm.

Throughout this paper, we do not use bra-ket notations. 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. We also denote by $\{e_i\}$ the usual orthonomal basis of $\mathbb{C}^n$, and $\{e_{ij}\}$ the usual matrix units of M_n. For natural numbers m and n, $m \wedge n$ means the minimum of m and n.

2. Characterization of extremal PPTES

We start with a brief review of the facial structures for the convex cone $\mathbb{T}$ [5]. 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 an $m \times n$ matrix $z = [z_{ik}] \in M_{m\times n}$, we define

$$
\begin{aligned}
z_i &= \sum_{k=1}^{n} z_{ik} e_k \in \mathbb{C}^n, \quad i = 1, 2, \cdots, m, \\
\tilde{z} &= \sum_{i=1}^{m} z_i \otimes e_i \in \mathbb{C}^n \otimes \mathbb{C}^m.
\end{aligned}
$$

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

$$
\begin{aligned}
\mathbb{V}_s &= \mathrm{conv}\{\tilde{z}\tilde{z}^* \in M_n \otimes M_m \,|\, \text{rank of } z \le s\} \\
\mathbb{V}^s &= \mathrm{conv}\{(\tilde{z}\tilde{z}^*)^\tau \in M_n \otimes M_m \,|\, \text{rank of } z \le s\}
\end{aligned}
$$

for $s = 1, 2, \cdots, m\wedge n$, where $\mathrm{conv}X$ means the convex set generated by X.

It is clear that $\mathbb{V}_{m\wedge n}$ coincides with the cone $(M_n \otimes M_m)^+$ of all positive semi-definite $mn \times mn$ matrices and so we get

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

It is well known that every face of $\mathbb{V}_{m\wedge n}$ and $\mathbb{V}^{m\wedge n}$ is of the form

$$
\begin{aligned}
\Psi_D &= \{A \in (M_n \otimes M_m)^+ \,:\, \mathcal{R}A \subset \widetilde{D}\}, \\
\Psi^E &= \{A \in M_n \otimes M_m \,:\, A^\tau \in \Psi_E\}
\end{aligned}
\tag{2.1}
$$

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

$$\begin{aligned} \operatorname{int}\Psi_D &= \{A \in \Psi_D : \mathcal{R}A = \widetilde{D}\}, \\ \operatorname{int}\Psi^E &= \{A \in \Psi^E : \mathcal{R}A^\tau = \widetilde{E}\} \end{aligned} \tag{2.2}$$

where $\operatorname{int} C$ denotes the relative interior of the convex set C with respect to the hyperplane spanned by C.

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

$$\tau(D, E) := \Psi_D \cap \Psi^E \tag{2.3}$$

of the convex cone $\mathbb{T}$, and every face of $\mathbb{T}$ is of the form (2.3) for a unique pair (D, E) of subspaces under the condition

$$\operatorname{int}\tau(D, E) \subset \operatorname{int}\Psi_D \cap \operatorname{int}\Psi^E \tag{2.4}$$

as was explained in [5].

In this section we will characterize extreme rays of the convex cone $\mathbb{T}$. Let $(M_n \otimes M_m)_h$ be the real Hilbert space of all $nm \times nm$ hermitian matrices in $M_n \otimes M_m$ with the inner product

$$\langle X, Y\rangle = \operatorname{Tr}(YX^t)$$

for X, $Y \in (M_n \otimes M_m)_h$. For a pair (D, E) of subspaces of $M_{m\times n}$, we define linear maps $\phi_{\widetilde{D}}$ and $\phi_{\widetilde{E}}$ from $(M_n \otimes M_m)_h$ to $(M_n \otimes M_m)_h$ by

$$\begin{aligned} \phi_{\widetilde{D}}(X) &= P_{\widetilde{D}} X P_{\widetilde{D}} - X \\ \phi_{\widetilde{E}}(X) &= (P_{\widetilde{E}} X^\tau P_{\widetilde{E}})^\tau - X \end{aligned}$$

where $P_{\widetilde{D}}$ denotes the orthogonal projection onto $\widetilde{D} \subset \mathbb{C}^n \otimes \mathbb{C}^m$. Note that the orthogonal projection $P_{\widetilde{D}}$ belongs to $(M_n \otimes M_m)_h$ and the map $X \mapsto X^\tau$ is an isomorphism of $(M_n \otimes M_m)_h$ preserving $\mathbb{T}$.

Let $\tau(D, E) = \Psi_D \cap \Psi^E$ be the face corresponding to the pair (D, E). Then for any $A \in \tau(D, E)$, we have

$$P_{\widetilde{D}} A P_{\widetilde{D}} = A, \quad P_{\widetilde{E}} A^\tau P_{\widetilde{E}} = A^\tau$$

since $\mathcal{R}A \subset \widetilde{D}$ and $\mathcal{R}A^\tau \subset \widetilde{E}$ by (2.1). Therefore we see that

$$\tau(D, E) \subset \operatorname{Ker}(\phi_{\widetilde{D}}) \cap \operatorname{Ker}(\phi_{\widetilde{E}}) \tag{2.5}$$

where $\operatorname{Ker}(\phi)$ denotes the kernel space of a linear map ϕ. Now, we characterize extreme rays of $\mathbb{T}$. Recall that every face of $\mathbb{T}$ is of the form $\tau(D, E)$ for a unique pair (D, E) of subspaces under the condition (2.4).

