Class of positive partial transposition states

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We construct a class of quantum bipartite $d\otimes d$ states which are positive under partial transposition (PPT states). This class is invariant under the maximal commutative subgroup of U(d) and contains as special cases many well-known examples of PPT states. States from our class provide criteria for testing the indecomposability of positive maps. Such maps are crucial for constructing entanglement witnesses.

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The interest on quantum entanglement has dramatically increased over the last two decades due to the emerging field of quantum information theory [1]. It turns out that quantum entangled states may be used as basic resources in quantum information processing and communication, such as quantum cryptography, quantum teleportation, dense coding, error correction, and quantum computation.

A fundamental problem in quantum information theory is to test whether a given state of a composite quantum system is entangled or separable. Several operational criteria have been proposed to identify entangled states [2]. The most famous Peres-Horodecki criterion [3,4] is based on the partial transposition: if a state ρ is separable then its partial transposition $(\mathbb{1}\otimes\tau)\rho$ is positive. States which are positive under partial transposition are called PPT states. Clearly each separable state is necessarily PPT but the converse is not true. It was shown by Horodecki *et al.* [5] that the PPT condition is both necessary and sufficient for separability for $2\otimes 2$ and $2\otimes 3$ systems.

Now, since all separable states belong to a set of PPT states, the structure of this set is of primary importance in quantum information theory. Unfortunately, this structure is still unknown, that is, one may check whether a given state is PPT but we do not know how to construct a general quantum state with PPT property. There are several well-known examples of PPT states. One class contains PPT states which are separable, e.g., Werner [6] and isotropic states [7]. Other examples present PPT states that are entangled. Actually there is a systematic method of construction of PPT entangled states which is based on a concept of unextendible product bases [8] (see also Ref. [9]). Other examples of PPT entangled states were constructed in Refs. [4,10–15]. PPT states also play a crucial role in mathematical theory of positive maps and, as is well known, these maps are very important in the study of quantum entanglement. Recently, the mathematical structure of quantum states with positive partial transposition were studied in Refs. [16,17].

In the present paper we propose a class of bipartite $d\otimes d$ PPT states. This class is important for the following reasons. (i) It contains many of the abovementioned examples of PPT states. (ii) We claim that this is the most general class of PPT states available at the moment. Moreover, unlike other examples it fully uses complex parametrization of density operators. (iii) Finally, it may be used to study important properties of positive maps, e.g., to test whether a given positive map is indecomposable and atomic. As is well known indecomposable positive maps are crucial in constructing entanglement witnesses.

The defining property of this class is very simple: it contains bipartite states invariant under the maximal commutative subgroup of U(d), i.e., d-dimensional torus $T^d=\mathrm{U}(1)\times\cdots\times\mathrm{U}(1)$. This commutative subgroup is generated by d mutually commuting operators

$$\hat{t}_k=|k\rangle\langle k|,\quad k=1,\ldots,d, \tag{1}$$

where $|k\rangle$ denotes an orthonormal base in $\mathbb{C}^d$. Now, any vector $\mathbf{x}\in\mathbb{R}^d$ gives rise to the following element from T^d:

$$U_{\mathbf{x}}=e^{-i\mathbf{x}\cdot\hat{\mathbf{t}}}, \tag{2}$$

where $\hat{\mathbf{t}}=(\hat{t}_1,\ldots,\hat{t}_d)$. Evidently, $U_{\mathbf{x}}U_{\mathbf{y}}=U_{\mathbf{x}+\mathbf{y}}$.

In the present paper we consider two classes of bipartite states each of which is invariant under a representation of T^d on $\mathbb{C}^d\otimes\mathbb{C}^d$.

