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by

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Abstract

We study certain quantum states for which the PPT criterion is both sufficient and necessary for separability. A class of $n \times n$ bipartite mixed states is presented and the conditions of PPT for these states are derived. The separable pure state decompositions of these states are explicitly constructed when they are PPT.

Quantum entangled states have become one of the key resources in quantum information processing. The study of quantum teleportation, quantum cryptography, quantum dense coding, quantum error correction and parallel computation [1–3] has spurred a flurry of activities in the investigation of quantum entanglement. Despite the potential applications of quantum entangled states, there are many open questions in the theory of quantum entanglement. The separability of quantum mixed states is one of the important problems in the theory of quantum entanglement.

Let H be an n-dimensional complex Hilbert space, with $|i\rangle$, $i = 1, ..., n$ the orthonormal basis. A bipartite mixed state in $H \otimes H$ is said to be separable if the density matrix can be written as

$$\rho = \sum_i p_i \rho_i^1 \otimes \rho_i^2, \tag{1}$$

where $0 < p_i \leq 1$, $\sum_i p_i = 1$, ρ_i^1 and ρ_i^2 are density matrices associated with the first and the second Hilbert spaces respectively. It is a challenge to find a decomposition like (1) or to prove that such a decomposition does not exist for a given state ρ. With considerable effort in analyzing the separability, there have been some (necessary) criterias for separability in recent years, for instance, Bell inequalities [4], PPT (positive partial transposition) [5], reduction criterion [6, 7], majorization criterion [8], entanglement witnesses [9, 10], realignment [11, 12] and generalized realignment [13], range criterion [14], criteria based on the local uncertainty relations [15], correlation matrix approach [16], as well as some necessary and sufficient criterias for low rank density matrices [17–19].

The PPT criterion is generally a necessary condition for separability. It becomes also sufficient for the cases of $2 \otimes 2$ and $2 \otimes 3$ bipartite states [21]. In [22], it has been shown that a state ρ supported on $m \times n$ Hilbert space ($m \leq n$) with $rank(\rho) \leq m$ is separable if and only if ρ is PPT. However, it is generally a difficult problem to find the concrete PPT conditions for a given such state within this class. Moreover, even if the PPT conditions are satisfied and hence the state is separable, it is still a challenging problem to find the detailed separable pure state decompositions (1). For separable two-qubit states, an elegant separable pure state decompositions has been given in [20].

In [23] a class of $3 \otimes 3$ mixed states ρ with $rank(\rho) = 3$ has been investigated. The PPT conditions are derived. And the explicit separable pure state decompositions are constructed. In this paper we generalize the results in [23] to a class of $n \otimes n$ quantum mixed states. We derive the PPT conditions and construct explicitly the separable pure state decompositions for states satisfying the PPT conditions.

We consider a set of mixed states defined in $H \otimes H$ space which has the following form of spectral decomposition:

$$\rho = \sum_{l=1}^{n} \lambda_l |V_l\rangle\langle V_l|, \tag{2}$$

with $\sum_{l=1}^{n} \lambda_l = 1$, $0 < \lambda_l < 1$, and

$$|V_l\rangle = \sum_{j=1}^{n} v_l^j |j\rangle \otimes |j+l-1\rangle, \quad l = 1, 2, \cdots, n, \tag{3}$$

where $0 \neq v_l^j \in \mathbb{C}$ and $\sum_j \overline{v_l}^j v_l^j = 1$. ($\overline{z}$ denoting the complex conjugation of z). When $n = 3$, the state ρ becomes the object of study in [23]. For simplicity we denote $x_l^j = \sqrt{\lambda_l} v_l^j$, $|X_l\rangle = \sqrt{\lambda_l}|V_l\rangle$. Then ρ has the form,

$$\rho = \sum_{l=1}^{n} |X_l\rangle\langle X_l| = \sum_{l,j,k=1}^{n} x_l^j \overline{x}_l^k |j\rangle\otimes|j+l-1\rangle\langle k|\otimes\langle k+l-1| = \sum_{l,j,k=1}^{n} x_l^j \overline{x}_l^k |j\rangle\langle k|\otimes|j+l-1\rangle\langle k+l-1|.$$