THEOREM 2.1. *For a face $\tau(D, E)$ of $\mathbb{T}$, the following are equivalent:*

(i) *The face $\tau(D, E)$ is an extreme ray in the cone $\mathbb{T}$.*

(ii) $\dim\bigl(\mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}})\bigr) = 1$

Proof. If $\mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}})$ is a 1-dimensional subspace of $(M_n \otimes M_m)_h$, then the face $\tau(D,E)$ is 1-dimensional, that is, $\tau(D,E)$ is an extreme ray of $\mathbb{T}$ by the inclusion (2.5).

Conversely, we assume (i), and choose an interior point A of $\tau(D,E)$. Then we see that

$$\mathcal{R}A = \widetilde{D}, \quad \mathcal{R}A^\tau = \widetilde{E} \tag{2.6}$$

by the relations (2.4) and (2.2). If $\dim\bigl(\mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}})\bigr) \geq 2$ then there exist a hermitian matrix $B \in \mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}})$, which is not a scalar multiple of A. We may assume that

$$\mathrm{Tr}(A) = \mathrm{Tr}(B) = 1.$$

Since both A and B bolong to $\mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}})$, the matrix $A' = B - A$ belong to $\mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}})$. Furthermore, the matrix A' is a nonzero hermitian matrix and $\mathrm{Tr}(A') = 0$. Therefore A' has both positive and negative eigenvalues. Now we define a hermitian matrix

$$\tilde{A}(t) = A + tA' \tag{2.7}$$

for real t. Since A' has both positive and negative eigenvalues, so has $\tilde{A}(t)$ for sufficiently large $|t|$. If $v \in \mathbb{C}^{nm}$ is an eigenvector of A corresponding to the eigenvalue 0 then $P_A v = 0$ for the orthogonal projection P_A onto $\mathcal{R}A$, and we see that

$$A'v = P_{\widetilde{D}} A' P_{\widetilde{D}} v = P_A A' P_A v = 0$$

because A' belong to $\mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}}) \subset \mathrm{Ker}(\phi_{\widetilde{D}})$ and $P_{\widetilde{D}} = P_A$ for an interior point A of $\tau(D,E)$ by the relations (2.6). Therefore $\tilde{A}(t)v = 0$ for all t. This means that only positive eigenvalues of A can be changed when tA' is added to A. Since positive eigenvalues of $\tilde{A}(t)$ change continuously with t, they remain positive for t in an open interval (t_1, t_2) containing $t = 0$. Consequently we can conclude that $\tilde{A}(t)$ is positive semi-definite for $t_1 \leq t \leq t_2$.

Since A' belong to $\mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}}) \subset \mathrm{Ker}(\phi_{\widetilde{E}})$, we have

$$A'^\tau = P_{\widetilde{E}} A'^\tau P_{\widetilde{E}}.$$

If $w \in \mathbb{C}^{nm}$ is an eigenvector of A^τ corresponding to the eigenvalue 0 then $P_{\widetilde{E}} w = 0$ for the orthogonal projection $P_{\widetilde{E}}$ because of $\widetilde{E} = \mathcal{R}A^\tau$ in (2.6), hence we see that

$$A'^\tau w = P_{\widetilde{E}} A'^\tau P_{\widetilde{E}} w = 0.$$

Therefore $(\tilde{A}(t))^\tau w = 0$ for all t by (2.7). By the same argument as the case of $\tilde{A}(t)$, we can conclude that there exist a $t_3 < 0$ and a $t_4 > 0$ such that $(\tilde{A}(t))^\tau$ is positive semi-definite for $t_3 \le t \le t_4$.

Consequently we conclude that for $\max\{t_1, t_3\} \le t \le \min\{t_2, t_4\}$

$$\tilde{A}(t) \in \mathbb{T}.$$

Since $\max\{t_1, t_3\} < 0 < \min\{t_2, t_4\}$ and $\tilde{A}(0) = A$, A is not extremal in the cone $\mathbb{T}$. This completes the proof. □

For a PPT entangled state A, we can find the pair (D, E) of subspaces of $M_{n\times m}$ such that $\widetilde{D} = \mathcal{R}A$ and $\widetilde{E} = \mathcal{R}A^\tau$. Then A generates an extreme ray if and only if the face $\tau(D, E)$ is an extreme ray. Therefore we have the following.

