Quantum states with strong positive partial transpose

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We construct a large class of bipartite $M \otimes N$ quantum states which defines a proper subset of states with positive partial transposes (PPT). Any state from this class is PPT but the positivity of its partial transposition is recognized with respect to canonical factorization of the original density operator. We propose to call elements from this class states with strong positive partial transposes (SPPT). We conjecture that all SPPT states are separable.

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Quantum entanglement is one of the most remarkable features of quantum mechanics and it leads to powerful applications like quantum cryptography, dense coding and quantum computing [1, 2].

One of the central problems in the theory of quantum entanglement is to check whether a given density matrix describing a quantum state of the composite system is separable or entangled. Let us recall that a state represented by a density operator ρ living in the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ is separable iff ρ is a convex combination of product states, that is, $\rho = \sum_k p_k \rho_k^{(A)} \otimes \rho_k^{(B)}$, with $\{p_k\}$ being a probability distribution, and $\rho_k^{(A)}$, $\rho_k^{(B)}$ are density operators describing states of subsystem A and B, respectively [3].

There are several operational criteria which enable one to detect quantum entanglement (see e.g. [2] for the recent review). The most famous Peres-Horodecki criterion [4, 5] is based on the partial transposition: if a state ρ is separable then its partial transposition $\rho^{\mathrm{T}_A} = (\mathrm{T} \otimes \mathbb{1})\rho$ is positive (such states are called PPT state). The structure of this set is of primary importance in quantum information theory. Unfortunately, this structure is still unknown, that is, one may easily check whether a given state is PPT but we do not know how to construct a general quantum state with PPT property.

Recently [6, 7] we proposed large classes of states where the PPT property is very easy to check. In the present Letter we propose a new class of states which are PPT by the very construction. This construction is based on the block structure of any density matrix living in the tensor product $\mathcal{H}_A \otimes \mathcal{H}_B$, that is, a density matrix in $\mathbb{C}^M \otimes \mathbb{C}^N$ may be considered as $M \times M$ matrix with $N \times N$ blocks. Partial transposition is an operation which acts on blocks and we show how to organize blocks to have a density matrix with PPT property. We propose to call PPT states constructed this way a strong PPT states (SPPT). Interestingly, known examples of SPPT states turn out to be separable. This observation supported by some numerical investigations encouraged us to conjecture that all SPPT states are separable.

The Letter is organized as follows: for pedagogical reason we start with $M = 2$ and arbitrary (but finite) N. This construction easily generalizes for arbitrary $M > 2$. We finish with some conclusions.

1. $2 \otimes N$ systems. Such systems are of primary importance in quantum information theory and they were extensively analyzed in [8]. It is clear that an (unnormalized) state of a bipartite system living in $\mathbb{C}^2 \otimes \mathbb{C}^N$ may be considered as a block 2×2 matrix with $N \times N$ blocks. Positivity of ρ implies that $\rho = \mathbf{X}^\dagger \mathbf{X}$ for some $2N \times 2N$ matrix $\mathbf{X}$. Again, this matrix may be considered as a block 2×2 matrix with $N \times N$ blocks. Consider now the following class of upper triangular block matrices $\mathbf{X}$:

$$\mathbf{X} = \left(\begin{array}{c|c} X_1 & SX_1 \\ \hline 0 & X_2 \end{array} \right) , \qquad (1)$$

with arbitrary $N \times N$ matrices X_1, X_2 and S. One finds

$$\rho = \mathbf{X}^\dagger \mathbf{X} = \left(\begin{array}{c|c} X_1^\dagger X_1 & X_1^\dagger S X_1 \\ \hline X_1^\dagger S^\dagger X_1 & X_1^\dagger S^\dagger S X_1 + X_2^\dagger X_2 \end{array} \right) , \qquad (2)$$

and its partial transposition is given by

$$\rho^{\mathrm{T}_A} = \left(\begin{array}{c|c} X_1^\dagger X_1 & X_1^\dagger S^\dagger X_1 \\ \hline X_1^\dagger S X_1 & X_1^\dagger S^\dagger S X_1 + X_2^\dagger X_2 \end{array} \right) . \qquad (3)$$