We first deduce the PPT conditions of ρ. The partial transposed matrix of ρ is given by

$$\rho^{T_1} = \sum_{l,j,k=1}^{n} x_l^j \, \overline{x}_l^k |k\rangle\langle j| \otimes |j+l-1\rangle\langle k+l-1|, \tag{4}$$

where T_1 stands for partial transpose with respect to the first Hilbert space. That ρ is PPT means that $\rho^{T_1} \geq 0$. Namely, for any vector $|Y\rangle = \sum_{r,s=1}^{n} y_r^{s+r-1} |r\rangle \otimes |s\rangle$ in $H \otimes H$, we obtain $\langle Y|\rho^{T_1}|Y\rangle \geq 0$. Here and later, we use $s + r - 1$ to represent $s + r - 1 \ mod \ n$, mod denoted modulo arithmetic. We have

$$\begin{aligned}
\langle Y|\rho^{T_1}|Y\rangle &= \langle Y| \sum_{l,j,k=1}^{n} x_l^j \, \overline{x}_l^k |k\rangle\langle j| \otimes |j+l-1\rangle\langle k+l-1| \sum_{r,s=1}^{n} y_r^{s+r-1} |r\rangle \otimes |s\rangle \\
&= \langle Y| \sum_{l,j,k=1}^{n} x_l^j \, \overline{x}_l^k \, y_r^{s+r-1} \delta_j^r \, \delta_s^{(k+l-1)} |k\rangle \otimes |j+l-1\rangle \\
&= \sum_{r',s'=1}^{n} y_{r'}^{s'+r'-1} |r'\rangle \otimes |s'\rangle \sum_{l,j,k=1}^{n} x_l^j \, \overline{x}_l^k \, y_j^{k+j+l-2} |k\rangle \otimes |j+l-1\rangle \\
&= \sum_{l,j,k,r',s'=1}^{n} x_l^j \, \overline{x}_l^k \, y_j^{k+j+l-2} \, \overline{y}_{r'}^{r'+s'-1} \, \delta_{r'}^k \, \delta_{s'}^{j+l-1} \\
&= \sum_{l,j,k=1}^{n} x_l^j \, \overline{x}_l^k \, y_j^{k+j+l-2} \, \overline{y}_k^{k+j+l-2} \geq 0.
\end{aligned}$$

Because of the independence of the variables y_r^{α}, the above inequality is equivalent to the following inequities:

$$
\begin{aligned}
< y^{n-1}|A_1|y^{n-1} > &\equiv \sum_{l,j,k=1,l+j+k=1\,mod\ n}^{n} x_l^j\,\overline{x}_l^k\,y_j^{n-1}\,\overline{y}_k^{n-1} \geq 0,\\
< y^{n}|A_2|y^{n} > &\equiv \sum_{l,j,k=1,l+j+k=2\,mod\ n}^{n} x_l^j\,\overline{x}_l^k\,y_j^{n}\,\overline{y}_k^{n} \geq 0,\\
&\cdots\\
< y^{n-3}|A_{n-3}|y^{n-1} > &\equiv \sum_{l,j,k=1,l+j+k=n-1\,mod\ n}^{n} x_l^j\,\overline{x}_l^k\,y_j^{n-3}\,\overline{y}_k^{n-3} \geq 0,\\
< y^{n-2}|A_n|y^{n-2} > &\equiv \sum_{l,j,k=1,l+j+k=0\,mod\ n}^{n} x_l^j\,\overline{x}_l^k\,y_j^{n-2}\,\overline{y}_k^{n-2} \geq 0,
\end{aligned}
$$

where $|y^i >= (y_1^i, y_2^i, ..., y_n^i)^t$ (t stands for transpose), $i = 1, 2, ..., n$. $A_1, A_1, \cdots, A_n$ are non-negative, hermitian matrices, with the entries of A_m given by $x_l^j\overline{x}_l^k$ for $l+j+k = m\,mod\,(n)$. For fixed m, $l = [m-(j+k)]\,mod\,n$ only depends on j, k.

