On separable decompositions of quantum states with strong positive partial transposes

B Bylicka, D Chruściński and J Jurkowski

Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5, 87-100 Toruń, Poland

E-mail: darch@fizyka.umk.pl

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Abstract

We analyze a class of positive partial transpose (PPT) states such that the positivity of its partial transposition is recognized with respect to the canonical factorization of the original density operator (Cholesky block decomposition). We call such PPT states strong PPT (SPPT) states. This property, in contrast to PPT, is basis dependent. It is shown that there exists a proper subset of SPPT states which are separable and provide a separable decomposition for any of these states.

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1. Introduction

Quantum entanglement is one of the most remarkable features of quantum mechanics and leads to powerful applications such as quantum cryptography, dense coding and quantum computing [1, 2]. One of the central problems in the theory of quantum entanglement is to discriminate between separable and entangled states of composite quantum systems. Let us recall that a state represented by a density operator \( \rho \) living in the Hilbert space \( \mathcal{H}_A \otimes \mathcal{H}_B \) is separable if and only if \( \rho \) 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 \( \rho_k^{(A)} \) and \( \rho_k^{(B)} \) the density operators of the subsystems A and B, respectively [3]. Despite its simplicity, the above definition does not tell us when such a separable decomposition does exist. It should be stressed that separable decomposition, if it exists, is highly non-unique. Moreover, knowing that \( \rho \) is separable, it is in general very hard to find even one separable decomposition (1). Therefore, the discrimination between separable and entangled (not separable) states is usually performed without looking for any specific decomposition. Instead, 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 \( \rho \) is separable, then its partial transposition \( \rho^\Gamma = (T \otimes \mathbb{1})\rho \) is positive (such states are called positive partial
transposed (PPT) states). It is well known that all PPT states in $2 \otimes 2$ and $2 \otimes 3$ systems are simultaneously separable, but this statement is no longer true for higher dimensional systems, where to discriminate separable and entangled PPT states, some more subtle methods should be used (see for instance [6]). Hence, the structure of the set of PPT states is of primary importance in quantum information theory. It would be very interesting to find a construction of PPT states which does guarantee separability. Such a construction would shed new light on the basic structure of PPT states. This is the basic motivation of our paper.

In what follows, we use the following convention: let $\dim \mathcal{H}_A = M$ and $\dim \mathcal{H}_B = N$. We call a composed system living in $\mathcal{H}_A \otimes \mathcal{H}_B$ a $M \otimes N$ system. Let $e_1 = |1\rangle, \ldots, e_M = |M\rangle$ be an arbitrary orthonormal basis in $\mathcal{H}_A$. Any $M \otimes N$ density operator $\rho$ may be represented as follows:

$$\rho = \sum_{i,j=1}^{M} |i\rangle \langle j| \otimes \rho_{ij},$$

(2)

where $\rho_{ij}$ are operators in $\mathcal{H}_B$, that is, $\rho$ is represented as a block $M \times M$ matrix with $N \times N$ blocks $\rho_{ij}$. Performing partial transposition with respect to the basis $|k\rangle$ in $\mathcal{H}_A$, one obtains

$$\rho^T = \sum_{i,j=1}^{M} |i\rangle \langle j| \otimes \rho_{ij} = \sum_{i,j=1}^{M} |i\rangle \langle i| \otimes \rho_{ij}.$$

(3)

We stress that $\rho^T$ is basis dependent; however, if $\rho^T \succeq 0$, then this property does not depend on the basis we use for block decompositions (2) and (3). Hence, the notion of a PPT state is basis independent. In this paper, we analyze a subclass of PPT states—strong positive partially transposed (SPPT) states—which, in contrast to PPT states, are basis dependent. Usually, in physics, we prefer notions which are basis or observer independent. We stress that in the case of SPPT states (or rather SPPT block matrices) it is not a drawback but the very essence of the construction. Note that in practice, we usually analyze not an abstract basis independent operator but a basis dependent density matrix.

In section 2, we investigate the case of $2 \otimes N$ SPPT states giving an explicit example that the notion of being an SPPT state is basis dependent. We also note that there are states which do not have the SPPT representation in any basis. Further, we recall that any super SPPT (SSPPT) $2 \otimes N$ state is separable [9], and we provide in section 3 a proof that this statement can be extended to an arbitrary $M \otimes N$ SSPPT state, giving an explicit separable expansion for such states.