Clearly, ρ is PPT iff there exists $\mathbf{Y}$ such that $\rho^{T_A} = \mathbf{Y}^\dagger \mathbf{Y}$. The choice of $\mathbf{Y}$ (if it exists) is highly nonunique. Note, however, that there is a 'canonical' candidate for $2N \times 2N$ matrix $\mathbf{Y}$ defined by (1) with S replaced by $S^\dagger$, that is

$$\mathbf{Y} = \left(\begin{array}{c|c} X_1 & S^\dagger X_1 \\ \hline 0 & X_2 \end{array} \right) \ , \tag{4}$$

and hence

$$\mathbf{Y}^\dagger \mathbf{Y} = \left(\begin{array}{c|c} X_1^\dagger X_1 & X_1^\dagger S^\dagger X_1 \\ \hline X_1^\dagger S X_1 & X_1^\dagger S S^\dagger X_1 + X_2^\dagger X_2 \end{array} \right) \ . \tag{5}$$

Now, we say that a state $\rho = \mathbf{X}^\dagger \mathbf{X}$ with $\mathbf{X}$ defined in (1) has **strong positive partial transpose** (SPPT) iff $\rho^{T_A} = \mathbf{Y}^\dagger \mathbf{Y}$ with $\mathbf{Y}$ defined in (4).

It is therefore clear that a $2 \otimes N$ state ρ is SPPT if and only if

$$X_1^\dagger S^\dagger S X_1 = X_1^\dagger S S^\dagger X_1 \ . \tag{6}$$

Note, that if S is normal, i.e. $S^\dagger S = S S^\dagger$, then ρ is necessarily SPPT. It was proved in [8] that if the rank of ρ is N, then PPT implies separability. Now, any PPT ρ of rank N may be constructed via (2) with $X_1 = \mathbb{I}$, $X_2 = 0$ and a normal matrix S giving rise to (so called canonical $2 \otimes N$ form [8])

$$\rho = \left(\begin{array}{c|c} \mathbb{I} & S \\ \hline S^\dagger & S^\dagger S \end{array} \right) \ .$$

Due to normality of S it does belong to our class, i.e. any rank N PPT state in $2 \otimes N$ is both SPPT and separable. Another example of SPPT states is provided by hermitian (and hence normal) S. It implies $\rho^{T_A} = \rho$. It is well known [8] that for $2 \otimes N$ systems this condition is sufficient for separability. Hence, for $2 \otimes N$ case all states defined by arbitrary X_1 , X_2 and arbitrary but hermitian S are SPPT from (6) and separable due to [8].

Consider other well known examples in $2 \otimes N$. The celebrated Werner state [3] in $2 \otimes 2$ is SPPT if and only if it is maximally mixed, i.e. $\frac{1}{4}\, \mathbb{I} \otimes \mathbb{I}$. The same is true for the isotropic state in $2 \otimes 2$. The seminal Horodecki entangled PPT state [5] in $2 \otimes 4$ parameterized by $b \in [0, 1]$ belongs to our class iff $b = 0$ (for $b = 0, 1$ Horodecki state is separable). In a recent paper [7] we constructed a class of so called circulant states in $N \otimes N$. For $N = 2$ they are given by

$$\rho = \left(\begin{array}{cc|cc} a_{11} & 0 & 0 & a_{12} \\ 0 & b_{11} & b_{12} & 0 \\ \hline 0 & b_{21} & b_{22} & 0 \\ a_{21} & 0 & 0 & a_{22} \end{array} \right) \ , \tag{7}$$

where $[a_{ij}]$ and $[b_{ij}]$ are 2×2 positive matrices. Partially transposed ρ has the same structure but with $[a_{ij}]$ and $[b_{ij}]$ replaced by $[\widetilde{a}_{ij}]$ and $[\widetilde{b}_{ij}]$

$$\widetilde{a} = \left(\begin{array}{cc} a_{11} & b_{21} \\ b_{12} & a_{22} \end{array} \right) \ , \quad \widetilde{b} = \left(\begin{array}{cc} b_{11} & a_{21} \\ a_{12} & b_{22} \end{array} \right) \ .$$