For example, when $n = 5$, one has

$$
A_1 = \begin{pmatrix}
x_4^1\overline{x}_4^1 & x_3^1\overline{x}_3^2 & x_2^1\overline{x}_2^3 & x_1^1\overline{x}_1^4 & x_5^1\overline{x}_5^5\\
x_3^2\overline{x}_3^1 & x_2^2\overline{x}_2^2 & x_1^2\overline{x}_1^3 & x_5^2\overline{x}_5^4 & x_4^2\overline{x}_4^5\\
x_2^3\overline{x}_2^1 & x_1^3\overline{x}_1^2 & x_5^3\overline{x}_5^3 & x_4^3\overline{x}_4^4 & x_3^3\overline{x}_3^5\\
x_1^4\overline{x}_1^1 & x_5^4\overline{x}_5^2 & x_4^4\overline{x}_4^3 & x_3^4\overline{x}_3^4 & x_2^4\overline{x}_2^5\\
x_5^5\overline{x}_5^1 & x_4^5\overline{x}_4^2 & x_3^5\overline{x}_3^3 & x_2^5\overline{x}_2^4 & x_1^5\overline{x}_1^5
\end{pmatrix}, \cdots. \tag{5}
$$

Due to the non-negativity of the matrices A_1, ..., A_n, all the principal minors of A_m, $m = 1, 2, ..., n$, are non-negative. We have

Theorem 1: The entries of the matrices A_m, $\forall\ m = 1, 2, \cdots, n$ satisfy the following quadratic relations,

$$
x^{ip}x^{jq} = x^{iq}x^{jp}, \tag{6}
$$

where $x^{ip} = x_{l(i,p)}^i\overline{x}_{l(i,p)}^p$, $l(i,p) = (m\,mod\,n) - (i+p) \equiv m - (i+p)$, the other marks have the same meaning.

Proof: First, we consider order two principal minors $\{(i,j),(i,j)\}$ of the matrix A_m. From the non-negativity of A_m, we get that $x^{ii}x^{jj} \geq x^{ij}x^{ji}$. The inequality is in fact an equality. Because if for some m, $x^{ii}x^{jj} > x^{ij}x^{ji}$, then $\prod_{m=1}^n x^{ii}x^{jj} > \prod_{m=1}^n x^{ij}x^{ji}$. On the other hand, from straightforward calculation, we have $\prod_{m=1}^n x^{ii}x^{jj} = \prod_{m=1}^n x^{ij}x^{ji}$ for fixed i, j.

Therefore, for any m we have

$$x^{ii}x^{jj} = x^{ij}x^{ji}. \tag{7}$$

Second, from the non-negativity of the order three principal minors $\{(i,j,k),(i,j,k)\}$ of the matrix A_m, we have $0 \le x^{ij}x^{jk}x^{ki} - x^{ii}x^{jk}x^{kj} + x^{ik}x^{ji}x^{kj} - x^{ik}x^{jj}x^{ki} = x^{ij}x^{jk}x^{ki} - 2x^{ii}x^{jj}x^{kk} + x^{ik}x^{ji}x^{kj} = 2Re(x^{ij}x^{jk}x^{ki}) - 2x^{ii}x^{jj}x^{kk} \le 2(|x^{ij}||x^{jk}||x^{ki}| - x^{ii}x^{jj}x^{kk}) = 2(\sqrt{x^{ii}x^{jj}}\sqrt{x^{jj}x^{kk}}\sqrt{x^{kk}x^{ii}} - x^{ii}x^{jj}x^{kk}) = 0$, where we have used the condition (7) in the first and the third equations. Therefore, we get the following relations:

$$x^{ij}x^{jk}x^{ki} = x^{ii}x^{jj}x^{kk}. \tag{8}$$

For a nonzero 3×3 hermitian matrix, if its order two and three principal minors are all 0, then it has only one eigenvalue, and all of its order two minors are 0. Therefore, we have

$$x^{ij}x^{jk} = x^{ik}x^{jj}. \tag{9}$$

Third, combining the non-negativity of the order four principal minors $\{(i,j,k,l),(i,j,k,l)\}$ of the matrix A_m with (7) and (8), we have

$$6x^{ii}x^{jj}x^{kk}x^{ll} - 2Re(x^{il}x^{lk}x^{kj}x^{ji} + x^{jl}x^{lk}x^{ki}x^{ij} + x^{jl}x^{li}x^{ik}x^{kj}) \ge 0.$$