(1) Werner-like state, or $U_{\mathbf{x}}\otimes U_{\mathbf{x}}$-invariant states

$$U_{\mathbf{x}}\otimes U_{\mathbf{x}}\rho=\rho U_{\mathbf{x}}\otimes U_{\mathbf{x}}. \tag{3}$$

(2) Isotropiclike state, or $U_{\mathbf{x}}\otimes U_{\mathbf{x}}^*$-invariant states

$$U_{\mathbf{x}}\otimes U_{\mathbf{x}}^*\rho=\rho U_{\mathbf{x}}\otimes U_{\mathbf{x}}^*, \tag{4}$$

for all $\mathbf{x}\in\mathbb{R}^d$. $U_{\mathbf{x}}^*$ denotes complex conjugation of $U_{\mathbf{x}}$ in a fixed basis.

Clearly, these two classes are related by a partial transposition, i.e., a bipartite operator $\hat{O}$ is $U_{\mathbf{x}}\otimes U_{\mathbf{x}}^*$ invariant iff $(\mathbb{1}\otimes\tau)\hat{O}$ is $U_{\mathbf{x}}\otimes U_{\mathbf{x}}$ invariant.

The most general state which is $U_{\mathbf{x}}\otimes U_{\mathbf{x}}^*$ invariant has the following form:

$$\rho=\sum_{i,j=1}^{d}a_{ij}|ii\rangle\langle jj|+\sum_{i\neq j=1}^{d}c_{ij}|ij\rangle\langle ij|. \tag{5}$$

Now, since $\rho^\dagger=\rho$ the matrix $\hat{a}=\|a_{ij}\|$ has to be hermitian and d^2-d coefficients c_{ij} have to be real. Moreover, ρ is positive iff

$$\hat{a}=\|a_{ij}\|\geqslant 0\quad\text{and } c_{ij}\geqslant 0. \tag{6}$$

Finally, normalization Tr $\rho=1$ leads to

$$\mathrm{Tr}\,\hat{a}+\sum_{i\neq j}c_{ij}=1. \tag{7}$$

Consider now the partial transposition of ρ:

$$(\mathbb{1} \otimes \tau)\rho = \sum_{i,j=1}^{d} a_{ij}|ij\rangle\langle ji| + \sum_{i\neq j=1}^{d} c_{ij}|ij\rangle\langle ij|. \tag{8}$$

Note, that the above formula may be rewritten as follows:

$$(\mathbb{1} \otimes \tau)\rho = \sum_{i=1}^{d} a_{ii}|ii\rangle\langle ii| + \sum_{i<j} \hat{X}_{ij}, \tag{9}$$

where the operator $\hat{X}_{ij}$ is given by

$$\hat{X}_{ij} = a_{ij}|ij\rangle\langle ji| + a_{ij}^{*}|ji\rangle\langle ij| + c_{ij}|ij\rangle\langle ij| + c_{ji}|ji\rangle\langle ji|.$$

Since two operators $\Sigma_i a_{ii}|ii\rangle\langle ii|$ and $\Sigma_{i<j}\hat{X}_{ij}$ live in a mutually orthogonal subspaces of $\mathbb{C}^d \otimes \mathbb{C}^d$, the positivity of $(\mathbb{1}\otimes\tau)\rho$ implies separately $\Sigma_i a_{ii}|ii\rangle\langle ii| \geqslant 0$, which is equivalent to $a_{ii}\geqslant 0$, and $\Sigma_{i<j}\hat{X}_{ij}\geqslant 0$. Now, for any pair $i<j$ an operator $\hat{X}_{ij}$ acts on a two-dimensional subspace of $\mathbb{C}^d\otimes\mathbb{C}^d$ spanned by $|ij\rangle$ and $|ji\rangle$:

$$\hat{X}_{ij}|ij\rangle = c_{ij}|ij\rangle + a_{ij}|ji\rangle,$$

$$\hat{X}_{ij}|ji\rangle = a_{ij}^{*}|ij\rangle + c_{ji}|ji\rangle, \tag{10}$$

and hence $\hat{X}_{ij}|ij\rangle \geqslant 0$ iff

$$\begin{bmatrix} c_{ij} & a_{ij} \\ a_{ij}^{*} & c_{ij} \end{bmatrix} \geqslant 0, \tag{11}$$