Corollary 2.2. *For a PPT entangled state A, the following are equivalent:*

(i) *A generates an extreme ray in $\mathbb{T}$.*
(ii) $\dim\big(\operatorname{Ker}(\phi_{\widetilde{D}}) \cap \operatorname{Ker}(\phi_{\widetilde{E}})\big) = 1$ *where $\widetilde{D} = \mathcal{R}A$ and $\widetilde{E} = \mathcal{R}A^\tau$.*

3. An algorithm for checking the extremality of PPTES

In this section, we give a practical algorithm that tries to check the extremality of an $n\otimes m$ PPTES. Let $A \in \mathbb{T} \subset (M_n \otimes M_m)^+$ be a PPTES of type (s, t). Then there is a unique face $\tau(D, E)$ containing A as an interior point, so we have $\widetilde{D} = \mathcal{R}A$ and $\widetilde{E} = \mathcal{R}A^\tau$. By the Corollary 2.2, we can construct the algorithm as follows.

step1: Compute the block transpose A^τ of A.
step2: Find the orthogonal projection $P_{\widetilde{D}}$ onto $\mathcal{R}A$. This process may be broken up into two steps:
 2-1) Apply Gram-Schmidt process to $\{Ae_1, \cdots, Ae_{nm}\}$ to get an orthonormal basis $\{p_1, \cdots, p_s\}$ where $\{e_i : 1 \le i \le nm\}$ is the usual basis of $\mathbb{C}^n \otimes \mathbb{C}^m$.
 2-2) Compute the orthogonal projection $P_{\widetilde{D}} = \sum_{i=1}^{s} p_i p_i^*$.
step3: Find the orthogonal projection $P_{\widetilde{E}}$ onto $\mathcal{R}A^\tau$. This process may be broken up into two steps:
 3-1) Apply Gram-Schmidt process to $\{A^\tau e_1, \cdots, A^\tau e_{nm}\}$ to get an orthonormal basis $\{q_1, \cdots, q_t\}$ where $\{e_i : 1 \le i \le nm\}$ is the usual basis of $\mathbb{C}^n \otimes \mathbb{C}^m$.
 3-2) Compute the orthogonal projection $P_{\widetilde{E}} = \sum_{i=1}^{t} q_i q_i^*$.

step4: Compute the $(nm)^2 \times (nm)^2$ matrices which represent the linear maps $\phi_{\widetilde{D}}$ and $\phi_{\widetilde{E}}$ respectively.
step5: Compute the basis $\mathcal{B}$ of $\mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}})$.
step6: if the number of $\mathcal{B}$=1 then
    print "A generates an extreme ray"
  else
    print "A does not generate an extreme ray"
  end if

We implemented this algorithm using the Maple's programming language. In step1 of the above algorithm, we made a procedure which compute the matrix $A^\tau \in M_n \otimes M_m$ for a given PPTES $A \in M_n \otimes M_m$, and used the Maple function *GramSchmidt* in step2 and step3. In step4, we considered a matrix in $M_n \otimes M_m = M_{m \times n}$ as a vector in $\mathbb{C}^{(nm)^2}$, so we could compute the $(nm)^2 \times (nm)^2$ matrices which represent the linear maps $\phi_{\widetilde{D}}$ and $\phi_{\widetilde{E}}$. Finally we used Maple functions *NullSpace* and *IntersectionBasis* to compute the basis of $\mathrm{Ker}(\phi_{\widetilde{D}}) \cap \mathrm{Ker}(\phi_{\widetilde{E}})$ in step5.

We confirmed all PPT entangled states of type $(4,4)$, $(5,5)$ and $(6,6)$ in [2, 6, 7] generate extreme rays in $\mathbb{T}$ using Maple program which implements our algorithm. As another application of our program, we checked that the PPT entangled state $A \in M_4 \otimes M_4$ in [3] is extremal. The author [3] constructed this PPTES to show that the Robertson map [15] is an atomic map.

For the reader's convenience, we restate this PPTES A. Define $z_i \in \mathbb{C}^4 \otimes \mathbb{C}^4$ and $A \in M_4 \otimes M_4$ by

$$
\begin{gathered}
z_1 = e_1 \otimes e_1,\ z_2 = e_1 \otimes e_3,\ z_3 = e_2 \otimes e_1,\ z_4 = e_2 \otimes e_4, \\
z_5 = e_3 \otimes e_1,\ z_6 = e_3 \otimes e_3,\ z_7 = e_3 \otimes e_4, \\
A := (z_1 - z_6)(z_1 - z_6)^* + (z_4 + z_5)(z_4 + z_5)^* + z_2 z_2^* + z_3 z_3^* + z_7 z_7^*.
\end{gathered}
$$

Then we see that

$$
A^\tau = (z_5 - z_2)(z_5 - z_2)^* + (z_3 + z_7)(z_3 + z_7)^* + z_1 z_1^* + z_4 z_4^* + z_6 z_6^*,
$$

and so A^τ is positive semi-definite, that is, $A \in \mathbb{T}$. Consequently, we get an example of PPTES of the type $(5,5)$, which generates an extreme ray in $\mathbb{T} \subset M_4 \otimes M_4$.

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