Using relations (9), we have $x^{ii}x^{jj}x^{kk}x^{ll} - Re(x^{il}x^{lk}x^{kj}x^{ji}) = x^{ii}x^{jj}x^{kk}x^{ll} - Re(x^{ii}x^{jj}x^{kk}x^{ll}) = x^{ii}x^{jj}x^{kk}x^{ll} - x^{ii}x^{jj}x^{kk}x^{ll} = 0$. Hence all order four principal minors are all 0 and $x^{il}x^{lk}x^{kj}x^{ji} = x^{ii}x^{jj}x^{kk}x^{ll}$. Since order two, three and four principal minors are equivalent to 0, therefore, the nonzero 4×4 hermitian matrix (order four principal minors) has only one eigenvalue, then all of its order two minors are 0. Furthermore, all order two minors are included in one order four principal minors. Therefore the entries of A_m satisfy the relations (6). $\square$

From the condition (7), $x^j_{m-2j}\,\overline{x}^j_{m-2j}\,x^k_{m-2k}\,\overline{x}^k_{m-2k} = x^j_{m-(j+k)}\,\overline{x}^k_{m-(j+k)}\,x^k_{m-(j+k)}\,\overline{x}^j_{m-(j+k)}$, we have the following relations:

$$x^j_{m-(j+k)}\,x^k_{m-(j+k)}\,e^{i\theta^{jk}_m} = x^j_{m-2j}\,x^k_{m-2k} \tag{10}$$

or

$$x^j_m\,x^k_m\,e^{i\theta^{jk}_m} = x^j_{m-(j-k)}\,x^k_{m+(j-k)}, \tag{11}$$

where $0 \leq \theta_m^{jk} \leq 2\pi$.

Theorem 2: The number of independent θ_m^{jk} is at most $n-1$.

proof: First, from (9),we have $x^{ij}x^{jk} = x^{ik}x^{jj}$, i.e, $x^i_{m-(i+j)}\overline{x}^j_{m-(i+j)}x^j_{m-(j+k)}\overline{x}^k_{m-(j+k)} = x^i_{m-(i+k)}\overline{x}^k_{m-(i+k)}x^j_{m-2j}\overline{x}^j_{m-2j}$. Let $j-i=k-j$. We obtain

$$x^i_{m-(i+j)}\overline{x}^j_{m-(i+j)}x^j_{m-(j+k)}\overline{x}^k_{m-(j+k)} = x^i_{m-2j}\overline{x}^k_{m-2j}x^j_{m-2j}\overline{x}^j_{m-2j},$$

which gives rise to $x^i_{m-i+j}\overline{x}^j_{m-i+j}x^j_{m+j-k}\overline{x}^k_{m+j-k} = x^i_m\overline{x}^k_m x^j_m\overline{x}^j_m$. Namely, $x^i_{m+s}\overline{x}^j_{m+s}x^j_{m-s}\overline{x}^k_{m-s} = x^i_m\overline{x}^k_m x^j_m\overline{x}^j_m$. However from (10) we have $x^i_{m+s}x^j_{m-s} = x^i_m x^j_m e^{i\theta_m^{ij}}$ and $\overline{x}^k_{m+s}\overline{x}^j_{m-s} = \overline{x}^k_m\overline{x}^j_m e^{i(-\theta_m^{kj})}$. Therefore,

$$\theta_m^{ij} = \theta_m^{kj} \qquad if\ j-i=k-j, \tag{12}$$

and θ_m^{ij} depends on the difference of i and j.

Set $s=|i-j|$. In the following, we denote θ_m^{ij} as θ_m^s. In particular, we denote θ_m^1 as θ_m. There are $[\frac{n}{2}]$ angles $\{\theta_m^s\}$ for given m, with $s=1,2,\cdots,[\frac{n}{2}]$, $[x]$ denoting the integer that is less or equal to x.