which is equivalent to the following condition:

$$c_{ij}c_{ji} - |a_{ij}|^2 \geqslant 0. \tag{12}$$

There is an evident example of isotropiclike PPT states. Let $\vec{\lambda}=(\lambda_1,\ldots,\lambda_d)$ be a normalized complex vector. Consider a state from the class (5) with $a_{ij}=\lambda_i\lambda_j^*$ and $c_{ij}=|\lambda_i\lambda_j^*|$. Evidently $\hat{a}\geqslant 0$, $c_{ij}\geqslant 0$, and $c_{ij}c_{ji}-|a_{ij}|^2=0$. Hence each complex vector $\vec{\lambda}$ gives rise to a PPT state.

Similarly one may analyze a general Werner-like $U_{\mathbf{x}}\otimes U_{\mathbf{x}}^{*}$-invariant state

$$\widetilde{\rho} = \sum_{i,j=1}^{d} b_{ij}|ij\rangle\langle ji| + \sum_{i\neq j=1}^{d} c_{ij}|ij\rangle\langle ij|. \tag{13}$$

Now, positivity of $\widetilde{\rho}$ is equivalent to $c_{ij}\geqslant 0$ and

$$c_{ij}c_{ji} - |b_{ij}|^2 = 0. \tag{14}$$

On the other hand, partial transposition

$$(\mathbb{1} \otimes \tau)\widetilde{\rho} = \sum_{i,j=1}^{d} b_{ij}|ii\rangle\langle jj| + \sum_{i\neq j=1}^{d} c_{ij}|ij\rangle\langle ij|, \tag{15}$$

is $U_{\mathbf{x}}\otimes U_{\mathbf{x}}^{*}$ invariant and, therefore, $\widetilde{\rho}$ is PPT iff

$$\hat{b} = \|b_{ij}\| \geqslant 0 \quad \text{and } c_{ij} \geqslant 0. \tag{16}$$

Examples. Now we show that many well-known examples of PPT states belong to our class.

(1) *Werner state* [6].

$$\mathcal{W}_p = (1-p)Q^{+} + pQ^{-}, \tag{17}$$

where

$$Q^{\pm} = \frac{1}{d(d\pm 1)}\left(I\otimes I \pm \sum_{i,j=1}^{d} |ij\rangle\langle ji|\right).$$

Clearly, $\mathcal{W}_p$ belongs to a class (13) with

$$b_{ij} = \begin{cases} x_{-}, & i\neq j, \\ x_{-}+x_{+}, & i=j, \end{cases}$$

and $c_{ij}=x_{+}$, where

$$x_{\pm} = \frac{1-p}{d^2+d} \pm \frac{p}{d^2-d}.$$

Condition (14) implies $p\in[0,1]$. To check condition (16) for PPT let us observe that the spectrum of $\hat{b}$ consists of only two points $\lambda_1=x_{+}$ with multiplicity $d-1$ and $\lambda_2=dx_{-}+x_{+}$. Therefore $\hat{b}$ is positive iff $\lambda_2\geqslant 0$ which is equivalent to $p\leqslant 1/2$ and hence it reproduces well known result for PPT property of Werner states [6].

(2) *Isotropic state* [7].

$$\mathcal{I} = \frac{1-\lambda}{d^2} I\otimes I + \frac{\lambda}{d}\sum_{i,j=1}^{d} |ii\rangle\langle jj| \tag{18}$$

belongs to a class (5) with $c_{ij}=(1-\lambda)/d^2$ and

$$a_{ij} = \begin{cases} \lambda/d, & i\neq j, \\ \lambda/d + (1-\lambda)/d^2, & i=j. \end{cases}$$

Positivity of $\hat{a}$ together with $c_{ij}\geqslant 0$ imply $-1/(d^2-1)\leqslant\lambda\leqslant 1$. PPT condition (12) leads to $\lambda\leqslant 1/d+1$ which reproduces well known result for PPT property of isotropic states [7].