Now, ρ is PPT iff $\widetilde{a} \geq 0$ and $\widetilde{b} \geq 0$. It is not difficult to see that a circulant $2 \otimes 2$ PPT state is SPPT iff $|a_{12}| = |b_{12}|$. A nice example of circulant state is provided by orthogonally invariant state [9], that is, a 2-qubit state ρ satisfying $U \otimes U \rho = \rho U \otimes U$, with $U \in U(2)$ and $\overline{U} = U$:

$$\rho = \frac{1}{4} \left(\begin{array}{cc|cc} a+2b & \cdot & \cdot & 2b-a \\ \cdot & a+2c & a-2c & \cdot \\ \hline \cdot & a-2c & a+2c & \cdot \\ 2b-a & \cdot & \cdot & a+2b \end{array} \right) \ , \tag{8}$$

where $a, b, c \geq 0$ and $a + b + c = 1$. It is easy to see that ρ is PPT iff $b, c \leq 1/2$ [9]. Moreover, ρ is SPPT iff it is PPT and $b = c$. Hence SPPT states define a 1-parameter family within 2-parameter class of PPT states.

2. General $M \otimes N$ systems. The above construction may be easily generalized for an arbitrary bipartite system living in $\mathbb{C}^M \otimes \mathbb{C}^N$. Now, a state ρ may be considered as an $M \times M$ matrix with entries being $N \times N$ matrices. Positivity of ρ implies that $\rho = \mathbf{X}^\dagger \mathbf{X}$ for some $MN \times MN$ matrix $\mathbf{X}$ — a block $M \times M$ matrix with $N \times N$ blocks. Let us consider the following class of upper triangular block matrices $\mathbf{X}$: diagonal blocks $X_{ii} = X_i$ and $X_{ij} = S_{ij} X_i$ for $i < j$

$$\mathbf{X} = \left(\begin{array}{c|c|c|c|c} X_1 & S_{12}X_1 & S_{13}X_1 & \dots & S_{1M}X_1 \\ \hline 0 & X_2 & S_{23}X_2 & \dots & S_{2M}X_2 \\ \hline \vdots & \vdots & \ddots & \vdots & \vdots \\ \hline 0 & 0 & 0 & X_{M-1} & S_{M-1,M}X_{M-1} \\ \hline 0 & 0 & 0 & 0 & X_M \end{array} \right) ,$$

where X_k and S_{ij} $(i < j)$ are $N \times N$ matrices. Simple calculation gives for diagonal blocks

$$\begin{aligned} \rho_{11} &= X_1^\dagger X_1 \ , \\ \rho_{22} &= X_1^\dagger S_{12}^\dagger S_{12} X_1 + X_2^\dagger X_2 \ , \\ \rho_{33} &= X_1^\dagger S_{13}^\dagger S_{13} X_1 + X_2^\dagger S_{23}^\dagger S_{23} X_2 + X_3^\dagger X_3 \ , \\ &\vdots \\ \rho_{MM} &= \sum_{k=1}^{M-1} X_k^\dagger S_{kM}^\dagger S_{kM} X_k + X_M^\dagger X_M \ , \end{aligned} \tag{9}$$

Off-diagonal blocks are defined as follows: for $i = 1$

$$\rho_{1j} = X_1^\dagger S_{1j} X_1 \ , \tag{10}$$

and for $1 < i < j$

$$\rho_{ij} = \sum_{k=1}^{i-1} X_k^\dagger S_{ki}^\dagger S_{kj} X_k + X_i^\dagger S_{ij} X_i \ . \tag{11}$$