Second, from (11) and (12), for any integer $j \leq [\frac{n}{2}]$ and given m, we can get the following equation: $\prod_{l=0}^s x^j_{m+l}x^{j+1}_{m+l}e^{i\sum_{l=0}^s\theta_{m+l}} = \prod_{l=0}^s x^j_{m+l+1}x^{j+1}_{m+l-1}$. That is

$$x^j_m x^{j+1}_{m+s}e^{i\sum_{l=0}^s\theta_{m+l}} = x^j_{m+s+1}x^{j+1}_{m-1}. \tag{13}$$

Following (13), we can get s equations: $x^j_m x^{j+1}_{m+s-1}e^{i\sum_{l=0}^{s-1}\theta_{m+l}} = x^j_{m+s}x^{j+1}_{m-1}$, $x^{j+1}_{m-1}x^{j+2}_{(m+s-1)-1}e^{i\sum_{l=0}^{s-1}\theta_{m-1+l}} = x^{j+1}_{m+s-1}x^{j+2}_{m-1-1}$, $\cdots$, $x^{j+s-1}_{m-(s-1)}x^{j+s}_m e^{i\sum_{l=0}^{s-1}\theta_{m-(s-1)+l}} = x^{j+s-1}_{m+s-(s-1)}x^{j+s}_{m-1-(s-1)}$. Multiplying these equations together, we get

$$x^j_m x^{j+s}_m e^{i(s\theta_m+(s-1)(\theta_{m-1}+\theta_{m+1})+\cdots+(\theta_{m+s-1}+\theta_{m-s+1}))} = x^j_{m+s}x^{j+s}_{m-1-(s-1)} = x^j_m x^{j+s}_m e^{i(\theta_m^s)},$$

i.e. any θ_m^s, $s \geq 2$, $m=1,2,\cdots,n$ can be expressed according to the angles θ_m, $m=1,2,\cdots,n$.

Furthermore, for fixed j,k or s, we have $\prod_{m=0}^{n-1} x^j_{m-2j}x^k_{m-2k} = \prod_{m=0}^{n-1} x^j_{m-(j+k)}x^k_{m-(j+k)}e^{i\Sigma_{m=0}^{n-1}\theta_m^{jk}}$. On the other hand, by direct computation, we have $\prod_{m=0}^{n-1} x^j_{m-2j}x^k_{m-2k} = \prod_{m=0}^{n-1} x^j_{m-(j+k)}x^k_{m-(j+k)}$. Hence $\Sigma_{m=0}^{n-1}\theta_m^{jk} = 0$, or $\sum_{m=0}^{n-1}\theta_m^s = 0$, $s=1,2,\cdots,[\frac{n}{2}]$. Therefore, there are in fact only $n-1$ independent angles θ_m. □

For example, using (11) we have $x_1^1 x_1^2 e^{i\theta_1} = x_2^1 x_n^2$, $x_2^1 x_2^2 e^{i\theta_2} = x_3^1 x_1^2$. Hence $x_1^1 x_2^2 e^{i(\theta_1+\theta_2)} = x_3^1 x_n^2$. From $x_1^2 x_1^3 e^{i\theta_1} = x_2^2 x_n^3$ and $x_n^2 x_n^3 e^{i\theta_n} = x_1^2 x_{n-1}^3$, we get $x_1^3 x_n^2 e^{i(\theta_1+\theta_n)} = x_2^2 x_{n-1}^3$, which give rise to $x_1^1 x_1^3 e^{i(\theta_1^{13})} = x_1^1 x_1^3 e^{i(\theta_1^{12}+\theta_2^{12}+\theta_1^{23}+\theta_n^{23})} = x_3^1 x_{n-1}^3$, i,e.

$$\theta_1^{13} = \theta_1^2 = (2\theta_1 + \theta_2 + \theta_n). \tag{14}$$

We are now ready to construct pure separable state decompositions of ρ when ρ is PPT. Let U be a unitary transformation, with its entries given by $u_{kl} = (\frac{1}{\sqrt{n}} e^{i((k-1)(l-1)\omega+\delta_k)})$, where δ_k $k = 1, 2, \cdots, n$ is an angle, ω is the n-th unit root, $\omega^n = 1$. Then $\rho = \sum_{l=1}^n |X_l\rangle\langle X_l| = \sum_{l=1}^n |Z_l\rangle\langle Z_l|$, where

$$|Z_l\rangle = \sum_{k=1}^n u_{kl}|X_l\rangle = \sum_{i,j=1}^n b_{rs}^l |rs\rangle. \tag{15}$$