(3) The authors of Ref. [11] considered the following two-parameter family:

$$\rho_{bc} = a\sum_{i=1}^{d} |ii\rangle\langle ii| + b\sum_{i<j=1}^{d} |\psi_{ij}^{-}\rangle\langle\psi_{ij}^{-}| + c\sum_{i<j=1}^{d} |\psi_{ij}^{+}\rangle\langle\psi_{ij}^{+}|, \tag{19}$$

where $|\psi_{ij}^{\pm}\rangle=(|ij\rangle\pm|ji\rangle)/\sqrt{2}$. Note, that the unit trace condition (7) enables one to compute a in terms of b and c: $a=1/d-(b+c)/(2d-2)$. Clearly, ρ_{bc} belongs to a Werner class (13) with

$$b_{ij} = \begin{cases} (c-b)/2, & i\neq j, \\ a, & i=j \end{cases}$$

and $c_{ij}=(c+b)/2$. Now, $c_{ij}\geqslant 0$ implies $c+b\geqslant 0$ whereas $\hat{b}\geqslant 0$ gives

$$1 - d(d-1)b \geqslant 0,$$

$$2 - d(d-2)b - d^2 c \geqslant 0,$$

which reproduce results of Ref. [11].

(4) Horodecki *et al.* [12] considered the following $3\otimes 3$ state:

$$\sigma_\alpha = \frac{2}{7}P^+ + \frac{\alpha}{7}\sigma_+ + \frac{5-\alpha}{7}\sigma_-, \quad 2 \leqslant \alpha \leqslant 5, \tag{20}$$

where P^+ denotes a projector onto the canonical maximally entangled state and

$$\sigma_+ = \frac{1}{3}(|01\rangle\langle 01| + |12\rangle\langle 12| + |20\rangle\langle 20|),$$

$$\sigma_- = \frac{1}{3}(|10\rangle\langle 10| + |21\rangle\langle 21| + |02\rangle\langle 02|).$$

Clearly, Eq. (20) belongs to isotropiclike class (5) with $a_{ij} = 2/21$, $c_{01}=c_{12}=c_{20}=\alpha/21$ and $c_{10}=c_{21}=c_{02}=(5-\alpha)/21$. One easily finds that PPT condition (12) reproduces well known fact that Eq. (20) is PPT for $\alpha \leqslant 4$. Recently, a one-parameter family (20) was generalized for $d\otimes d$ systems as follows [15]:

$$\rho = \frac{a_1}{d}P^+ + \sum_{i=1}^{d}\sum_{j=2}^{d}\frac{a_j}{d}|i,i+j-1\rangle\langle i,i+j-1|, \tag{21}$$

where the positive numbers a_i satisfy $\Sigma_i a_i = 1$. Clearly, it belongs to an isotropiclike family (5). If $a_{i+1}a_{d-i+1} \geqslant a_1^2$ then the state is PPT.

(5) Bound entangled states considered in Ref. [13] belong to our class (5) with $a_{ij}=1$.

(6) *Størmer state*. Størmer [18] analyzed an un-normalized $3\otimes 3$ positive PPT matrix with $a_{ij}=1$ and

$$c_{ij} = 2\mu, \quad i<j; \quad c_{ij} = 1/2\mu, \quad i>j.$$

This example may be immediately generalized for $d\otimes d$ case as follows: $a_{ij}=\alpha$ and

$$c_{ij} > 0, \quad i<j; \quad c_{ij} = \alpha^2 c_{ji}^{-1}, \quad i>j,$$

where $\alpha>0$ is a normalization constant. One has $c_{ij}c_{ji} = |a_{ij}|^2$, and Eq. (12) implies that the corresponding state is PPT.