Partially transposed ρ^{T_A} is therefore given by the following block matrix: diagonal blocks

$$\rho_{ii}^{T_A} = \rho_{ii} \ , \tag{12}$$

and off-diagonal blocks: for $i = 1$

$$\rho_{1j}^{T_A} = \rho_{j1}^\dagger = X_1^\dagger S_{1j}^\dagger X_1 \ , \tag{13}$$

and for $1 < i < j$

$$\rho_{ij}^{T_A} = \rho_{ji}^\dagger = \sum_{k=1}^{i-1} X_k^\dagger S_{kj}^\dagger S_{ki} X_k + X_i^\dagger S_{ij}^\dagger X_i \ . \tag{14}$$

Now, in analogy to $2 \otimes N$ case we say that ρ is SPPT iff $\rho^{T_A} = \mathbf{Y}^\dagger \mathbf{Y}$ where $\mathbf{Y}$ is given by the following 'canonical' block matrix

$$\mathbf{Y} = \left(\begin{array}{c|c|c|c|c} X_1 & S_{12}^\dagger X_1 & S_{13}^\dagger X_1 & \ldots & S_{1M}^\dagger X_1 \\ \hline 0 & X_2 & S_{23}^\dagger X_2 & \ldots & S_{2M}^\dagger X_2 \\ \hline \vdots & \vdots & \ddots & \vdots & \vdots \\ \hline 0 & 0 & 0 & X_{M-1} & S_{M-1,M}^\dagger X_{M-1} \\ \hline 0 & 0 & 0 & 0 & X_M \end{array} \right) .$$

It is clear that blocks $(\mathbf{Y}^\dagger \mathbf{Y})_{ij}$ are defined by the same formulae as $(\mathbf{X}^\dagger \mathbf{X})_{ij}$ with S_{ij} replaced by $S_{ij}^\dagger$ — formulae (9)–(11). Therefore, the SPPT condition $\rho^{T_A} = \mathbf{Y}^\dagger \mathbf{Y}$ is equivalent to:

- for $j = 2, \ldots, M$

$$\sum_{k=1}^{j-1} X_k^\dagger S_{kj}^\dagger S_{kj} X_k = \sum_{k=1}^{j-1} X_k^\dagger S_{kj} S_{kj}^\dagger X_k \ , \tag{15}$$

- for $2 \leq i < j = 3, \ldots, M$

$$\sum_{k=1}^{i-1} X_k^\dagger S_{kj}^\dagger S_{ki} X_k = \sum_{k=1}^{i-1} X_k^\dagger S_{ki} S_{kj}^\dagger X_k \ . \tag{16}$$

In particular the above conditions are satisfied if

$$S_{ki} S_{kj}^\dagger = S_{kj}^\dagger S_{ki} \ , \tag{17}$$

for $k < i \leq j$. Formula (17) shows that there are $\frac{1}{2}M(M-1)$ normal matrices S_{ij} $(i < j)$ such that each matrix S_{ki} commutes with $S_{kj}^\dagger$ for $i < k$. It introduces $\frac{1}{6}(M-1)M(M+1)$ independent conditions for matrices S_{ij}. For $M = 2$ it reduces to exactly one condition (6) for one matrix S. The special class of SPPT states corresponds to a family of hermitian (and hence normal) matrices S_{ij} satisfying

$$[S_{ki} \, , \, S_{kj}] = 0 \ , \quad k < i \leq j \ .$$

In this case one simply has $\rho^{T_A} = \rho$.

Let us analyze known examples of $M \otimes N$ states belonging to our class of SPPT states. Now, the situation is much more complicated since our knowledge about general $M \otimes N$ case is very limited.

Example 1) Similarly as in $2 \otimes 2$ case both Werner and isotropic states in $N \otimes N$ are SPPT iff they are maximally mixed.

Example 2) The seminal Horodecki $3 \otimes 3$ PPT but entangled state [5] is SPPT if and only if $a = 0$ (in this case it is separable).