Denoting $B_l = (b_{rs}^l)$, one has

$$B_l = (b_{rs}^l) = ((e^{i((s-r)(l-1)\omega+\delta_{s-r+1})} x_{s-r+1}^r)_{rs}).$$

For example, when $n = 5$, one has

$$B_l = \begin{pmatrix} u_{1l}x_1^1 & u_{2l}x_2^1 & u_{3l}x_3^1 & u_{4l}x_4^1 & u_{5l}x_5^1 \\ u_{5l}x_5^2 & u_{1l}x_1^2 & u_{2l}x_2^2 & u_{3l}x_3^2 & u_{4l}x_4^2 \\ u_{4l}x_4^3 & u_{5l}x_5^3 & u_{1l}x_1^3 & u_{2l}x_2^3 & u_{3l}x_3^3 \\ u_{3l}x_3^4 & u_{4l}x_4^4 & u_{5l}x_5^4 & u_{1l}x_1^4 & u_{2l}x_2^4 \\ u_{2l}x_2^5 & u_{3l}x_3^5 & u_{4l}x_4^5 & u_{5l}x_5^5 & u_{1l}x_1^5 \end{pmatrix}. \tag{16}$$

Theorem 3: There exist δ_k such that every order two minors $\{(m,k),(\alpha,\beta)\}$ in B_l is zero, and so that $\rho = \sum_{l=1}^n |Z_l\rangle\langle Z_l|$ is a pure separable state decomposition for ρ that is PPT.

Proof That any order two minors $\{(m,k),(\alpha,\beta)\}$ of B_l are zero implies:

$$e^{i(\delta_{\alpha-m+1}+\delta_{\beta-k+1}-\delta_{\alpha-k+1}-\delta_{\beta-m+1})} x_{\alpha-m+1}^m x_{\beta-k+1}^k = x_{\beta-m+1}^m x_{\alpha-k+1}^k. \tag{17}$$

Namely, any order two minors $\{(m,m+1),(\alpha,\alpha+1)\}$ should be zero,

$$e^{i(2\delta_{\alpha-m+1}-\delta_{\alpha-m+2}-\delta_{\alpha-m})} x_{\alpha-m+1}^m x_{\alpha-m+1}^{m+1} = x_{\alpha-m+2}^m x_{\alpha-m}^{m+1}. \tag{18}$$

From the PPT conditions, we have: $x_m^j x_m^{j+1} e^{i\theta_m} = x_{m+1}^j x_{m-1}^{j+1}$. Applying Theorem 2, we have $x_m^j x_m^{j+1} e^{i(2\delta_m-\delta_{m+1}-\delta_{m-1})} = x_{m+1}^j x_{m-1}^{j+1} = x_m^j x_m^{j+1} e^{i\theta_m}$. Therefore

$$2\delta_i - \delta_{i+1} - \delta_{i-1} = \theta_i, i = 1, 2, \cdots, n. \tag{19}$$

Eq. (19) has always solutions for δ_i with the relationship $\sum_{i=1}^{n}\theta_i = 0$. As every order two minors $\{(m,k),(\alpha,\beta)\}$ of B_l is zero, the rank of B_l is one. Therefore, $|Z_l\rangle$ is separable. $\square$

In fact the solutions of Eq. (19) are not unique. By calculating, we know that there is a free variable of the parameters δ_m, $m = 1, 2, \cdots, n$, therefore exist many different separable pure state decompositions for such ρ.

We have investigated a class of $n \otimes n$ bipartite mixed states for which the PPT criterion is both sufficient and necessary for separability. The PPT conditions for these states are derived. We have presented a general approach to find the separable pure state decompositions of this class, and the separable pure state decompositions have been explicitly constructed.

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