(7) Ha [16] performed very sophisticated construction of a one-parameter family of $d^2\times d^2$ (un-normalized) positive matrices and showed that this family remains positive after performing partial transposition. It turns that Ha's family is a special example of an isotropiclike class (5) with $a_{ij}=1$ and

$$c_{i\oplus 1,i} = \lambda, \quad c_{i,i\oplus 1} = \lambda',$$

and the remaining $c_{ij}=1$. In the above formula "$\oplus$" denotes addition modulo d, and

$$\lambda = \frac{\gamma^2 + d - 1}{d}, \quad \lambda' = \frac{\gamma^{-2}+d-1}{d},$$

with $\gamma>0$. Now, conditions for positivity (6) are trivially satisfied. Moreover, due to $\lambda\lambda' \geqslant 1$, the PPT condition (12) is also satisfied which shows that Ha's family is PPT.

Another example constructed in Ref. [16] is a family of (un-normalized) $3\otimes 3$ positive PPT matrices but the construction may be generalized to an arbitrary d as follows. Let

$$u_i = |ii\rangle, \quad z_i = \frac{1}{s}|i+1,i\rangle + s|i,i+1\rangle,$$

with $s>0$ and $i=1,\ldots,d$. Define the following family of positive $d^2\times d^2$ matrices

$$B_s = \sum_{i=1}^{d}(|u_i\rangle\langle u_i| + |z_i\rangle\langle z_i|). \tag{22}$$

Observe, that Eq. (22) belongs to a Werner-like class (13) with

$$b_{ii} = b_{i,i\oplus 1} = b_{i\oplus 1,i} = 1,$$

$$c_{i,i\oplus 1} = s^2, \quad c_{i\oplus 1,i} = s^{-2},$$

and the remaining b_{ij} and c_{ij} vanish. Note, that PPT condition (16) is trivially satisfied.

(8) *PPT states which do not belong to our class*. It turns out that apart from bound entangled states constructed *via* unextendible product bases [8] almost all other examples of PPT states do belong to our class. We are aware of only few exceptions: one is the family of $O\otimes O$-invariant states [19] (see also Ref. [24]) and the second one is the celebrated family of $3\otimes 3$ states which are nonseparable but PPT constructed by Horodecki [4]. Note that the d-dimensional torus $\mathrm{U}(1)\times\cdots\times\mathrm{U}(1)$ does not allow for an orthogonal subgroup and hence states with orthogonal symmetry has to be considered separately. Now, the Horodecki state ρ_a may be rewritten as $\rho_a = \rho_a' + \rho_a''$, where

$$\rho_a' = \alpha a\left(\sum_{i,j=1}^{3}|ii\rangle\langle jj| + \sum_{i\neq j=1}^{3}|ij\rangle\langle ij|\right)$$

and

$$\rho_a'' = \frac{\alpha}{2}\sqrt{1-a^2}(|31\rangle\langle 33| + |33\rangle\langle 31|),$$

with $\alpha = 1/(8a+1)$ being a normalization constant. Note, that ρ_a' is an isotropiclike matrix and does belong to Eq. (5). However, ρ_a'' is not invariant under the maximal commutative subgroup of $U(3)$. Note, that ρ_a'' is invariant only under the one-parameter subgroup generated by $\hat{t}_2 = |2\rangle\langle 2|$. It shows that Horodecki state ρ_a is also symmetric but with respect to smaller symmetry group.

Separability. A state from a class (5) is separable iff there exists a separable state σ such that $\rho = \mathbf{P}\sigma$, where $\mathbf{P}$ denotes a projector operator projecting an arbitrary state onto the class (5), i.e., $\mathbf{P}\sigma$ belongs to Eq. (5) with "pseudo-fidelities" $a_{ij} = \mathrm{Tr}(\sigma|ii\rangle\langle jj|)$ and $c_{ij} = \mathrm{Tr}(\sigma|ij\rangle\langle ij|)$. Taking $\sigma = |\alpha\otimes\beta\rangle\langle\alpha\otimes\beta|$ one finds the following sufficient condition for separability:

$$a_{ij} = \alpha_i^*\alpha_j\beta_i^*\beta_j, \quad c_{ij} = |\alpha_i|^2|\beta_j|^2, \tag{23}$$

where $\alpha_i = \langle i|\alpha\rangle$ and $\beta_i = \langle i|\beta\rangle$.