Example 3) In [6] we have proposed a class of $N \otimes N$ states defined as follows

$$\rho = \sum_{i,j=1}^{N} a_{ij} \, |ii\rangle\langle jj| + \sum_{i \neq j=1}^{N} b_{ij} \, |ij\rangle\langle ij| \ , \tag{18}$$

where $[a_{ij}]$ is $N \times N$ positive matrix and b_{ij} $(i \neq j)$ are positive coefficients. It was shown [6] that ρ is PPT iff $|a_{ij} a_{ji}| \leq b_{ij}^2$ for $i \neq j$. It turns out that this class contains many well known PPT states (for example an isotropic state are there). If $N = 3$ this state has the following block form (to have more transparent picture we represent zeros by dots)

$$\rho = \left(\begin{array}{ccc|ccc|ccc} a_{11} & \cdot & \cdot & \cdot & a_{12} & \cdot & \cdot & \cdot & a_{13} \\ \cdot & b_{12} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & b_{13} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & b_{21} & \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{21} & \cdot & \cdot & \cdot & a_{22} & \cdot & \cdot & \cdot & a_{23} \\ \cdot & \cdot & \cdot & \cdot & \cdot & b_{23} & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & b_{31} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & b_{32} & \cdot \\ a_{31} & \cdot & \cdot & \cdot & a_{32} & \cdot & \cdot & \cdot & a_{33} \end{array} \right) .$$

It is clear that ρ is SPPT iff $a_{ij} = 0$ for $i \neq j$, that is, ρ is diagonal and hence separable. We stress that both Werner and isotropic states do belong to this class.

Example 4) In a recent paper [7] we proposed a class of so called circulant PPT states in $N \otimes N$. It is easy to show that for odd N circulant PPT states are SPPT if and only if they are diagonal (hence separable). However, for even N we may have circulant states with more complicated structure (cf. [7]). Circulant SPPT state for $N = 2$ was already presented in (7). It is not difficult to show that again SPPT property implies separability.

Conclusions. We constructed a large class of PPT states in $\mathbb{C}^M \otimes \mathbb{C}^N$ — we called them SPPT states since they satisfy one extra condition which is *strong* enough to guarantee PPT. All known to us examples of such states turn out to be separable. Moreover, we have strong numerical evidence (realignment criterion) that SPPT states in $\mathbb{C}^3 \otimes \mathbb{C}^3$ are separable. Therefore, we are encouraged to conjecture that all SPPT states are separable. If this conjecture is true it gives rise to new sufficient criterion for separability: if ρ is SPPT, then it is separable.

Note, that constructed states give rise to new family of quantum channels $\Phi : M_M(\mathbb{C}) \longrightarrow M_N(\mathbb{C})$, where $M_K(\mathbb{C})$ denotes a set of $K \times K$ complex matrices. If $e_{ij} = |i\rangle\langle j|$ denotes a base in $M_M(\mathbb{C})$, then the action of the channel corresponding to state ρ is given by

$$\Phi(e_{ij}) = \rho_{ij} \ , \qquad (19)$$

where ρ_{ij} defined in (9)–(11) are elements from $M_N(\mathbb{C})$. Now, if our conjecture about SPPT states is true any quantum channel defined via (19) corresponding to SPPT state ρ is entanglement breaking [10, 11] (see also [12] for classification of channels), i.e. $(\mathbb{1}_M \otimes \Phi)P^+_M$ is separable, where P^+_M denotes a projector onto maximally entangled state in $\mathbb{C}^M \otimes \mathbb{C}^M$. Therefore, as a byproduct we derive a large class of entanglement breaking quantum channels.

In a recent paper [13] authors developed new necessary and sufficient criterion for separability which is based on the existence of a set of normal commuting matrices. SPPT states may therefore provide a laboratory of states where the methods of [13] may be applied. They may shed new light on the intricate structure of quantum states of composed systems.

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