2. $2 \otimes N$ SPPT states

To illustrate our construction, let us start with a $2 \otimes N$ system (such systems were carefully investigated in [10]). Let us fix an orthonormal basis $e_1 = |1\rangle, e_2 = |2\rangle$ in $\mathcal{H}_A$ and introduce the following upper triangular block matrices $X$ and $Y$:

$$X = \begin{pmatrix} X_1 & S X_1 \\ \emptyset & X_2 \end{pmatrix}, \quad Y = \begin{pmatrix} X_1 & S' X_1 \\ \emptyset & X_2 \end{pmatrix},$$

(4)

with arbitrary $N \times N$ matrices $X_1, X_2$ and $S$. $\emptyset$ denotes here the null operator in $\mathcal{H}_B$. Define the (unnormalized) density matrix $\rho = X^\dagger X$. One finds

$$\rho = \begin{pmatrix} X_1^\dagger X_1 & X_1^\dagger S X_1 \\ X_1^\dagger S' X_1 & X_1^\dagger S' S X_1 + X_2^\dagger X_2 \end{pmatrix}, \quad \rho^T = \begin{pmatrix} X_1^\dagger X_1 & X_1^\dagger S X_1 \\ X_1^\dagger S' S X_1 + X_2^\dagger X_2 & X_1^\dagger S' X_1 \end{pmatrix}.$$

(5)

On the other hand,

$$Y^\dagger Y = \begin{pmatrix} X_1^\dagger X_1 & X_1^\dagger S X_1 \\ X_1^\dagger S' X_1 & X_1^\dagger S' S X_1 + X_2^\dagger X_2 \end{pmatrix}.$$

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Definition 1 ([7]). One says that $\rho$ is SPPT (with respect to $\{e_1, e_2\}$) iff
$$\rho^T = Y^*Y,$$
that is, iff the following condition is satisfied:
$$X_1^*S^*SX_1 = X_1^*SS^*X_1.$$ (6)

Remark 1. A sufficient condition for $\rho$ to be SPPT is that $S$ is normal, i.e. $S^*S = SS^*$. In a recent paper [11], such a state was called SSPPT. One has a chain of obvious implications: SSPPT $\Rightarrow$ SPPT $\Rightarrow$ PPT.

Remark 2. If $X_1$ has a full rank (rank $X_1 = N$), then formula (7) implies that $S$ is normal.

Remark 3. If $\rho$ is SPPT with respect to $\{e_1, e_2\}$, it need not be SPPT with respect to another basis $\{f_1, f_2\}$. Consider for example
$$X_1 = \begin{pmatrix} 2 & 1 \\ 1 & -1 \end{pmatrix}, \quad S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$ (8)
It is SPPT since $S$ is normal. However, if we perform a local unitary transformation
$$\rho \rightarrow (U \otimes I)\rho(U^* \otimes I),$$ (9)
with $U$ being a Hadamard gate,
$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$
the transformed $\rho$ is no longer SPPT. Indeed, one finds after the Hadamard transformation that
$$\tilde{X}_1 = \frac{1}{\sqrt{26}} \begin{pmatrix} \sqrt{127} + 2\sqrt{51} \\ \sqrt{2(8 - \sqrt{51})} \end{pmatrix}, \quad \tilde{S} = \begin{pmatrix} 1 & -5 \\ 2(1 - 3\sqrt{51}) & -11 \end{pmatrix}.$$ (10)

Remark 4. Interestingly, there are PPT states which are not SPPT with respect to any basis. Consider for example the Werner states for two qubits represented in the computational basis as
$$W_p = \frac{1}{6} \begin{pmatrix} 2p & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 - 2p & 4p - 3 & 0 & 0 & 0 \\ 0 & 4p - 3 & 3 - 2p & 0 & 0 & 0 \\ 0 & 0 & 0 & 2p \end{pmatrix}, \quad 0 \leq p \leq 1.$$ (11)
$W_p$ is PPT (and hence separable) for $p \geq \frac{1}{2}$. One easily finds that
$$X_1 = \begin{pmatrix} \sqrt{\frac{p}{3}} & 0 \\ 0 & \sqrt{\frac{3 - 2p}{6}} \end{pmatrix}, \quad S = \begin{pmatrix} 0 & 0 \\ 4p - 3 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} \sqrt{\frac{2p(p - 1)}{2p - 3}} & 0 \\ 0 & \sqrt{\frac{p}{3}} \end{pmatrix}.$$ (11)
Note that rank $X_1 = 2$ and condition (7) implies $S^†S = SS^†$, which is not the case unless $p = 3/4$. This shows that $W_p$ is not SPPT for $p \neq \frac{3}{4}$ ($W_{\frac{3}{4}} = \frac{1}{2}\mathbb{I} \otimes \mathbb{I}$ and hence it is SPPT in all bases). Now, according to the defining property of the Werner state one has