Positive maps. PPT states are also important in the study of positive maps [16,18,20] (see also Ref. [12] for a useful review). It has been shown [5] that there exists a strong connection between the classification of the entanglement of quantum states and the structure of positive linear maps: a state ρ living in $\mathbb{C}^d \otimes \mathbb{C}^d$ is separable iff $(\mathbb{1}\otimes\Phi)\rho \geqslant 0$ for all positive maps $\Phi: M_d \to M_d$, where M_d denotes the set of $d \times d$ complex matrices. Now, let V_k be the cone of positive matrices $A \in (M_d \otimes M_d)^+$ such that Schmidt number Sch$(A) \leqslant k$ [21]. Now, one says that A belongs to a cone V^l iff A is PPT and SN$[(\mathbb{1}\otimes\tau)A] \leqslant l$. It is clear that $V_1 = V^1$ defines a cone of separable elements. Recall that a positive map $\Phi: M_d \to M_d$ is k positive iff $(\mathbb{1}\otimes\Phi)$ is positive when restricted to V_k. Similarly, Φ is k copositive iff $(\mathbb{1}\otimes\Phi\circ\tau)$ is positive on V^k. Clearly, k-positive map is necessarily l positive for $l<k$ (the same is true for k copositivity). If $k=d$ then the d-positive (d-copositive) map is called completely positive (completely copositive).

Concerning the PPT states the crucial role is played by so called indecomposable maps: a linear positive map is indecomposable iff it cannot be decomposed into the sum of completely positive and completely copositive maps. The most basic class of indecomposable maps consists of so-called atomic ones [22]—Φ is atomic iff it cannot be decomposed into the sum of two-positive and two-copositive maps. Atomic maps posses the "weakest" positivity property and hence may be used to detect the bipartite states with the "weakest" entanglement, i.e., states from $V_2 \cap V^2$. Conversely, PPT states may be used to check the atomic property of positive maps. Suppose that we are given an indecomposable positive map Φ. If for some $A \in V_2 \cap V^2$ one finds that $(\mathbb{1}\otimes\Phi)A$ is not positive then Φ is necessarily atomic. Now, it would be interesting to know when PPT states from our class belong to $V_2 \cap V^2$. Consider, e.g., a state ρ from an isotropiclike class (5). Note, that if ρ is PPT then, due to Eq. (10), ρ necessarily belongs to V^2. Hence, it is enough to check when $\rho \in V_2$. It is clear that $\rho \in V_2$ iff there is $\sigma' \in V_2$ such that $\rho = \mathbf{P}\sigma'$. Taking $\sigma' = \frac{1}{2}|\alpha\otimes\beta + \psi\otimes\phi\rangle\langle\alpha\otimes\beta+\psi\otimes\phi|$ one finds the following sufficient condition for ρ to be an element from a cone V_2:

$$a_{ij} = \frac{1}{2}(\alpha_i^* \beta_i^* [\alpha_j\beta_j + \psi_j\phi_j] + \psi_i^*\phi_i^*[\alpha_j\beta_j + \psi_j\phi_j]),$$

$$c_{ij} = \frac{1}{2}(\alpha_i\beta_j[\alpha_i^*\beta_j^* + \psi_i^*\phi_j^*] + \psi_i\phi_j[\alpha_i^*\beta_j^* + \psi_i^*\phi_j^*]),$$

where $\alpha_i = \langle i|\alpha\rangle$ and similarly for β_i, ψ_i and ϕ_i. Interestingly, any Werner-like state from (13) belongs to V_2. Hence it suffices to check wether it belongs to V^2. One may easily derive sufficient conditions for b_{ij} and c_{ij} in analogy to the above conditions for a_{ij} and c_{ij}. It would be interesting to generalize PPT states analyzed in this paper to multipartite case following the construction presented recently in Ref. [23,24].

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