$$U \otimes UW_p U \otimes U = W_p$$

(12)

for each unitary operator $U$ in $\mathbb{C}^2$. This invariance shows that $W_p$ is not SPPT also in the transformed basis $\{U|1\}, U|2\rangle$).

In a recent paper [9], Ha shows that if $N \leq 4$, any SPPT state is separable. However, for $N \geq 5$, there are SPPT entangled states. Interestingly, for arbitrary $N$, one has the following.

**Theorem 1** ([9]). If $\rho$ is SSPPT, then it is separable.

### 3. $M \otimes N$ SPPT states

In the general case, a state $\rho$ may be considered as an $M \times M$ matrix with entries being operators from $\mathfrak{B}(\mathcal{H}_B)$. The positivity of $\rho$ implies that $\rho = X^†X$. Let us consider the following class of upper triangular block matrices $X$:

$$X = \begin{pmatrix}
X_1 & S_{12}X_1 & S_{13}X_1 & \cdots & S_{1M}X_1 \\
\mathbb{0} & X_2 & S_{23}X_2 & \cdots & S_{2M}X_2 \\
\mathbb{0} & \mathbb{0} & X_3 & \cdots & S_{3M}X_3 \\
\mathbb{0} & \mathbb{0} & \mathbb{0} & \cdots & X_{M-1} \\
\mathbb{0} & \mathbb{0} & \mathbb{0} & \cdots & X_M \\
\end{pmatrix},$$

(13)

where $X_k$ and $S_{ij}$ ($i < j$) belong to $\mathfrak{B}(\mathcal{H}_B)$. This block matrix may be written in a compact form

$$X = \sum_{i,j=1}^M |i\rangle\langle j| \otimes X_{ij},$$

(14)

with $X_{ij} = S_{ij}X_i$, where we assume that $S_{ii} = \mathbb{I}$ and $S_{ij} = \mathbb{0}$ for $i > j$. One has

$$\rho = X^†X = \sum_{i,j=1}^M |i\rangle\langle j| \otimes \rho_{ij},$$

(15)

where the blocks are defined by

$$\rho_{ij} = \sum_{k=1}^i X_k^†S_{ij}X_k,$$

(16)

for $i \leq j$, and for a partially transposed block matrix

$$\rho^Γ = \sum_{i,j=1}^M |j\rangle\langle i| \otimes \rho_{ij} = \sum_{i,j=1}^M |i\rangle\langle j| \otimes \tilde{\rho}_{ij},$$

(17)

with

$$\tilde{\rho}_{ij} = \rho_{ji} = \sum_{k=1}^i X_k^†S_{ij}^†X_k,$$

(18)

for $i \leq j$ (one obviously has $\rho_{ij} = \rho_{ji}^†$). Now, in analogy to the $2 \otimes N$ case, we have the following.

**Definition 2.** $\rho$ is SPPT (with respect to $\{e_1, \ldots, e_M\}$) if $\rho^Γ = Y^†Y$, where $Y$ is given by (13) with $S_{ij}$ replaced by $S_{ij}^†$. 4
One easily finds that $\rho$ is SPPT if
\[
\sum_{k=1}^{i} X_k^\dagger S_k X_k = \sum_{k=1}^{j} X_k^\dagger S_k X_k, \quad i \leq j.
\]
(19)

In particular, the above conditions are satisfied if
\[
S_k S_k^\dagger = S_k^\dagger S_k,
\]
for $k < i \leq j$. Following [11], we call SPPT states satisfying (20) SSPPT states.

**Theorem 2.** An SSPPT state is separable.

**Proof.** It is clear from (16) and (17) that
\[
\rho = \rho_1 + \rho_2 + \cdots + \rho_M,
\]
(21)

where
\[
\rho_k = \sum_{i,j=k}^{M} |i\rangle \langle j| \otimes X_k^\dagger S_k X_k.
\]
(22)

Note that the sum starts with $i, j = k$ due to the fact that $S_k = 0$ for $i < k$. We show that all $\rho_k$ are separable and hence (21) provides the separable decomposition of $\rho$. Condition (20) implies that $S_k$ for $k < i$ defines a family of normal and mutually commuting operators. Hence $S_k = \sum_{l=1}^{N} \lambda^{(k)}_l P^{(k)}_l$, (23)

where $\lambda^{(k)}_l$ are complex and $P^{(k)}_l$ are rank-1 projectors. It gives therefore
\[
\rho_k = \sum_{l=k}^{M} \sigma^{(k)}_l \otimes X_k^\dagger P^{(k)}_l X_k,
\]
(24)

where $\sigma^{(k)}_l = \sum_{i,j=k}^{N} \lambda^{(k)}_l |i\rangle \langle j|$. Note that $\sigma^{(k)}_l = |\psi^{(k)}_l\rangle \langle \psi^{(k)}_l|$ with $|\psi^{(k)}_l\rangle = \sum_{l=1}^{N} \lambda^{(k)}_l |i\rangle$, which proves that $\sigma^{(k)}_l$ are positive operators and hence $\rho_k$ is separable. □

**Remark 5.** A statement similar to theorem 2 has been raised already in [11], but some technical details of the proof are questionable. To avoid this, we presented the complete proof which gives, in fact, a different separable decomposition of $\rho$. Condition (20) implies that $S_k$ for $k < i$ defines a family of normal and mutually commuting operators. Hence

An interesting class of SSPPT states is provided by the so-called classical-quantum (CQ) states
\[
\rho = \sum_{n} p_n |e_n\rangle \langle e_n| \otimes \sigma_n,
\]
(25)

where $|e_n\rangle$ defines an orthonormal basis in $\mathcal{H}_A$, $\sigma_n$ are density operators in $\mathcal{H}_B$ and $p_n$ is a probability distribution. Such states have vanishing quantum discord and were recently intensively investigated (see recent review [12]). It was shown in [13] that $2 \otimes N$ states with vanishing discord are SSPPT with respect to an arbitrary basis in the qubit Hilbert space. However, it is no longer true for $M \otimes N$ states with $M > 2$ (actually, the authors of [11] provided a proof that this statement is true but their proof is not correct).
Remark 6. A subclass of CQ defines so-called classical-classical (CC) states, i.e. states for which $\sigma_n$ are mutually commuting. It implies that there exists an orthonormal basis $|f_m\rangle$ in $\mathcal{H}_B$ such that

$$\rho = \sum_n p_{nm} |e_n\rangle \langle e_n| \otimes |f_m\rangle \langle f_m|.$$  

(26)

CC states are, therefore, fully characterized by the classical joint probability distribution $p_{nm}$.

Let us observe that a CC state rewritten in another basis $|\tilde{e}_n\rangle$ in $\mathcal{H}_A$ has the following form $\rho = \sum_{n,m} |\tilde{e}_n\rangle \langle \tilde{e}_m| \otimes \rho_{nm}$ and the blocks $\rho_{nm}$ are diagonal in the basis $|f_m\rangle$. It is therefore clear that a CC state is SSPPT with respect to an arbitrary basis in $\mathcal{H}_A$.

For a recent discussion on quantifying classical and quantum correlations see the series of papers in [14]. CQ and CC states and the corresponding CQ and CC quantum channels have been recently analyzed in [15, 16].

4. Conclusions

We analyzed a class of SPPT states in $\mathcal{H}_A \otimes \mathcal{H}_B$ with respect to a fixed orthonormal basis $\{e_1, \ldots, e_M\}$ in $\mathcal{H}_A$ with $M = \dim \mathcal{H}_A$. We stress that the property of being SPPT is always defined with respect to a fixed basis and hence it is basis dependent. It is not a drawback but the very essence of the construction. In particular, we showed that a state which is SSPPT is separable. Moreover, we provided separable decomposition for any SSPPT state.

Now, any SPPT state is PPT and any SSPPT is separable. We have shown, providing a counterexample, that the converse statements are not always true. However, it would be interesting to find a class of states with the following property: if $\rho$ is PPT (separable), then there exists an orthonormal basis $\{e_1, \ldots, e_M\}$ in $\mathcal{H}_A$ such that $\rho$ is SPPT (SSPPT) with respect to this basis. Note that this class of separable states provides natural separable decomposition. Finally, it would be interesting to generalize SPPT states for multipartite setting.

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